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Renewable Para-Xylene

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Renewable Para-Xylene

Abstract

This report details a process designed to renewably produce 400 million pounds of para-xylene per year from corn dry grind, sugar cane molasses (SCM), or woody biomass while minimizing water use. The para-xylene should be suitable for the production of polymers and plastics, and should be economical and green. All three feedstocks are equally suitable for the process and available for use.

The process is designed for SCM and consumes a total feed of 9.35 billion pounds of molasses per year. Corn dry grind is simply too expensive, and biomass, while cheaper per pound, imposes too many additional pre-processing costs. The molasses first undergoes hydrolysis then hydrogenation, followed by condensation and separation involving distillation and crystallization. Transalkylation and aqueous phase reforming are also employed to boost yield and create a self-contained process.

Several key assumptions are inherent in this process's design. First, all reactor yields come directly from specific examples in the literature. Second, results found in the patents for glycerol were assumed valid for sorbitol as well, since not all patents used the same materials for their examples. Third, the economic analysis assumes that raw materials for catalyst manufacture can be purchased in bulk for a quarter of the price for small quantities. This assumption was suggested by Dr. Fabiano.

Based on these assumptions, the process designed herein meets the desired non-financial criteria, but results in an investor's rate of return of negative 2.90% and a net present value of negative $196 million. However, further research into the catalyst or reactor yields could easily allow the process to break even or offer an attractive return.

CBE 459: PROCESS SYSTEM DESIGN PROJECTS
Professors Leonard Fabiano and Warren Seider

Renewable Para-Xylene

Senior Design Project

Eric Castillo, Tyler Ernst, Corey Lerch, J. Parker Winchester

4/10/2012

Department of Chemical and Biomolecular Engineering
University of Pennsylvania

Faculty Advisor: Dr. Miriam Wattenbarger, University of Pennsylvania
Project Author: Mr. Stephen M. Tieri, DuPont Engineering Research & Technology

University of Pennsylvania
School of Engineering and Applied Science
Chemical and Biomolecular Engineering

April 10, 2012

Dear Dr. Wattenbarger, Dr. Fabiano, and Mr. Stephen Tieri,

Following our original Senior Design Project Statement, we have designed a process for the renewable production of para-xylene, enclosed herein. As requested, this process produces 400 million pounds of para-xylene per annum from our chosen input, sugar cane molasses. In spite of the limited information available on cutting-edge technology, we believe the following process accurately estimates the costs and challenges associated with the renewable production of para-xylene, as well as identifies the key drivers of feasibility and profitability for further investigation.

Based on para-xylene and benzene selling prices of $0.83 and $0.45 per pound, respectively, and a purchase cost of $0.03 per pound for sugar cane molasses, as well as further considerations contained within this report, we believe that the renewable production of para-xylene is not profitable, and recommend against construction of the process. However, we recommend further research into yields obtainable in aqueous phase reforming and in condensation, as well as the cost to manufacture zeolite or similarly-capable catalysts; both will profoundly alter our economic analysis and may enable this project to offer significant returns to the investor.

Sincerely,

Eric Castillo　　Tyler Ernst　　Corey Lerch　　Parker Winchester

Contents

Section I

Introduction

I. INTRODUCTION

Abstract

This report details a process designed to renewably produce 400 million pounds of para-xylene per year from corn dry grind, sugar cane molasses (SCM), or woody biomass while minimizing water use. The para-xylene should be suitable for the production of polymers and plastics, and should be economical and green. All three feedstocks are equally suitable for the process and available for use.

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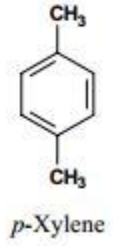
Process Overview



This process aims to produce 400 million pounds of para-xylene per year from woody biomass, corn dry grind, or sugar cane juice, and must be both environmentally friendly and water-conserving. The para-xylene must be suitable for use in the manufacture of polymeric fibers and plastics such as polyethylene terephthalate (PET).

Para-xylene is a critical component in the manufacture of PET, used in high quantities to produce fibers, bottles, and other synthetic plastics and polymers. The market for para-xylene has grown by five to ten percent annually over the last several years, and is predicted to continue doing so in the near future. Current para-xylene production consumes valuable and non-renewable hydrocarbon-based feed materials. As demand continues to rise and these resources continue to dwindle, consumers of para-xylene foresee an unwelcome increase in the monetary and societal cost of these processes, and are actively seeking renewable alternatives as part of their environmental initiatives. Other than its more desirable environmental impact, renewably-produced para-xylene is indistinguishable from conventionally-produced para-xylene when used by the consumer. While somewhat small in comparison to the large para-xylene producers, 400 million pounds per year would signify a key first step towards renewable production in this market. There are currently no commercially operational plants that renewably produce para-xylene.

The process contained herein aims to renewably produce 400 million pounds of para-xylene per year. In addition to producing the specified quantity of para-xylene, the process also generates additional water which is recovered and reused. Significant quantities of benzene are also produced, which can be sold off for use in other industries. The process was designed to produce as many of its own materials as possible, including the water recovered from the process and the hydrogen generated in the aqueous phase reforming. The process also takes advantage of recycle loops to ensure high levels of conversion and recovery, but does so without the use of additional costly units and equipment, aside from the increase in size associated with recycle streams. Only the sugar cane juice must be purchased externally, and is available from sugar cane ethanol facilities already acquired by the investigating company.

Molasses was chosen over corn dry grind due to its superior upfront cost, and over woody biomass due to the pre-processing costs bypassed by using a material already composed of sucrose. The process's demand for molasses will, however, be significant enough to be noticed by the molasses market at large, and will likely affect the equilibrium market price.

Information used to design individual blocks within the process comes from patents and other relevant literature. The design adhered strictly to specific examples within the literature in order to ensure a conservative and accurate assessment of the process's feasibility. Most notably, yields from the aqueous phase reforming, condensation, and transalkylation reactors were constrained to remain consistent with examples found in patents. However, the number of specific examples was limited, and as a result the process hinges on several key parameters, such as catalyst prices and reactor yields, that must be further investigated to provide a final assessment of the project's economic viability. Based on the information available at present, the process is not profitable, but a small and reasonable shift in any one of several key parameters, discussed in greater detail in the report, would dramatically alter this prognosis.

Input Analysis

A major component of the design objectives is the identification of the optimal raw material input for a green para-xylene production process. The company commissioning this design recently acquired corn dry-grind (Nebraska) and sugar-cane ethanol (São Paolo) facilities; additionally, the company is negotiating a woody biomass supply from Washington. In order to determine the optimal raw material input(s), a sequential analysis was performed. In phase one of the analysis, corn dry-grind outputs were eliminated on the basis of cost; in phase two, sugar cane molasses (SCM) won out as the optimal input on the basis of cost and availability.

Phase One: Screening by Cost Estimation

Corn Dry-Grind

The production of ethanol requires that whole grain corn be ground into a powder, which enters aqueous slurry and is fermented. The waste from this process is called the whole stillage. Whole stillage undergoes phase separation, the solids portion of which is called wet distillers' grains with solubles (WDGS). WDGS is frequently dried and sold as dried distillers' grains with solubles (DDGS). DDGS is used as livestock feed, and the drying process helps extend its shelf life. It was assumed that both WDGS and DDGS would be available to the designed facility. Information on these inputs is available in Figure 1, but the important takeaway is that DDGS and WDGS contain 29.4% and 33.4% sugar (glucan and xylan), respectively (Kim, 2008).

Figure 1

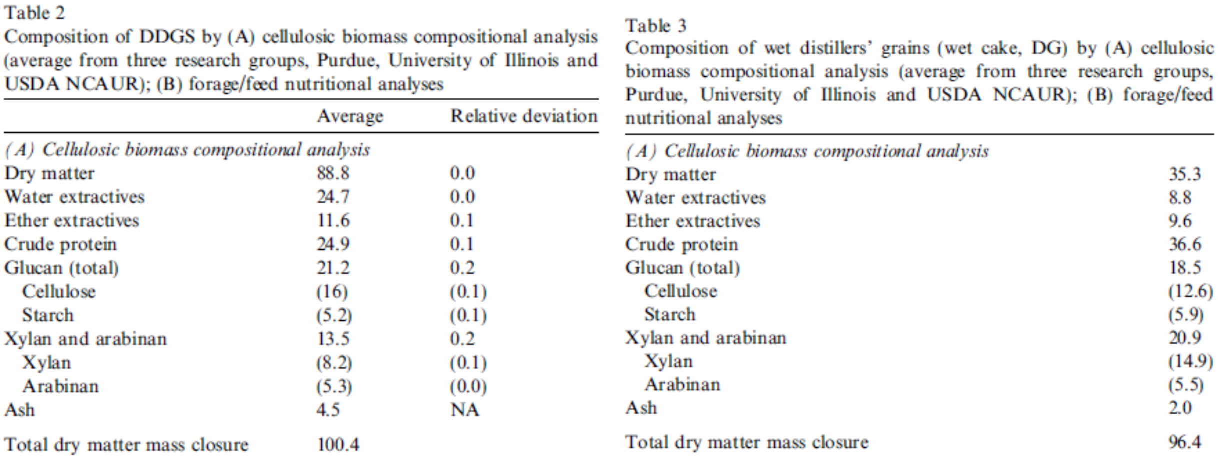


Table 2

Composition of DDGS by (A) cellulosic biomass compositional analysis (average from three research groups, Purdue, University of Illinois and USDA NCAUR); (B) forage/feed nutritional analyses

	Average	Relative deviation
(A) Cellulosic biomass compositional analysis		
Dry matter	88.8	0.0
Water extractives	24.7	0.0
Ether extractives	11.6	0.1
Crude protein	24.9	0.1
Glucan (total)	21.2	0.2
Cellulose	(16)	(0.1)
Starch	(5.2)	(0.1)
Xylan and arabinan	13.5	0.2
Xylan	(8.2)	(0.1)
Arabinan	(5.3)	(0.0)
Ash	4.5	NA
Total dry matter mass closure	100.4	

Table 3

Composition of wet distillers' grains (wet cake, DG) by (A) cellulosic biomass compositional analysis (average from three research groups, Purdue, University of Illinois and USDA NCAUR); (B) forage/feed nutritional analyses

(A) Cellulosic biomass compositional analysis	
Dry matter	35.3
Water extractives	8.8
Ether extractives	9.6
Crude protein	36.6
Glucan (total)	18.5
Cellulose	(12.6)
Starch	(5.9)
Xylan and arabinan	20.9
Xylan	(14.9)
Arabinan	(5.5)
Ash	2.0
Total dry matter mass closure	96.4

Suppliers for both WDGS and DDGS were located, which showed Midwest market prices to be ~$90/ton and ~$225/ton, respectively (Horner, 2012). The Scoular Company is an exemplary supplier due to its theoretical proximity (headquartered in Kansas), its scale (376M bushels and $4.9B sales annually), and its product line (i.e., availability of WDGS in addition to the more common DDGS) (Scoular). These factors were advantageous because Scoular represents likely the lowest transportation costs and an accurate reflection of market-wide prices.

Sugar-Cane By-products

The primary material of-interest in the sugar-cane ethanol process is a raw cane juice and molasses mixture, which is typically used as the primary feedstock after the sugarcane is initially processed. Unfortunately, market information for the molasses mixture is not easily attainable. Since it is a feedstock produced *in situ*, it does not have a secondary market like DGS. That said, Gopal (2009) identified a rough market price of Brazilian sugar cane molasses at ~$60/ton. The same article notes higher real and opportunity costs for cane juice - "molasses has a significantly lower opportunity cost than raw cane juice" – so molasses became the sole focus of the evaluation henceforth. Note that the standard molasses concentration of total reducible sugars (TRS) was initially taken to be 50%. Finally, note that world production is estimated at 61.7 million tons, with roughly 25% of the world's supply produced in Brazil, the proposed location of this facility (Licht, 2011).

Woody Biomass

The source of woody biomass identified in the project is located in the state of Washington. The description notes forest-thinning, mill residue, and land-clearing debris would be available. In a 2005 report by funded by the state government, Biomass Inventory and Bioenergy Assessment, the supply of such biomass in WA is noted as 6.3 million tons (Frear). Furthermore, in a 2000 study, it was estimated that mill residue could be delivered at a price of $30/ton (Antares Group). This latter figure is inflation-adjusted to $39.49 (CNM Group). It should be noted that this figure is optimistic since the original price quote was for a scale of 45 million tons, which significantly exceeds Washington's total availability.

Initial Screening Results

Using the above figures, an initial screening solely on the basis of price permitted easy insight into the profitability ceiling of the proposed models. The comparative basis chosen was the maximum margin attainable. This is defined as the profit margin where the sole cost is input procurement (i.e., not factoring in the costs of equipment, transportation, utilities, etc.). This figure imposes a ceiling on process profitability and enabled the prioritization of research into the most theoretically profitable input materials. Woody biomass (WB), with a maximum margin of 93-97%, and SCM (at 94%) became the focus of effort. Note that WDS was found to be a viable alternative, but that it appears substantially more expensive than the other two inputs. DDGS was ruled out completely because it would cost ~3-10x more than the other inputs.

Phase Two: In-Depth Screening

The second phase of the input screening involved a closer look at getting raw materials to usable process inputs. It was quickly conclusive that SCM was favorable. Given that both substances are produced in enormous quantities, it was necessary to distinguish between them along another dimension - the question became one of whether the $20/ton savings from using biomass was worth the added enzymatic or acid-catalyzed processing to convert cellulose to glucose. Enzymes were quickly ruled out on the basis of cost and the necessity of a batch process. Acid-catalyzed processing was appealing, but ultimately, the route from SCM to glucose appeared both simpler and easier -- largely just adding water and decanting --, well in excess of the $20 savings per ton.

Section II

Market & Competitive Analysis

II. MARKET & COMPETITIVE ANALYSIS

Porter's Five Forces

The *Porter's Five Forces* framework, developed by Michael Porter of the Harvard Business School in 1989, provides a framework to identify and evaluate less tangible aspects of a prospective market. The framework allows the user to evaluate attractiveness of the market based on (1) the bargaining power of suppliers, (2) the bargaining power of customers, (3) the threat of new entrants (4) the threat of substitute products, and (5) competitive rivalry within the industry. Based on the prevalence of each of these forces, prospective entrants can better evaluate a project's potential.

Bargaining power of suppliers

The molasses used as feedstock is the only material that must be purchased externally. Fermentation processes use molasses to produce baker's and brewer's yeast, citric acid, industrial alcohol, monosodium glutamate, and lysine. In addition, many industries, in particular agricultural feed manufacturing, use molasses for its binding properties (DMH Website). The presence of these additional buyers implies a high bargaining power among suppliers. Furthermore, suppliers are likely to lower production in response to a predicted surplus (DMH MB), which would further increase suppliers' leverage.

However, Cuba recently replaced its Ministry of Sugar with 13 separate state enterprises. The number of active sugar mills fell from 61 to 56, but overall bargaining power will fall without the ability to negotiate collectively. In addition, Beet molasses prices in eastern Europe have fallen dramatically (DMH MB), which will decrease the demand for cane molasses and further reduce suppliers' bargaining power. Overall, bargaining power of suppliers, while moderately high, should decay somewhat in the near future.

Bargaining power of customers

Xylene and particularly para-xylene are already produced in high volumes within the United States. It serves as a solvent in the printing, rubber, and leather industries, as well as a cleaning agent, a thinner for paint, and a component of many varnishes. Gasoline also contains para-xylene in small quantities. Most importantly, producers of synthetic fibers and plastics rely on para-xylene to manufacture polyester and related compounds like polyethylene terephthalate (PET); plastic bottle production alone represents 98% of global para-xylene consumption (Habeck 1995). These industries are dominated by large companies, such as Koch industries, who can use their size to exert high bargaining power.

In addition, supplies of para-xylene more than satisfy demand. Worldwide production capacity exceeded demand by over 4.5 million metric tons, meaning that average capacity utilization resides below 80%. In the short term, this likely counteracts any disadvantages in bargaining power that plague para-xylene customers. However, in the long term, the demand for para-xylene is expected to continue growing at 7% per annum, which should eliminate this excess capacity (Primary Information Services). Overall, the bargaining power of customers is high, but should decay steadily in the future.

Threat of new entrants

Demanders of para-xylene are actively encouraging a fiercely competitive para-xylene market inhabited by numerous new entrants, particularly those focused on renewable production. Most recently, Coca-cola, whose bottle manufacturing represents a significant fraction of annual para-xylene demand, recently invested in partnerships with three separate companies developing renewable para-xylene or substitute production processes: Gevo, Virent, and Avantium. In fact, Virent’s technology served as the basis for this process’s design. Pepsi, Coca-Cola’s chief competitor, responded with in-house development of their own renewable para-xylene production process. Both Coca-Cola and Pepsi expect to use these processes commercially by 2015 (Lane

2011). This means that even as demand continues to grow, new entrants will maintain a fierce level of competition in the para-xylene market.

The Threat of Substitute products

Para-xylene and its enabled polymer, polyethylene terephthalate (PET), have long served the markets mentioned under "Bargaining Power of Customers." However, Avantium, a company that recently partnered with both Coca-Cola and Danone Research, is currently developing what they claim to be a viable alternative, polyethylene furanoate (PEF) using its patented YXY ("icksy") catalyst technology. Independent studies by the Copernicus Institute at Utrecht University showed that PEF has a 50-60% lower carbon footprint that oil-based PET, and Avantium further claims that PEF is both lighter and more thermally resistant than PET (Danone, 2012).

However, the process has not yet proven industrially viable. In addition, a renewable para-xylene production process would mitigate or eliminate the carbon footprint advantages of PEF, dramatically lowering the incentive for bottle manufactures to invest in a transition to PEF. Because of these mitigating factors, the threat of substitutes is moderate.

Competitive Rivalry

Due to economies of scale, as well as consumer tendencies to require high quantities of para-xylene, the market is dominated by a significant number of high-capacity firms that operate internationally. Some, such as Invsita, a subsidiary previously owned by DuPont and recently purchased by Koch Industries, are vertically integrated, and provide their own demand for para-xylene in the form of polymers and polymer intermediates used in surfaces, materials, resins, and apparel (Koch, 2012). Others, such as Reliance Industries, have a more diversified portfolio. These companies produce para-xylene in quantities far exceeding the 200,000 tons of this process's design (Reliance Industries is the 5th largest at 1.86 million tons) (Reliance, 2012). With so many large competitors, competitive rivalry is expected to be high.

SWOT Analysis

SWOT stands for Strengths, Weaknesses, Opportunities, and Threats. After analyzing the state of Porter's Five Forces above, a SWOT framework enables the user to contextualize the information, draw conclusions, and make decisions.

Strengths

The first strength of this process is renewability. Para-xylene is not a new chemical, and the market has many large and well-established players. However, in the new age of environmental responsibility, the largest consumers of para-xylene are search for, and willing to invest heavily in, renewable alternatives to their current supplies. This creates competitive advantage over large incumbents in the market.

Second, the process was designed to take advantage of excess benzene produced during condensation and transalkylation. Although not quite as lucrative as para-xylene, benzene is still a valuable chemical. In addition to the additional profit offered by this benzene on a regular basis, it provides greater financial stability for the process. Both para-xylene and benzene demand and prices have been historically volatile, but have not always followed one another. As such, should the price of para-xylene drop unexpectedly, the process will still generate revenue from the sale of benzene.

Third, the para-xylene market in general is growing at an expected rate of 7% per annum. At this rate, there should be sufficient demand for para-xylene in general to sustain the process. Furthermore, if the market continues to grow, this process could be expanded or replicated elsewhere in order to establish a stronger foothold in the market at large.

Weaknesses

First, the process is dependent on molasses as a feedstock. Because suppliers of molasses are expected to exert a large amount of bargaining power in the near future, they could easily negotiate higher prices in response to an increase in demand, which would have a direct impact on the process's profitability. Unfortunately, the process's molasses requirements represent a significant fraction of molasses production in Brazil, essentially ensuring that prices will rise.

Second, the dominance of large and established para-xylene suppliers implies that this process will have to compete fiercely for customers, as well as accept market prices as given. Should the operating or materials costs rise for this particular process, it will be difficult to negotiate higher prices when larger competitors continue to sell at historical levels.

Third, the current excess para-xylene production capacity suggests that finding customers immediately upon market entry will be difficult. Most likely, the process will have to cater to smaller niche buyers, which will increase organizational costs and directly affect profitability.

Opportunities

First and foremost, the largest consumers of para-xylene are actively searching for a renewable source of para-xylene. These buyers are large. They are adverse to change in general, and place a high value on mitigating risk. As already demonstrated by Virent, Gevo, and Avantium, these companies are willing to subsidize further research. In addition, whichever company is first to market will capture a large customer, who will have little incentive to switch to any new entrant without a significantly superior value proposition.

Second, many industries, both those mentioned in the "Bargaining Power of Customers," and others, that could either begin using or make greater use of para-xylene are largely overlooked by the large players in the market. A smaller plant, such as this one, could better serve these smaller customers in a smaller, more profitable niche market while simultaneously contributing to increased total demand.

Third, although molasses prices are predicted to rise in response to this new para-xylene production process, the current slump in demand for cane molasses provides an opportunity to mitigate these rises. Molasses suppliers will dislike falling prices, and should be more willing to enter into long-term contracts at the current market price in order to avoid short-term losses.

Threats

First, Virent and Gevo are already developing similar processes for the renewable production of para-xylene. If either succeeds and enters the market first, they are likely to capture most or all of the demand for renewable para-xylene. This will leave later entrant to either battle to steal market share or compete with non-renewable suppliers for customers. Either represents a challenge for late entrants to operate at full-capacity.

Second, Avantium's prototype process for PEF threatens to decrease demand for para-xylene overall. This will have the direct effect of lowering the market price of para-xylene. Indirectly, many of Porter's Five Forces are currently unfavorable for a new entry, but are expected to improve as a result of steady increase in demand. If PEF proves viable and superior to PET, these conditions will remain unfavorable and make profitable operation in the market difficult.

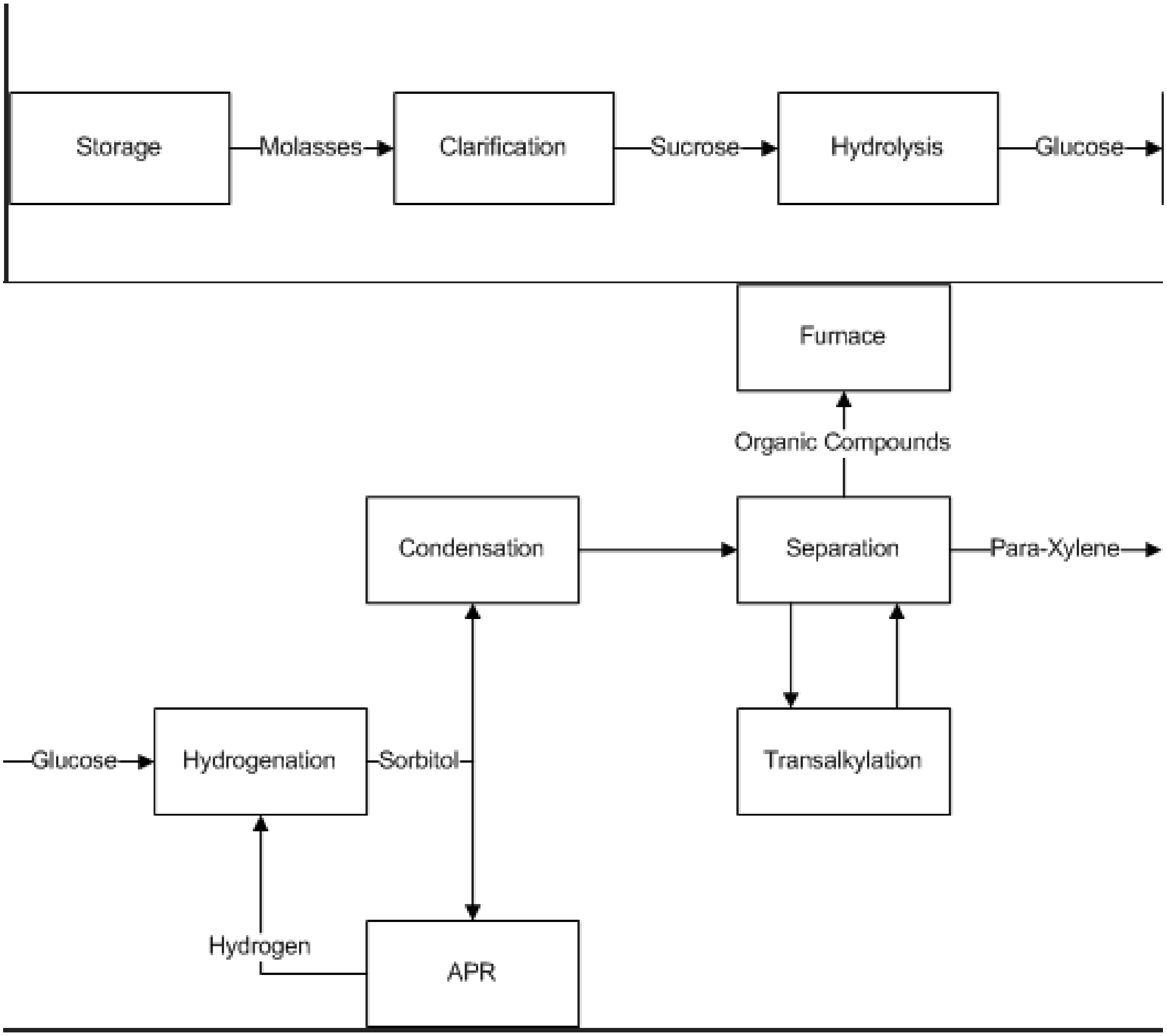
Section III

Process Overview, Flowsheets, & Material Balances

III. OVERVIEW, FLOWSHEETS, and MATERIAL BALANCES

Overview

The goal of this process is to produce para-xylene from sugar cane molasses. From storage, molasses is pumped to the clarifying section in which ash and other impurities are removed to form a sucrose and water solution. The sucrose is then hydrolyzed to form glucose and fructose. The glucose and fructose are then hydrogenated to form sorbitol. Sorbitol is used in the aqueous phase reforming to produce hydrogen, which is consumed in the hydrogenation reaction. The majority of the sorbitol is reacted in the condensation section to form aromatics and other organic compounds. These compounds are then separated through distillation. Certain alkanes and aromatics are then reacted in the transalkylation section through which additional para-xylene is formed, which is then sent back to the separation section. In the separation section, para-xylene is separated from similar compounds through crystallization to yield the final product.


Storage
Molasses
Clarification
Sucrose
Hydrolysis
Glucose
Furnace
Organic Compounds
Condensation
Separation
Para-Xylene
Transalkylation
Glucose
Hydrogenation
Sorbitol
Hydrogen
APR

Section 000: Input Storage & Clarification

Molasses is produced only nine months per year, which means that storage to maintain output levels throughout the three dry months is a key process consideration. This section details the storage of molasses, which requires 15 cone-roof tanks. One-third of these tanks will be in active use at any given time during the molasses season. The other two-thirds will be used to build up molasses supply throughout the year so that production can continue for the 92 days without raw material supply.

Molasses is a raw material produced from sugar cane and has many impurities in it such as ash and various minerals and carbohydrates besides the desired sugars, sucrose, glucose, and fructose. In order to remove these impurities and produce a sugar and water stream to be fed into the hydrolysis section, the molasses must undergo clarification. Molasses is first diluted with water in a heated continuously stirred mixer. Phosphoric acid and sodium hydroxide are added to precipitate impurities. Once diluted, the mixture is fed to a large concrete clarifying vessel. This allows the precipitated material to settle on the bottom of the clarifier, where it is scraped away by a rotating rake and leaves the clarifier as a sludge. The liquid overflow from the clarifier is pumped through a rotary drum filter where impurities are further removed from the mixture. Excess water is then evaporated to form a 50% sugar by mass solution, which is then pumped to the hydrolysis section.

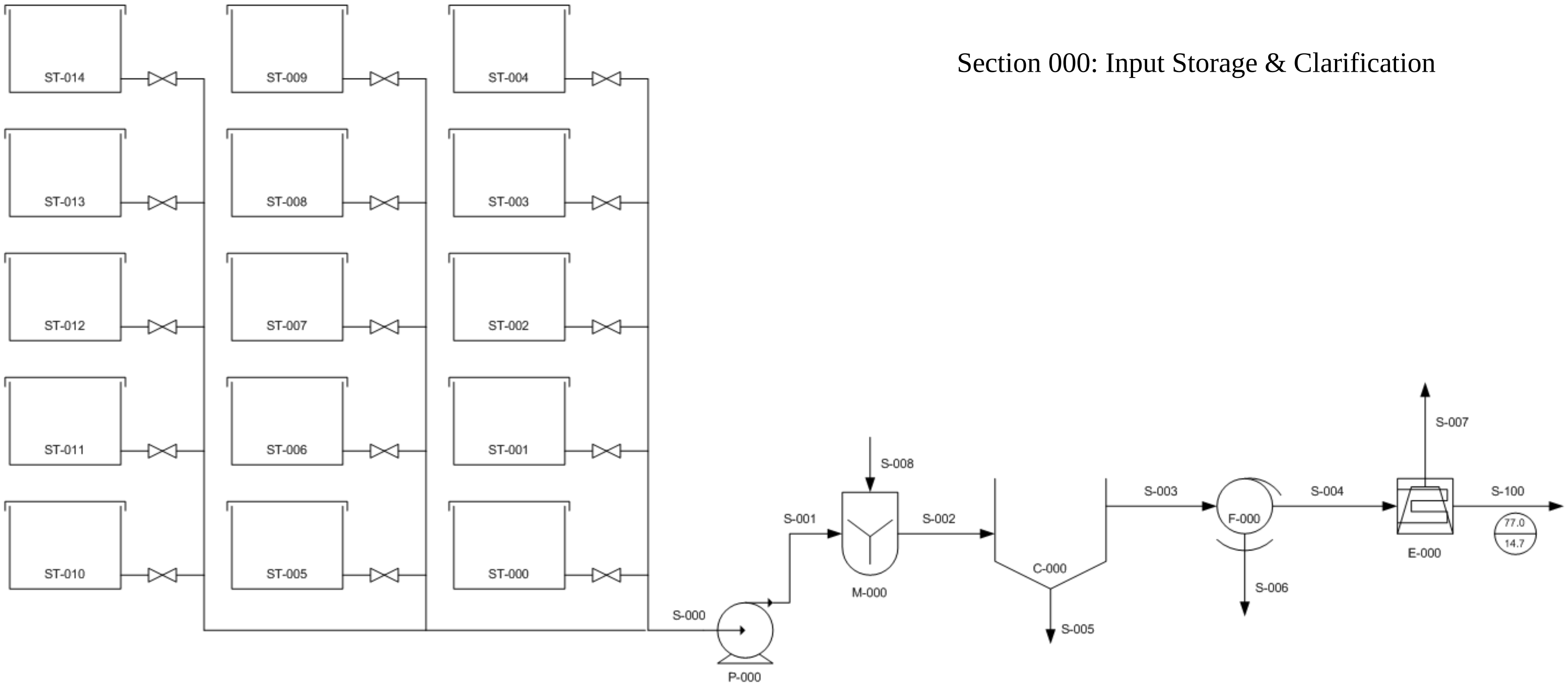
Since the project description states that the company has recently acquired “sugar-cane ethanol facilities” in Brazil, it is a reasonable assumption that the facilities are capable of molasses clarification and processing. Because of this assumption, we focused on the aspects of the process downstream of the conversion of raw molasses into a sugar and water solution.

However, a qualitative analysis of molasses clarification was examined and conservative estimates for the equipment and materials required were performed.

For each pound of molasses fed into the clarification process, .003 pounds of phosphoric acid and .004 pounds of sodium hydroxide would be required. Additionally, .00006 pounds of flocculant would be necessary. For our process, 1183104 pounds per hour of molasses are required. At a cost of $850 per ton of phosphoric acid, $12 million per year would be spent on phosphoric acid. At a cost of $500 per ton, $9 million per year would go to sodium hydroxide. Flocculant would cost only $295,000 per year.

A concrete clarifier with settling area of 88,258 square feet would cost $1,255,988 to purchase. The rotary drum filter, removing 1500 pounds of filtrate per day per square foot, would have to have an area of 115 square feet and would cost $130,000. In addition to this, an evaporator would likely be necessary to evaporate some of the water to turn the dilute sugar solution into a 50% sugar solution.

Section 000: Input Storage & Clarification



Section 100: Hydrolysis

$$C_{12}H_{22}O_{11} + H_2O \rightarrow 2\ C_6H_{12}O_6$$

The hydrolysis reaction converts sucrose and water into glucose. Sucrose is hydrolyzed by an HY faujasite zeolite catalyst, with a Si/Al ratio of 15. While sucrose hydrolysis could take place by itself in water, it would take years to fully hydrolyze. The catalyst is put in place to expedite the process to a much more reasonable reaction velocity. The product, glucose, is the necessary feed materials for the hydrogenation reactor needed to generate sorbitol.

The hydrolysis reaction process involves a splitter (SPT-100), six pumps (P-100, P-101,P-102, P-103, P-104, and P-105), three heat exchangers (HX-100, HX-101, and HX-102), and three fixed bed reactors (R-100, R-101, and R-102) to convert sucrose and water to glucose.

Pre-hydrolysis

The system input is fed into a splitter to make three identical streams and fed into the first three pumps (P-100, P-101, and P-102). The pumps are used to begin the flow of material throughout the process and make up for the frictional losses caused by the pipes. These pumps, feed the three heat exchangers (HX-100, HX-101, and HX-102). The heat exchangers are used to heat up the reactor feed streams to 100°C, while simultaneously cooling the condensation product stream.

Catalyst

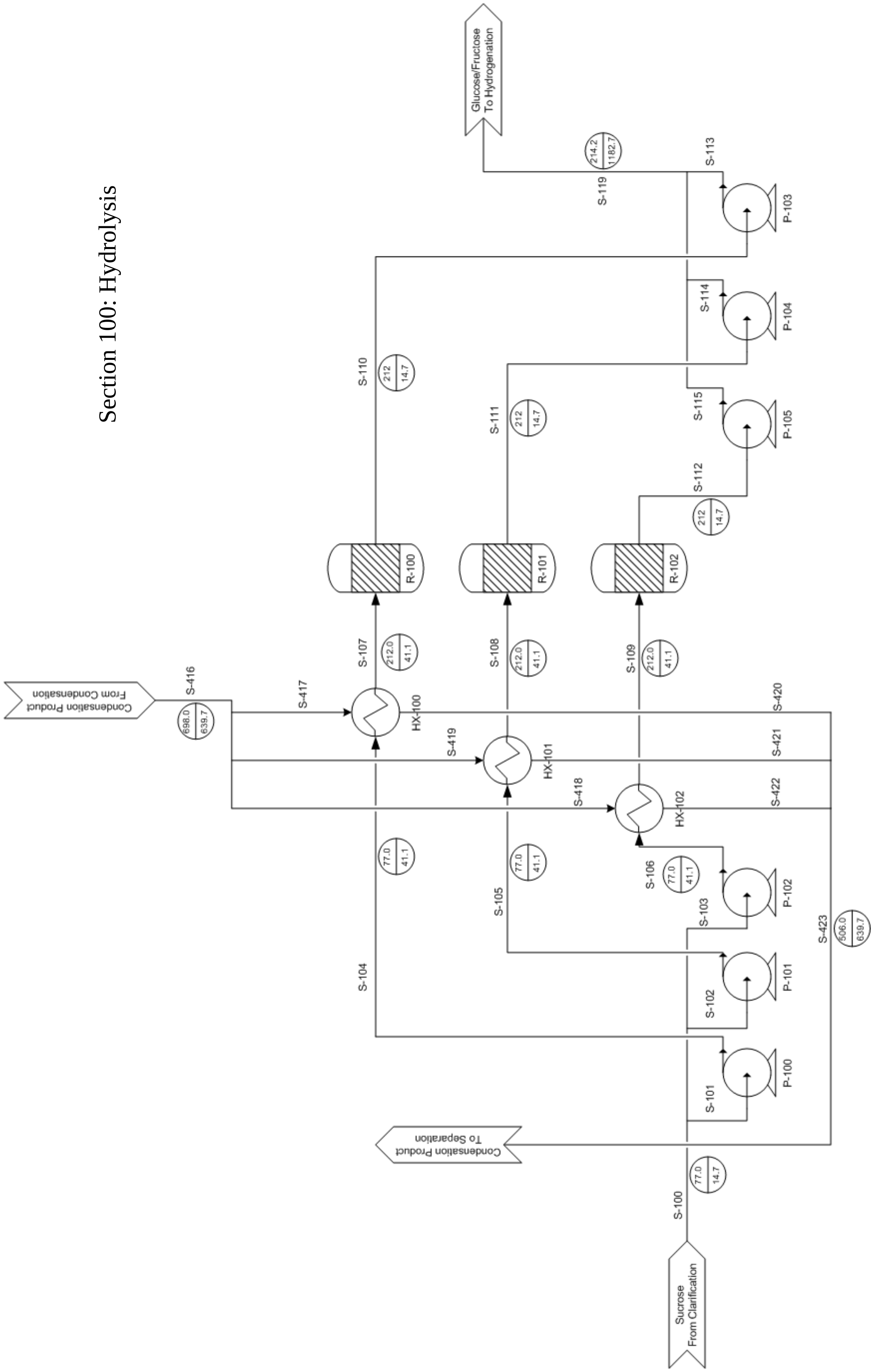
The HY faujasite catalyst can easily made by feeding H4SiO4 and NaAlO2 in a ratio of about 12 to 1 in the presence of NaOH and excess water. Faujasite crystals are formed through the use of steam aging HY crystals at 500°C for about 2 hours. To adjust the Si/Al ratio, after the steam aging, aqueous (NH4)2SiF6 is used until the Si/Al ratio is 15. The catalyst deactivation is estimated to be 13.9 g catalyst/lbmol sucrose fed, based on the deactivation rate of a similar catalyst, however the deactivation rate may actually be lower than estimated. The reason for the possibility of lower deactivation is evidenced by the claim that by running the reactor for 7 days, at a low flow, rate no deactivation was observed. The catalyst can also easily be regenerated through a thermal treatment, in which hot air at 500°C is passed through the catalyst for 2 hours, when it has lost significant activity a limited number of times.

Hydrolysis

Once the streams are heated up they are fed into the three reactors (R-100, R-101, and R-102). The reactors are typical industrial fixed bed reactors. They are essentially a series of tubes, filled with catalyst, in parallel. The tubes are laid out in such a way as to look similar to a shell and tube heat exchanger with many tubes. The reactors used for this process have over 10000 tubes per reactor. All three reactors operate at atmospheric pressure and 100°C and convert 100% of the sucrose to glucose. Once the reaction has taken place the three product streams are fed into the other three pumps to raise their pressure to 80 bar, after which they are mixed and fed into the next section.

These reactors were based off of examples found in the literature, in particular Moreau (1999). To hydrolyze sucrose, an approximately 600 g/l solution of sucrose is fed through a tubular reactor charged with the HY faujasite catalyst. The fixed bed reactor is held at 100°C. It was observed that approximately 99.9% of all sucrose fed into the reactor was converted to glucose.

Section 100: Hydrolysis



Hydrolysis Stream Report (1 of 3)

	S-100	S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108	S-109
Mass Flow (lb/hr)										
Sorbitol	0	0	0	0	0	0	0	0	0	0
Para-Xylene	0	0	0	0	0	0	0	0	0	0
Ortho-Xylene	0	0	0	0	0	0	0	0	0	0
Meta-Xylene	0	0	0	0	0	0	0	0	0	0
Methane	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0	0	0	0
N-Butane	0	0	0	0	0	0	0	0	0	0
N-Pentane	0	0	0	0	0	0	0	0	0	0
N-Hexane	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	0	0	0	0	0	0	0	0	0	0
Water	618205	206068	206068	206068	206068	206068	206068	206068	206068	206068
Hydrogen	0	0	0	0	0	0	0	0	0	0
Glucose	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0
Sucrose	618205	206068	206068	206068	206068	206068	206068	206068	206068	206068
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	0	0	0	0	0	0	0	0
Toluene	0	0	0	0	0	0	0	0	0	0
Benzene	0	0	0	0	0	0	0	0	0	0
Napthalene	0	0	0	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0	0	0	0	0	0	0	0	0	0
Isopropylbenzene	0	0	0	0	0	0	0	0	0	0
N-Heptane	0	0	0	0	0	0	0	0	0	0
1-Butene	0	0	0	0	0	0	0	0	0	0
1-Pentene	0	0	0	0	0	0	0	0	0	0
1-Hexene	0	0	0	0	0	0	0	0	0	0
1-Heptene	0	0	0	0	0	0	0	0	0	0
Air	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	36122	12041	12041	12041	12041	12041	12041	12041	12041	12041
Total Flow (lb/hr)	1236410	412136	412136	412136	412136	412136	412136	412136	412136	412136
Total Flow (cuft/hr)	16714	5571	5571	5571	5571	5571	5571	5953	5953	5953
Temperature (°F)	77.00	77.00	77.00	77.00	77.04	77.04	77.04	212.00	212.00	212.00
Pressure (psia)	14.70	14.70	14.70	14.70	40.41	41.15	41.15	40.41	41.15	41.15
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Hydrolysis Stream Report (2 of 3)

	S-110	S-111	S-112	S-113	S-114	S-115	S-119	S-416	S-417	S-418
Mass Flow (lb/hr)										
Sorbitol	0	0	0	0	0	0	0	0	0	0
Para-Xylene	0	0	0	0	0	0	0	41138	13712	13713
Ortho-Xylene	0	0	0	0	0	0	0	763	254	254
Meta-Xylene	0	0	0	0	0	0	0	85	28	28
Methane	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0	0	0	0
N-Butane	0	0	0	0	0	0	0	6059	2020	2020
N-Pentane	0	0	0	0	0	0	0	23225	7741	7742
N-Hexane	0	0	0	0	0	0	0	32312	10771	10771
Carbon Dioxide	0	0	0	0	0	0	0	0	0	0
Water	195221	195221	195221	195221	195221	195221	585662	792890	264294	264302
Hydrogen	0	0	0	0	0	0	0	389	130	130
Glucose	216916	216916	216916	216916	216916	216916	650747	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	0	0	0	0	0	424	141	141
Toluene	0	0	0	0	0	0	0	9087	3029	3029
Benzene	0	0	0	0	0	0	0	2019	673	673
Napthalene	0	0	0	0	0	0	0	20195	6732	6732
1,2,4-Trimethylbenzene	0	0	0	0	0	0	0	20195	6732	6732
Isopropylbenzene	0	0	0	0	0	0	0	30293	10098	10098
N-Heptane	0	0	0	0	0	0	0	7068	2356	2356
1-Butene	0	0	0	0	0	0	0	972	324	324
1-Pentene	0	0	0	0	0	0	0	2934	978	978
1-Hexene	0	0	0	0	0	0	0	4081	1360	1361
1-Heptene	0	0	0	0	0	0	0	893	298	298
Air	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	12040	12040	12040	12040	12040	12040	36121	46295	15432	15432
Total Flow (lb/hr)	412136	412136	412136	412136	412136	412136	1236410	995023	331671	331681
Total Flow (cuft/hr)	5745	5745	5745	5753	5753	5753	17259	822002	273998	274006
Temperature (°F)	212.00	212.00	212.00	214.16	214.16	214.16	214.16	698.00	698.00	698.00
Pressure (psia)	14.70	14.70	14.70	1181.70	1181.70	1181.70	1181.70	639.70	639.70	639.70
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00

Hydrolysis Stream Report (3 of 3)

	S-419	S-420	S-421	S-422	S-423
Mass Flow (lb/hr)					
Sorbitol	0	0	0	0	0
Para-Xylene	13712	13712	13712	13713	41138
Ortho-Xylene	254	254	254	254	763
Meta-Xylene	28	28	28	28	85
Methane	0	0	0	0	0
Ethane	0	0	0	0	0
Propane	0	0	0	0	0
N-Butane	2020	2020	2020	2020	6059
N-Pentane	7741	7741	7741	7742	23225
N-Hexane	10771	10771	10771	10771	32312
Carbon Dioxide	0	0	0	0	0
Water	264294	264294	264294	264302	792890
Hydrogen	130	130	130	130	389
Glucose	0	0	0	0	0
Oxygen	0	0	0	0	0
Nitrogen	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0
Sucrose	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0
Ethylbenzene	141	141	141	141	424
Toluene	3029	3029	3029	3029	9087
Benzene	673	673	673	673	2019
Napthalene	6732	6732	6732	6732	20195
1,2,4-Trimethylbenzene	6732	6732	6732	6732	20195
Isopropylbenzene	10098	10098	10098	10098	30293
N-Heptane	2356	2356	2356	2356	7068
1-Butene	324	324	324	324	972
1-Pentene	978	978	978	978	2934
1-Hexene	1360	1360	1360	1361	4081
1-Heptene	298	298	298	298	893
Air	0	0	0	0	0
DowthermA	0	0	0	0	0
Total Flow (lbmol/hr)	15432	15432	15432	15432	46295
Total Flow (lb/hr)	331671	331671	331671	331681	995023
Total Flow (cuft/hr)	273998	208888	208889	208897	626674
Temperature (°F)	698.00	505.98	505.98	505.98	505.98
Pressure (psia)	639.70	639.70	639.70	639.70	639.70
Vapor Fraction	1.00	1.00	1.00	1.00	1.00

Section 200: Hydrogenation

$$C_6H_{12}O_6 + H_2 \Rightarrow C_6H_{14}O_6$$

Hydrogenation reacts glucose with hydrogen gas and converts it to sorbitol. There are several ways to successfully convert glucose to sorbitol, in the presence of hydrogen and certain catalysts. Some combinations of catalysts, hydrogen pressures, and reactor temperature yield much better results in terms of overall conversion of glucose to sorbitol. Many of these variables were experimented with in search of the best results.

Pre-Hydrogenation

The hydrogenation process consists of a heat exchanger (HX-200), a splitter (SPT-200), twelve pumps (P-200, P-201, P-202, P-203, P-204, P-205, P-206, P-207, P-208, P-209, P-210, and P-211), and six trickle bed reactors (R-200, R-201, R-202, R-203, R-204, and R-205). HX-200 cools the streams to 100^0C from the hydrolysis process before feeding them into the splitter, SPT-200 to create six identical streams. They are fed into the first six pumps (P-200, P-201, P-202, P-203, P-204, and P-205) to get them flowing into the six trickle bed reactors (R-200, R-201, R-202, R-203, R-204, and R-205) and make up for the frictional losses in the pipes. Hydrogen created in the APR process is fed into the reactors as well.

Catalyst

In typical glucose hydrogenation Ni used to be the preferred catalyst metal because of its high activity and low costs. Unfortunately Ni catalysts can leach and have their activity decreased rapidly and require possibly expensive separation processes to purify the product of the Ni particles. Ru catalysts however don’t suffer from the same drawbacks as Ni which makes it much more appealing as a commercial catalyst. The catalyst which yielded the best result for glucose hydrogenation was a Ru05Ai catalyst.

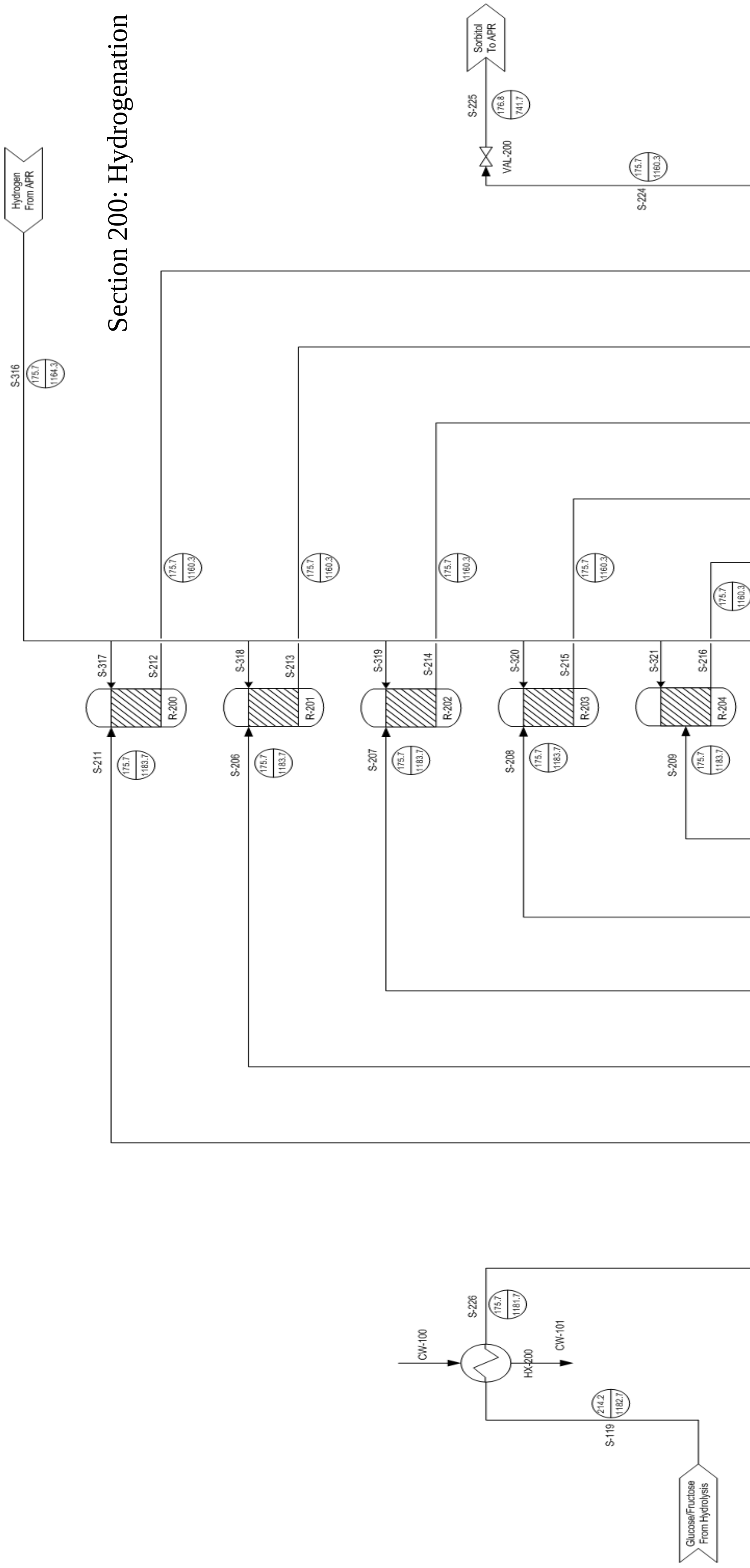
The Ru05Ai catalyst creation process would be prepared by the impregnation of Al2O3 with Ruthenium (III) Acetylacetonate. The Al2O3 is used as the support metal for the activation of the ruthenium. To begin the preparation of the catalyst 73 g Al2O3 is mixed with 150 ml of toluene and stirred for 15 minutes. Once the Al2O3/toluene slurry is prepared, 2.907 g Ruthenium (III) Acetylacetonate is dissolved in a separate 150 ml of toluene and this solution is added to the slurry. This new slurry is stirred for one hour while being swirled occasionally to homogenize it. The toluene is also left to evaporate at room temperature at this time. The catalyst is then heated in by a helium stream within four hours to 250°C and held at this temperature for two more hours. To reduce the catalyst it is heated to 350°C within one hour by a hydrogen stream and held at this temperature for threemore hours. However based on the cost of buying of the raw materials needed and additional labor costs needed for creating the catalyst it was found to be much cheaper to purchase a catalyst that is believed to be similar from a supplier. Catalyst deactivation was assumed to be seven years because of Ruthenium’s use as a precious metal. It was also assumed that the catalyst could be sold back to the supplier for half of the purchase price.

Hydrogenation

There are two possible ways to do a glucose hydrogenation, either discontinuously or continuously. The discontinuous process involves feeding an autoclave with the feedstock and pressurizing it to 3 bar with hydrogen followed by increasing the temperature to its reaction temperature and then finally pressurizing the hydrogen to its desired pressure. This process unfortunately would take too much time and the continuous process is preferred in practice. The continuous process involves a trickle bed reactor. A typical reaction condition for this is a 40-wt% glucose solution with a large of excess of hydrogen gas at about 80 bar fed into a reactor at approximately 353K. A conversion of 99.9% of the glucose fed with selectivity to sorbitol of 99.0% was reported.

A trickle bed reactor is different from most conventional fixed bed reactors in that both the gas and liquid flow are pumped into the top of the reactor co-currently as opposed to having liquid flow downward and gas flow upward counter-currently. The hydrogenation reaction takes place at 353K and 80 bar and converts 100% of the glucose into sorbitol. The products streams are then fed into the other six pumps (P-206, P-207, P-208, P-209, P-210, and P-211) to get them flowing into the aqueous phase reforming and condensation processes and make up for the frictional losses caused by the reactor and pipes.

Section 200: Hydrogenation



Hydrogenation Stream Report (1 of 4)

	CW-100	CW-101	S-119	S-200	S-201	S-202	S-203	S-204	S-205	S-206	S-207
Mass Flow (lb/hr)											
Sorbitol	0	0	0	0	0	0	0	0	0	0	0
Para-Xylene	0	0	0	0	0	0	0	0	0	0	0
Ortho-Xylene	0	0	0	0	0	0	0	0	0	0	0
Meta-Xylene	0	0	0	0	0	0	0	0	0	0	0
Methane	0	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0	0	0	0	0
N-Butane	0	0	0	0	0	0	0	0	0	0	0
N-Pentane	0	0	0	0	0	0	0	0	0	0	0
N-Hexane	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	0	0	0	0	0	0	0	0	0	0	0
Water	1284910	1284910	585662	97610	97610	97610	97610	97610	97610	97610	97610
Hydrogen	0	0	0	0	0	0	0	0	0	0	0
Glucose	0	0	650747	108458	108458	108458	108458	108458	108458	108458	108458
Oxygen	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Toluene	0	0	0	0	0	0	0	0	0	0	0
Benzene	0	0	0	0	0	0	0	0	0	0	0
Napthalene	0	0	0	0	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Isopropylbenzene	0	0	0	0	0	0	0	0	0	0	0
N-Heptane	0	0	0	0	0	0	0	0	0	0	0
1-Butene	0	0	0	0	0	0	0	0	0	0	0
1-Pentene	0	0	0	0	0	0	0	0	0	0	0
1-Hexene	0	0	0	0	0	0	0	0	0	0	0
1-Heptene	0	0	0	0	0	0	0	0	0	0	0
Air	0	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	71323	71323	36121	6020	6020	6020	6020	6020	6020	6020	6020
Total Flow (lb/hr)	1284910	1284910	1236410	206068	206068	206068	206068	206068	206068	206068	206068
Total Flow (cuft/hr)	20854	21196	17259	2809	2809	2809	2809	2809	2809	2809	2809
Temperature (°F)	90.00	119.17	214.16	175.73	175.73	175.73	175.73	175.73	175.73	175.73	175.73
Pressure (psia)	14.70	14.70	1181.70	1181.70	1181.70	1181.70	1181.70	1181.70	1181.70	1183.70	1183.70
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

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	S-209	S-210	S-211	S-212	S-213	S-214	S-215	S-216	S-217	S-218	S-219
Mass Flow (lb/hr)											
Sorbitol	0	0	0	109680	109680	109680	109680	109682	109680	109680	109680
Para-Xylene	0	0	0	0	0	0	0	0	0	0	0
Ortho-Xylene	0	0	0	0	0	0	0	0	0	0	0
Meta-Xylene	0	0	0	0	0	0	0	0	0	0	0
Methane	0	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0	0	0	0	0
N-Butane	0	0	0	0	0	0	0	0	0	0	0
N-Pentane	0	0	0	0	0	0	0	0	0	0	0
N-Hexane	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	0	0	0	0	0	0	0	0	0	0	0
Water	97610	97610	97610	97616	97616	97616	97616	97617	97616	97616	97616
Hydrogen	0	0	0	0	0	0	0	0	0	0	0
Glucose	108458	108458	108458	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Toluene	0	0	0	0	0	0	0	0	0	0	0
Benzene	0	0	0	0	0	0	0	0	0	0	0
Napthalene	0	0	0	0	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Isopropylbenzene	0	0	0	0	0	0	0	0	0	0	0
N-Heptane	0	0	0	0	0	0	0	0	0	0	0
1-Butene	0	0	0	0	0	0	0	0	0	0	0
1-Pentene	0	0	0	0	0	0	0	0	0	0	0
1-Hexene	0	0	0	0	0	0	0	0	0	0	0
1-Heptene	0	0	0	0	0	0	0	0	0	0	0
Air	0	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	6020	6020	6020	6021	6021	6021	6021	6021	6021	6021	6021
Total Flow (lb/hr)	206068	206068	206068	207296	207296	207296	207296	207299	207296	207296	207296
Total Flow (cuft/hr)	2809	2809	2809	2821	2821	2821	2821	2821	2821	2821	2821
Temperature (°F)	175.73	175.73	175.73	175.73	175.73	175.73	175.73	175.73	175.73	175.73	175.73
Pressure (psia)	1183.70	1183.70	1183.70	1160.30	1160.30	1160.30	1160.30	1160.30	1160.30	1162.30	1162.30
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Hydrogenation Stream Report (4 of 4)

	S-220	S-221	S-222	S-223	S-224	S-225	S-226	S-316	S-317	S-318	S-319
Mass Flow (lb/hr)											
Sorbitol	109680	109680	109682	109680	658083	658083	0	0	0	0	0
Para-Xylene	0	0	0	0	0	0	0	0	0	0	0
Ortho-Xylene	0	0	0	0	0	0	0	0	0	0	0
Meta-Xylene	0	0	0	0	0	0	0	0	0	0	0
Methane	0	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0	0	0	0	0
N-Butane	0	0	0	0	0	0	0	0	0	0	0
N-Pentane	0	0	0	0	0	0	0	0	0	0	0
N-Hexane	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	0	0	0	0	0	0	0	0	0	0	0
Water	97616	97616	97617	97616	585695	585695	585662	0	0	0	0
Hydrogen	0	0	0	0	0	0	0	7369	1228	1228	1228
Glucose	0	0	0	0	0	0	650747	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Toluene	0	0	0	0	0	0	0	0	0	0	0
Benzene	0	0	0	0	0	0	0	0	0	0	0
Napthalene	0	0	0	0	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Isopropylbenzene	0	0	0	0	0	0	0	0	0	0	0
N-Heptane	0	0	0	0	0	0	0	0	0	0	0
1-Butene	0	0	0	0	0	0	0	0	0	0	0
1-Pentene	0	0	0	0	0	0	0	0	0	0	0
1-Hexene	0	0	0	0	0	0	0	0	0	0	0
1-Heptene	0	0	0	0	0	0	0	0	0	0	0
Air	0	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	6021	6021	6021	6021	36123	36123	36121	3656	609	609	609
Total Flow (lb/hr)	207296	207296	207299	207296	1243780	1243780	1236410	7369	1228	1228	1228
Total Flow (cuft/hr)	2821	2821	2821	2821	16928	16938	16852	22167	3693	3693	3693
Temperature (°F)	175.73	175.73	175.73	175.73	175.74	176.80	175.73	175.73	175.73	175.73	175.73
Pressure (psia)	1162.30	1162.30	1162.30	1162.30	1160.30	741.70	1181.70	1164.30	1164.30	1164.30	1164.30
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	1.00

Hydrogenation Stream Report (4 of 4)

	S-320	**S-321**	**S-322**
Mass Flow (lb/hr)			
Sorbitol	0	0	0
Para-Xylene	0	0	0
Ortho-Xylene	0	0	0
Meta-Xylene	0	0	0
Methane	0	0	0
Ethane	0	0	0
Propane	0	0	0
N-Butane	0	0	0
N-Pentane	0	0	0
N-Hexane	0	0	0
Carbon Dioxide	0	0	0
Water	0	0	0
Hydrogen	1228	1231	1228
Glucose	0	0	0
Oxygen	0	0	0
Nitrogen	0	0	0
Carbon Monoxide	0	0	0
Sucrose	0	0	0
Sodium Hydroxide	0	0	0
Ethylbenzene	0	0	0
Toluene	0	0	0
Benzene	0	0	0
Napthalene	0	0	0
1,2,4-Trimethylbenzene	0	0	0
Isopropylbenzene	0	0	0
N-Heptane	0	0	0
1-Butene	0	0	0
1-Pentene	0	0	0
1-Hexene	0	0	0
1-Heptene	0	0	0
Air	0	0	0
DowthermA	0	0	0
Total Flow (lbmol/hr)	609	610	609
Total Flow (lb/hr)	1228	1231	1228
Total Flow (cuft/hr)	3693	3702	3693
Temperature (°F)	175.73	175.73	175.73
Pressure (psia)	1164.30	1164.30	1164.30
Vapor Fraction	1.00	1.00	1.00

Section 300: Aqueous Phase Reforming

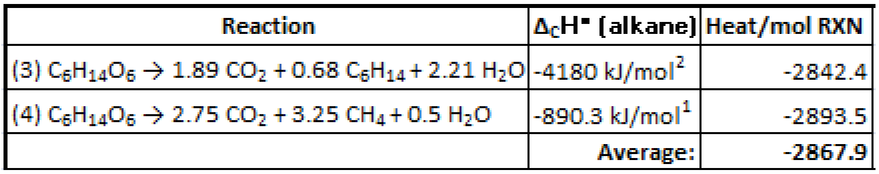
(1) $C_6H_{14}O_6 + 6H_2O \rightarrow 6CO_2 + 13H_2$

(2) $C_6H_{14}O_6 + xH_2 \rightarrow aH_2O + bCH_4 + cC_2H_6 + dC_3H_8 + eC_4H_{10} + fC_5H_{12} + gC_6H_{14}$

Aqueous phase reforming (APR) is a novel technology for the catalytic conversion of oxygenated hydrocarbons into hydrogen, alkanes, and carbon dioxide (WO/2007075476-A2). It is a more sustainable alternative to fossil fuel reforming for processes that require an endogenous supply of hydrogen. In this process, APR can convert readily-available sugar alcohols into hydrogen, over a RhReCe catalyst, which is used to create sorbitol, a necessary intermediate in the production of para-xylene.

Although hydrogen is the goal output of this section, the light alkane by-products can be used to generate heat for other portions of the process. However, the data supplied in the patent detail conversion and output composition in lump sum “alkanes.” The relative breakdowns of alkanes in the final product is unknown. However, a sensitivity analysis of heats of combustion (Figure 2) showed that the actual composition of C1-C6 alkanes made little differential impact on the overall energy output (Pittam, 1972; SI Chemical Data Book).

Figure 2



Reaction	$\Delta_C H^\circ$ (alkane)	Heat/mol RXN
(3) $C_6H_{14}O_6 \rightarrow 1.89\ CO_2 + 0.68\ C_6H_{14} + 2.21\ H_2O$	-4180 kJ/mol[2]	-2842.4
(4) $C_6H_{14}O_6 \rightarrow 2.75\ CO_2 + 3.25\ CH_4 + 0.5\ H_2O$	-890.3 kJ/mol[1]	-2893.5
	Average:	**-2867.9**

Therefore, propane, which has a middling heat of combustion, was chosen as the sole alkane for all ASPEN calculations in this portion of the analysis.

The aqueous phase reforming process utilizes four heat exchangers (HX-300, HX-301, HX-302, and HX-303), three pumps (P-300, P-301, and P-302), two valves (VAL-300 and VAL 301), two flash separators (F-300 and F-301), a mixer (MIX-300), a pressure swing adsorption separator (SEP-300), a compressor (CMP-300) and a fixed bed reactor (R-300).

Catalyst

The catalyst presentation in the patent was presented independent of the operating conditions discussion. The most optimal conditions range from 150-300°C and from 10-50 bar. 182°C and 50 bar were selected as the duty-minimizing conditions, over which the specified conversions were assumed to apply. This is certainly a questionable assumption, but there was no other basis for condition selection available. The catalyst was made by adding 3.86g of Rhodium(III) Nitrate, 1.64g of Perrhenic acid, and 2.21g of Cerium(III) Nitrate hexahydrate to 12 ml of deionized water in the presence of titania modified carbon and dried overnight under a vacuum at 100°C. The titania modified carbon was created by adding 1.95g of Titanium n-butoxide to 12 ml of anhydrous isopropanol in the presence of 10g of activated carbon. However due to the high costs of Rhodium(III) Nitrate it was assumed that the metals were purchased at market price and could be sold back to the supplier after deactivation for half the purchase price to be regenerated. It was also assumed that because rhodium is a precious metal the deactivation would take place over 5 years.

Aqueous Phase Reforming

The patented technology (Cortright 2007) - assumed to be available for use in this plant - presents a range of operating conditions, inputs, and catalysts. Since sorbitol is a key component of the process, Example 31 from Table 7 was chosen for the design, as it maximizes hydrogen from a sorbitol input. Specifically, this embodiment converts a 50 wt% aqueous sorbitol solution to a gas that is 57 mol% hydrogen over a RhReCe catalyst in the presence of NaOH. Note that the patent is extraordinarily difficult to interpret, as the molar percentage of alkanes is uninterpretable on a mass basis, since the breakdown of alkanes is unknown. To overcome this, Excel solver was used to backout the actual yields for the process via a mole balance. The fixed bed reactor, R-300, is used to generate hydrogen, alkanes, and carbon dioxide from sorbitol.

Heat Exchange and Recovery

The first heat exchanger, HX-300, is used to cool the carbon dioxide, water, hydrogen and alkane stream from F-300 while simultaneously heating the new and recycled sorbitol mix stream from MIX-300. The second heat exchanger, HX-301, is used to heat the inlet sorbitol stream, fed to R-300, to 182°C, the reaction temperature by using the heat generated from the furnace. The third heat exchanger, HX-302, is used to cool the hydrogen stream coming from HX-400 to 353K the reaction temperature of the hydrogenation reaction. The fourth heat exchanger, HX-303, is used to cool the hydrogen, carbon dioxide, and alkane stream from HX-300 and is fed into F-301.

Pressurization and Depressurization

The first pump, P-300, is used to pump the new and recycled sorbitol mix stream from HX-300 to HX-301 and make up for any frictional losses.The second pump, P-301, is used to pump the recycled sorbitol from F-300 into MIX-300 and to make up for frictional losses. The third pump, P-302, is used to pump the new and recycled sorbitol mix from MIX-300 to HX-300 and to combat the frictional losses. The first valve, VAL-300, is used to decrease the pressure of the product stream mixed with the recyclable sorbitol from R-300. The second valve, VAL-301, is used to decrease the pressure of the hydrogen, carbon dioxide, water, and alkane stream from F-300. The compressor, CMP-300, is used to compress the hydrogen separated in SEP-300 to 80 bar to be fed to the hydrogenation process.

Separations

To recover hydrogen from the aqueous phase reforming reactor, the vapor product is separated using pressure swing adsorption (PSA). Hydrogen, carbon dioxide, water, and various light alkanes are flowed across several adsorption columns at 20 bar. The zeolites in the columns adsorb the polar components and carbon dioxide, while the hydrogen exits the column. Once the column becomes saturated, the outlet valve is shut off and a vacuum is pulled on the column, causing the polar components and carbon dioxide to desorb from the adsorbent and regenerate the column. Once the column is regenerated, the cycle is repeated. Multiple adsorption columns are necessary to make optimal use of the compressor and vacuum, ensuring that at least one column is being fed vapor at any moment.

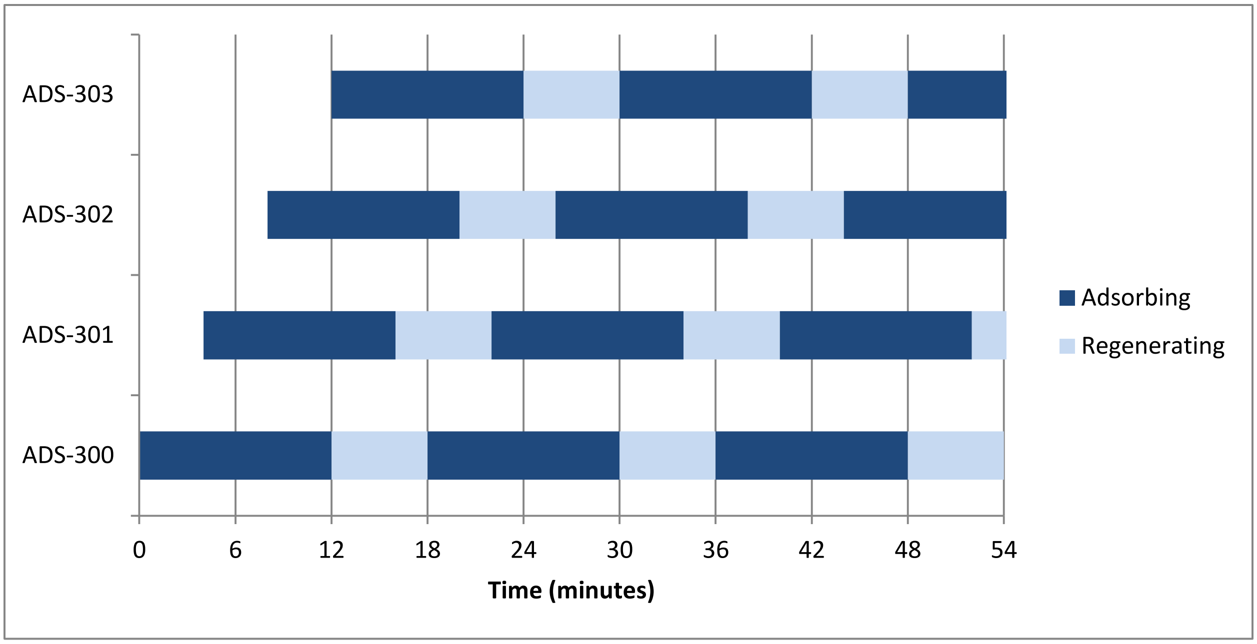
The first flash separator, F-300, is used to separate sorbitol from R-300 products so the sorbitol can be recycled. The second flash separator is used to separate water from the carbon dioxide, hydrogen, and alkane stream that is going to be fed in SEP-300.

To recover hydrogen from the aqueous phase reforming reactor, the vapor product is separated using pressure swing adsorption (PSA). Hydrogen, carbon dioxide, water, and various light alkanes are flowed across several adsorption columns at 20 bar. The 13x zeolite in the columns adsorb the polar components, alkanes, and carbon dioxide, while the hydrogen exits the column, unadsorbed. Once the column nears saturation, or the exit concentration of hydrogen falls below a desired point, the inlet and outlet valves are shut off and a small amount of product purity hydrogen is sent through the column, causing the polar components, alkanes, and carbon dioxide to desorb from the adsorbent and regenerate the column. Once the column is regenerated, the cycle is repeated. Multiple adsorption columns are necessary to make optimal use of the compressor and inlet streams, ensuring that at least one column is being fed gas at any point, preventing the need for a storage tank before the PSA.

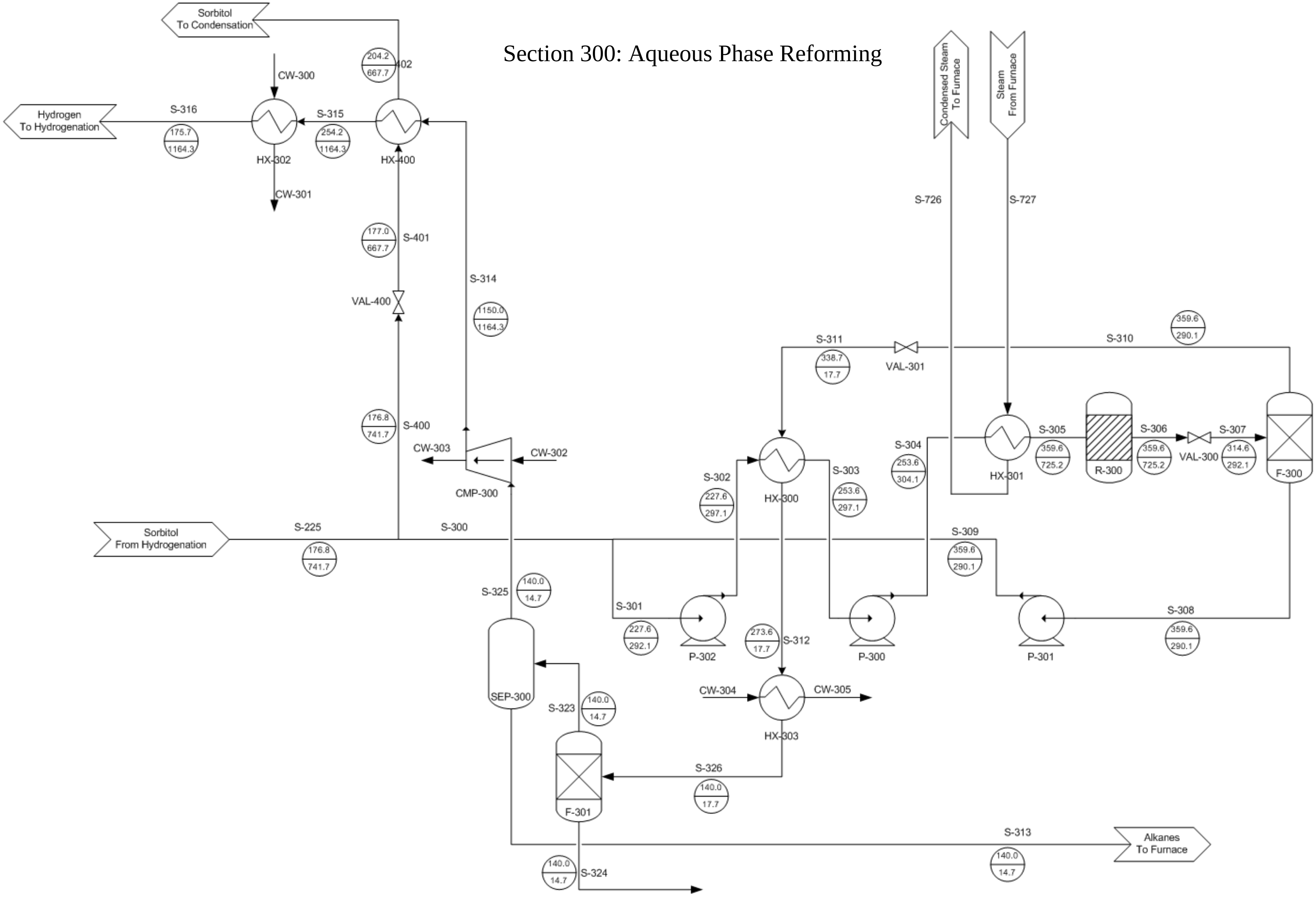
Because pressure swing adsorption is a batch process, it was left out of the ASPEN simulation. On the block diagram for APR, it is represented by SEP-300. A storage tank is used to collect excess hydrogen from the adsorption columns so that downstream of the storage tank, the hydrogen appears to come from a continuous source.

Four columns are used for the PSA system in order to make the system as flexible as possible. Since some assumptions had to be made, it was decided to make a conservative estimate of the breakthrough time for each adsorber. Each adsorber will have gas flowed through it for 12 minutes, and then be desorbed at atmospheric pressure for 6 minutes. The adsorbers will start running at 0, 4, 8, and 12 minutes so that at any given moment three of the four adsorbers will be adsorbing gas, while one adsorber is being regenerated. This ensures the lowest flowrate possible through the adsorbers, which increases the amount of unwanted gases that adsorb to the zeolite, increasing the recovery of hydrogen. This schedule is summarized in Figure 3 (Cavenati, 2004).

Figure 3



Section 300: Aqueous Phase Reforming



APR Stream Report (1 of 4)

	CW-300	CW-301	CW-304	CW-305	S-225	S-300	S-301	S-302	S-303	S-304	S-305
Mass Flow (lb/hr)											
Sorbitol	0	0	0	0	658083	131617	174447	174447	174447	174447	174447
Para-Xylene	0	0	0	0	0	0	0	0	0	0	0
Ortho-Xylene	0	0	0	0	0	0	0	0	0	0	0
Meta-Xylene	0	0	0	0	0	0	0	0	0	0	0
Methane	0	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	13	13	13	13	13
N-Butane	0	0	0	0	0	0	0	0	0	0	0
N-Pentane	0	0	0	0	0	0	0	0	0	0	0
N-Hexane	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	0	0	0	0	0	0	89	89	89	89	89
Water	60786	60786	1395680	1395680	585695	117139	162433	162433	162433	162433	162433
Hydrogen	0	0	0	0	0	0	1	1	1	1	1
Glucose	0	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Toluene	0	0	0	0	0	0	0	0	0	0	0
Benzene	0	0	0	0	0	0	0	0	0	0	0
Napthalene	0	0	0	0	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Isopropylbenzene	0	0	0	0	0	0	0	0	0	0	0
N-Heptane	0	0	0	0	0	0	0	0	0	0	0
1-Butene	0	0	0	0	0	0	0	0	0	0	0
1-Pentene	0	0	0	0	0	0	0	0	0	0	0
1-Hexene	0	0	0	0	0	0	0	0	0	0	0
1-Heptene	0	0	0	0	0	0	0	0	0	0	0
Air	0	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	3374	3374	77472	77472	36123	7225	9977	9977	9977	9977	9977
Total Flow (lb/hr)	60786	60786	1395680	1395680	1243780	248756	336982	336982	336982	336982	336982
Total Flow (cuft/hr)	987	1004	22057	23040	16938	3388	4751	4751	4825	4825	5173
Temperature (°F)	90.00	120.67	40.00	120.50	176.80	176.80	227.58	227.59	253.57	253.59	359.60
Pressure (psia)	14.70	14.70	14.70	14.70	741.70	741.70	292.08	297.08	297.08	304.08	725.19
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

APR Stream Report (2 of 4)

	S-306	**S-307**	**S-308**	**S-309**	**S-310**	**S-311**	**S-312**	**S-313**	**S-314**	**S-315**	**S-316**
Mass Flow (lb/hr)											
Sorbitol	42830	42830	42830	42830	0	0	0	0	0	0	0
Para-Xylene	0	0	0	0	0	0	0	0	0	0	0
Ortho-Xylene	0	0	0	0	0	0	0	0	0	0	0
Meta-Xylene	0	0	0	0	0	0	0	0	0	0	0
Methane	0	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0	0
Propane	27996	27996	13	13	27983	27983	27983	27983	0	0	0
N-Butane	0	0	0	0	0	0	0	0	0	0	0
N-Pentane	0	0	0	0	0	0	0	0	0	0	0
N-Hexane	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	93122	93122	89	89	93033	93033	93033	93032	0	0	0
Water	165664	165664	45294	45294	120370	120370	120370	24372	0	0	0
Hydrogen	7370	7370	1	1	7369	7369	7369	0	7369	7369	7369
Glucose	0	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Toluene	0	0	0	0	0	0	0	0	0	0	0
Benzene	0	0	0	0	0	0	0	0	0	0	0
Napthalene	0	0	0	0	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Isopropylbenzene	0	0	0	0	0	0	0	0	0	0	0
N-Heptane	0	0	0	0	0	0	0	0	0	0	0
1-Butene	0	0	0	0	0	0	0	0	0	0	0
1-Pentene	0	0	0	0	0	0	0	0	0	0	0
1-Hexene	0	0	0	0	0	0	0	0	0	0	0
1-Heptene	0	0	0	0	0	0	0	0	0	0	0
Air	0	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	15838	15838	2752	2752	13086	13086	13086	4101	3656	3656	3656
Total Flow (lb/hr)	336982	336982	88227	88227	248756	248756	248756	145387	7369	7369	7369
Total Flow (cuft/hr)	101208	253325	1380	1380	382110	6320480	5800240	1450210	55020	24831	22167
Temperature (°F)	359.60	314.62	359.60	359.61	359.60	338.74	273.58	140.00	1150.00	254.16	175.73
Pressure (psia)	725.19	292.08	290.08	292.08	290.08	17.70	17.70	14.70	1164.30	1164.30	1164.30
Vapor Fraction	0.53	0.57	0.00	0.00	1.00	1.00	1.00	0.81	1.00	1.00	1.00

APR Stream Report (3 of 4)

	S-317	S-318	S-319	S-320	S-321	S-322	S-323	S-324	S-325	S-326	S-400
Mass Flow (lb/hr)											
Sorbitol	0	0	0	0	0	0	0	0	0	0	526467
Para-Xylene	0	0	0	0	0	0	0	0	0	0	0
Ortho-Xylene	0	0	0	0	0	0	0	0	0	0	0
Meta-Xylene	0	0	0	0	0	0	0	0	0	0	0
Methane	0	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	27983	0	0	27983	0
N-Butane	0	0	0	0	0	0	0	0	0	0	0
N-Pentane	0	0	0	0	0	0	0	0	0	0	0
N-Hexane	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	0	0	0	0	0	0	93032	1	0	93033	0
Water	0	0	0	0	0	0	24372	95998	0	120370	468556
Hydrogen	1228	1228	1228	1228	1231	1228	7369	0	7369	7369	0
Glucose	0	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Toluene	0	0	0	0	0	0	0	0	0	0	0
Benzene	0	0	0	0	0	0	0	0	0	0	0
Napthalene	0	0	0	0	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Isopropylbenzene	0	0	0	0	0	0	0	0	0	0	0
N-Heptane	0	0	0	0	0	0	0	0	0	0	0
1-Butene	0	0	0	0	0	0	0	0	0	0	0
1-Pentene	0	0	0	0	0	0	0	0	0	0	0
1-Hexene	0	0	0	0	0	0	0	0	0	0	0
1-Heptene	0	0	0	0	0	0	0	0	0	0	0
Air	0	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	609	609	609	609	610	609	7757	5329	3656	13086	28899
Total Flow (lb/hr)	1228	1228	1228	1228	1231	1228	152756	96000	7369	248756	995023
Total Flow (cuft/hr)	3693	3693	3693	3693	3702	3693	3390850	1603	1601510	2720670	13550
Temperature (°F)	175.73	175.73	175.73	175.73	175.73	175.73	140.00	140.00	140.00	140.00	176.80
Pressure (psia)	1164.30	1164.30	1164.30	1164.30	1164.30	1164.30	14.70	14.70	14.70	17.70	741.70
Vapor Fraction	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.00	1.00	0.57	0.00

APR Stream Report (4 of 4)

	S-401	**S-402**
Mass Flow (lb/hr)		
Sorbitol	526467	526467
Para-Xylene	0	0
Ortho-Xylene	0	0
Meta-Xylene	0	0
Methane	0	0
Ethane	0	0
Propane	0	0
N-Butane	0	0
N-Pentane	0	0
N-Hexane	0	0
Carbon Dioxide	0	0
Water	468556	468556
Hydrogen	0	0
Glucose	0	0
Oxygen	0	0
Nitrogen	0	0
Carbon Monoxide	0	0
Sucrose	0	0
Sodium Hydroxide	0	0
Ethylbenzene	0	0
Toluene	0	0
Benzene	0	0
Napthalene	0	0
1,2,4-Trimethylbenzene	0	0
Isopropylbenzene	0	0
N-Heptane	0	0
1-Butene	0	0
1-Pentene	0	0
1-Hexene	0	0
1-Heptene	0	0
Air	0	0
DowthermA	0	0
Total Flow (lbmol/hr)	28899	28899
Total Flow (lb/hr)	995023	995023
Total Flow (cuft/hr)	13552	13757
Temperature (°F)	176.99	204.16
Pressure (psia)	667.70	667.70
Vapor Fraction	0.00	0.00

Section 400: Condensation

The condensation reaction converts sorbitol produced during hydrolysis and hydrogenation into water and a mixture of alkane and aromatic products that includes the final product, para-xylene. In the reactor, water and hydrogen vapor are driven off during the formation of the new carbon-carbon bonds present in the final product. In theory, any sugar alcohol or other "oxygenated hydrocarbon" can be used; in particular, US patent 2008/0300435 A1 contained one example with an acetone feed over gallium-loaded catalyst which converts nearly 80% of carbon in the feed into aromatics. However, the current design relies on a feed containing 50% sorbitol by mass in order to maintain comparability with other examples in the literature; consequently, the process only achieves a single pass yield of 48.4% aromatics. Other patents, such as US Patent 6372680, report less specific but similar results.

Catalyst

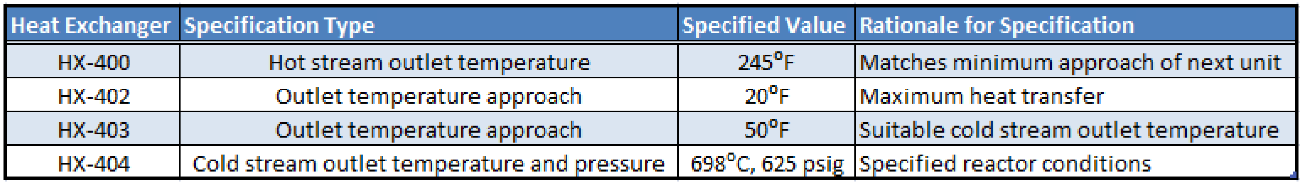
An activated zeolite or aluminosilicate catalyst, normally pentasil (more commonly called ZSM-5), facilitates the reaction. Zeolites have a porous structure that can accommodate a wide variety of cations. The cations are loosely held and exchange easily with cations in the contacted solution. Similar catalysts are used in the aqueous phase reforming and transalkylation portions of this process, and information on their manufacture and properties can be found in US patent 2008/0300435 A1. For the condensation of sorbitol to produce para-xylene, ZSM-5, with a thirty-to-one silicon dioxide to aluminum oxide ratio, is treated with a gallium nitrate solution, dried overnight in a vacuum oven, and subsequently calcined in flowing air at 400 degrees Celsius to effect 1.2% loading by weight of gallium (Example 46 in the patent). The prior cost-benefit analysis favors purchasing the catalyst from an external supplier to manufacturing the catalyst in-house.

Pre-Heating and Depressurization

The condensation section of the process begins with a valve, VAL-400), which releases the excess pressure generated during the aqueous phase reforming in order to establish conditions suitable for condensation. The outlet pressure is specified at 653 psig, which results in a 74 psig pressure drop across the valve.

Between the valve and reactor is a series of four heat exchangers (HX-400, HX-402, HX-403, HX-404), each followed by a small pump (P-400, P-401, P-402, P-403) that restores pressure lost to friction with a 2 psi pressure increase (industry heuristic). The heat exchangers then transfer heat from the hydrogen APR product, the pre-crystallization para-xylene stream, the transalkylation product, and the hot Dowtherm A stream to the condensation feed, respectively. Each exchanger conservatively assumes an overall heat transfer coefficient, U, of 50 BTU per hr-ft2-Rankine (Product and Process Design Principles; hereafter, PPDP) and allows for a conservative minimum temperature approach of 20 degrees Fahrenheit. The first exchanger (HX-400) is specified such that outlet temperatures approach to within 50 degrees Fahrenheit; this maximizes heat transfer while abiding by industry heuristics for streams above 300 degrees Fahrenheit. The second exchanger brings the pre-crystallization xylene stream and condensation feed to within 20 degrees Fahrenheit; this maximizes heat transfer while abiding by industry heuristics for streams under 300 degrees Fahrenheit. The third exchanger brings the transalkylation product and feed to within 50 degrees Fahrenheit; again, this maximizes heat transfer subject to heuristic-based constraints on the minimum allowable temperature approach. The fourth exchanger provides the final requisite heat to the condensation feed while cooling the refrigerant, Dowtherm A; this serves the simultaneous purpose of cooling the Dowtherm A in the refrigeration cycle used to cool the xylene stream for crystallization. See Figure 4 for a summary.

Figure 4

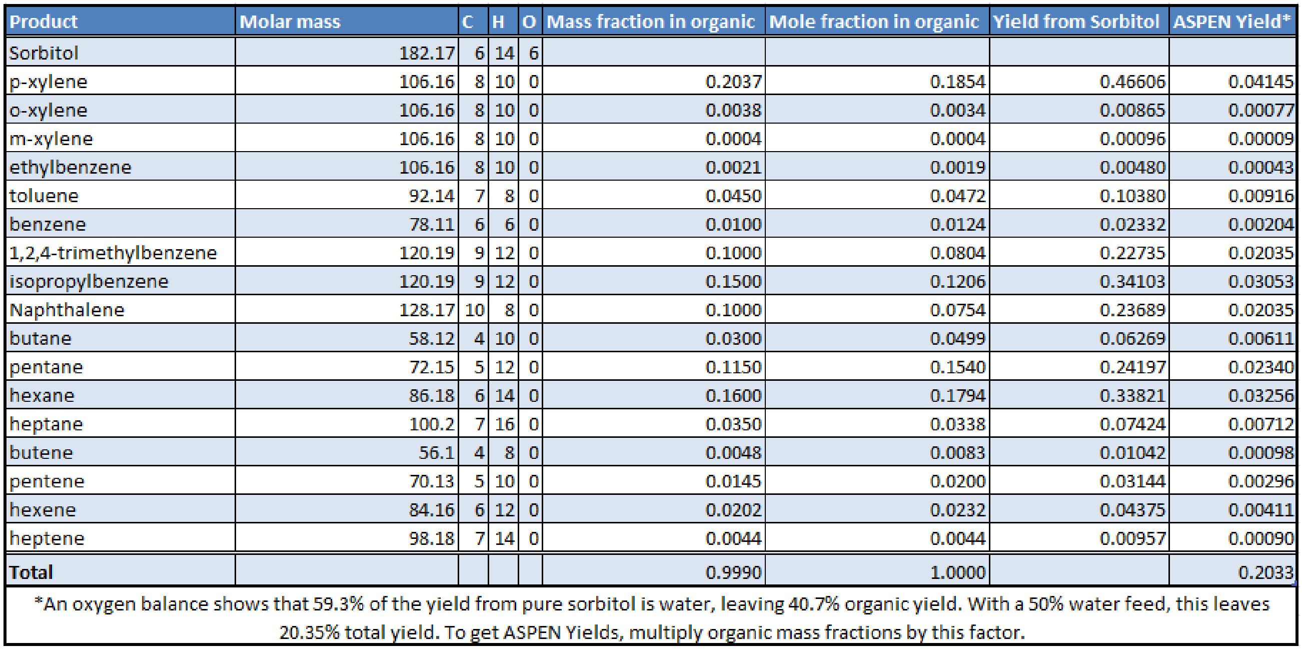


Heat Exchanger	Specification Type	Specified Value	Rationale for Specification
HX-400	Hot stream outlet temperature	245°F	Matches minimum approach of next unit
HX-402	Outlet temperature approach	20°F	Maximum heat transfer
HX-403	Outlet temperature approach	50°F	Suitable cold stream outlet temperature
HX-404	Cold stream outlet temperature and pressure	698°C, 625 psig	Specified reactor conditions

Condensation

The feed is then split into four equal streams using a conventional splitter (Spt-401) and fed into four identical condensation reactors; a single reactor would be prohibitively large. Specifically, the splitter takes a 995,000 lb/hr aqueous feed of 50% sorbitol (by mass) at 698 degrees Fahrenheit and 642 psia and splits it into four 249,000 lb/hr streams of the same composition, temperature, and pressure. Each reactor (R-400, R-401, R-402, and R-403) is an identical packed bed reactor, operated at 625 psig and 370 degrees Celsius, as specified in example 55 (PP) of US patent 2008/0300435 A1, and catalyzed by the catalyst prescribed in example 46 of the same. Each processes a 249,000 lb/hr feed stream of 50% sorbitol (by mass) in water. In ASPEN, the reactors were modeled using identical RYIELD blocks. Based on the information in Table 13 (pg. 37) and Figure 17, which offered mass fractions in the organic stream for generalized product categories (e.g. C5+ olefins), the following mass fractions were assumed for each representative species identified in Figure 5 below. Although some error is expected when manually interpreting figures, these estimates yielded an overall mass fraction of unity with very little post-measurement manipulation. Yields for the RYIELD blocks were then calculated for a pure sorbitol stream, then adjusted to account for the 50% water by mass in the feed, as illustrated in Figure 5.

Figure 5



Product	Molar mass	C	H	O	Mass fraction in organic	Mole fraction in organic	Yield from Sorbitol	ASPEN Yield*
Sorbitol	182.17	6	14	6				
p-xylene	106.16	8	10	0	0.2037	0.1854	0.46606	0.04145
o-xylene	106.16	8	10	0	0.0038	0.0034	0.00865	0.00077
m-xylene	106.16	8	10	0	0.0004	0.0004	0.00096	0.00009
ethylbenzene	106.16	8	10	0	0.0021	0.0019	0.00480	0.00043
toluene	92.14	7	8	0	0.0450	0.0472	0.10380	0.00916
benzene	78.11	6	6	0	0.0100	0.0124	0.02332	0.00204
1,2,4-trimethylbenzene	120.19	9	12	0	0.1000	0.0804	0.22735	0.02035
isopropylbenzene	120.19	9	12	0	0.1500	0.1206	0.34103	0.03053
Naphthalene	128.17	10	8	0	0.1000	0.0754	0.23689	0.02035
butane	58.12	4	10	0	0.0300	0.0499	0.06269	0.00611
pentane	72.15	5	12	0	0.1150	0.1540	0.24197	0.02340
hexane	86.18	6	14	0	0.1600	0.1794	0.33821	0.03256
heptane	100.2	7	16	0	0.0350	0.0338	0.07424	0.00712
butene	56.1	4	8	0	0.0048	0.0083	0.01042	0.00098
pentene	70.13	5	10	0	0.0145	0.0200	0.03144	0.00296
hexene	84.16	6	12	0	0.0202	0.0232	0.04375	0.00411
heptene	98.18	7	14	0	0.0044	0.0044	0.00957	0.00090
Total					0.9990	1.0000		0.2033

*An oxygen balance shows that 59.3% of the yield from pure sorbitol is water, leaving 40.7% organic yield. With a 50% water feed, this leaves 20.35% total yield. To get ASPEN Yields, multiply organic mass fractions by this factor.

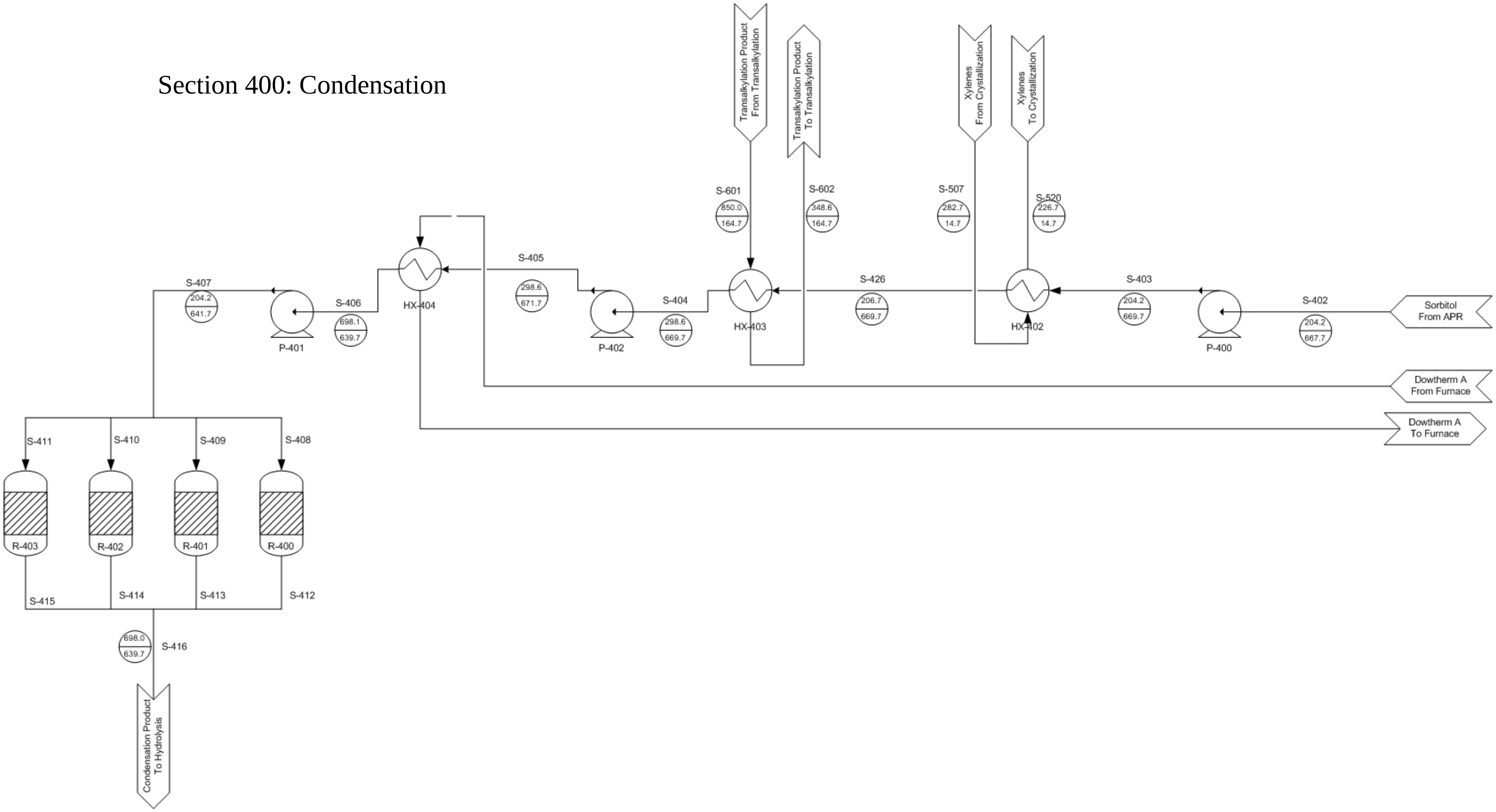
Post-Condensation Cooling and Heat Recovery

After reacting, a mixer (MIX-400) takes each 249,000 lb/hr para-xylene-containing product stream at 698 degrees Fahrenheit and 640 psia, present entirely in the vapor phase, and combines them into a single 995,000 lb/hr stream at the same composition and conditions. A splitter (SPT-400) then splits this combined product stream into three 332,000 lb/hr streams for at the same composition and conditions; this provides three streams which can preheat the feed to each of the three Hydrolysis reactors.

Each of the three identical 332,000 lb/hr product streams, still hot, is then fed through one of three pre-hydrolysis heat exchangers (HX-100, HX-101, HX-102); these exchangers each cool an effluent stream while pre-heating a feed to one of three hydrolysis reactors. Each exchanger conservatively assumes an overall heat transfer coefficient, U, of 50 BTU per hr-ft2-Rankine (industry heuristic) and a minimum temperature approach of 20 degrees Fahrenheit. With these parameters, each exchanger then specified a cold stream outlet temperature of 212 degrees Fahrenheit, the desired temperature for hydrolysis. The partially-cooled reactor effluents exit each exchanger at 506 degrees Fahrenheit, well above the temperature desired for distillation. All three streams are then combined by a mixer (MIX-401) for further phase and temperature changes prior to distillation.

The combined partially-cooled condensation product, flowing at 995,000 lb/hr, then passes through a valve (VAL-401) which vents the stream to a specified pressure of 1.5 psig. This pressure causes the condensation product to reach distillation at approximately atmospheric pressure. This pressure is cheap and easy to achieve; in addition, major components in the effluent can be isolated with high recoveries, and these distillations can all use cooling water to serve the condenser duties. The effluent then passes through a final heat exchanger (HX-401), which uses cooling water to cool the effluent to 50 degrees Celsius in anticipation of 3-phase separation. In accordance with industry standard, the heater specifies that cooling water that enters at 90 degrees Fahrenheit exit at 120. The flow rate of cooling water was then adjusted to 60,000 gallons per minute in order to achieve the desired hot-stream outlet temperature.

Section 400: Condensation



Condensation Stream Report (1 of 3)

	S-400	S-401	S-402	S-403	S-404	S-405	S-406	S-407	S-408	S-409	S-410
Mass Flow (lb/hr)											
Sorbitol	526467	526467	526467	526467	526467	526467	526467	526467	131617	131617	131617
Para-Xylene	0	0	0	0	0	0	0	0	0	0	0
Ortho-Xylene	0	0	0	0	0	0	0	0	0	0	0
Meta-Xylene	0	0	0	0	0	0	0	0	0	0	0
Methane	0	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0	0	0	0	0
N-Butane	0	0	0	0	0	0	0	0	0	0	0
N-Pentane	0	0	0	0	0	0	0	0	0	0	0
N-Hexane	0	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	0	0	0	0	0	0	0	0	0	0	0
Water	468556	468556	468556	468556	468556	468556	468556	468556	117139	117139	117139
Hydrogen	0	0	0	0	0	0	0	0	0	0	0
Glucose	0	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Toluene	0	0	0	0	0	0	0	0	0	0	0
Benzene	0	0	0	0	0	0	0	0	0	0	0
Napthalene	0	0	0	0	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0	0	0	0	0	0	0	0	0	0	0
Isopropylbenzene	0	0	0	0	0	0	0	0	0	0	0
N-Heptane	0	0	0	0	0	0	0	0	0	0	0
1-Butene	0	0	0	0	0	0	0	0	0	0	0
1-Pentene	0	0	0	0	0	0	0	0	0	0	0
1-Hexene	0	0	0	0	0	0	0	0	0	0	0
1-Heptene	0	0	0	0	0	0	0	0	0	0	0
Air	0	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	28899	28899	28899	28899	28899	28899	28899	28899	7225	7225	7225
Total Flow (lb/hr)	995023	995023	995023	995023	995023	995023	995023	995023	248756	248756	248756
Total Flow (cuft/hr)	13550	13552	13757	13758	14561	14561	22455	22458	5614	5614	5614
Temperature (°F)	176.80	176.99	204.16	204.16	298.62	298.62	698.10	698.15	698.15	698.15	698.15
Pressure (psia)	741.70	667.70	667.70	669.70	669.70	671.70	639.70	641.70	641.70	641.70	641.70
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

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	S-411	S-412	S-413	S-414	S-415	S-416	S-417	S-418	S-419	S-420	S-421
Mass Flow (lb/hr)											
Sorbitol	131617	0	0	0	0	0	0	0	0	0	0
Para-Xylene	0	10284	10284	10284	10284	41138	13712	13713	13712	13712	13712
Ortho-Xylene	0	191	191	191	191	763	254	254	254	254	254
Meta-Xylene	0	21	21	21	21	85	28	28	28	28	28
Methane	0	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0	0	0	0	0
N-Butane	0	1515	1515	1515	1515	6059	2020	2020	2020	2020	2020
N-Pentane	0	5806	5806	5806	5806	23225	7741	7742	7741	7741	7741
N-Hexane	0	8078	8078	8078	8078	32312	10771	10771	10771	10771	10771
Carbon Dioxide	0	0	0	0	0	0	0	0	0	0	0
Water	117139	198222	198222	198222	198222	792890	264294	264302	264294	264294	264294
Hydrogen	0	97	97	97	97	389	130	130	130	130	130
Glucose	0	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	106	106	106	106	424	141	141	141	141	141
Toluene	0	2272	2272	2272	2272	9087	3029	3029	3029	3029	3029
Benzene	0	505	505	505	505	2019	673	673	673	673	673
Napthalene	0	5049	5049	5049	5049	20195	6732	6732	6732	6732	6732
1,2,4-Trimethylbenzene	0	5049	5049	5049	5049	20195	6732	6732	6732	6732	6732
Isopropylbenzene	0	7573	7573	7573	7573	30293	10098	10098	10098	10098	10098
N-Heptane	0	1767	1767	1767	1767	7068	2356	2356	2356	2356	2356
1-Butene	0	243	243	243	243	972	324	324	324	324	324
1-Pentene	0	733	733	733	733	2934	978	978	978	978	978
1-Hexene	0	1020	1020	1020	1020	4081	1360	1361	1360	1360	1360
1-Heptene	0	223	223	223	223	893	298	298	298	298	298
Air	0	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	7225	11574	11574	11574	11574	46295	15432	15432	15432	15432	15432
Total Flow (lb/hr)	248756	248756	248756	248756	248756	995023	331671	331681	331671	331671	331671
Total Flow (cuft/hr)	5614	205500	205500	205500	205500	822002	273998	274006	273998	208888	208889
Temperature (°F)	698.15	698.00	698.00	698.00	698.00	698.00	698.00	698.00	698.00	505.98	505.98
Pressure (psia)	641.70	639.70	639.70	639.70	639.70	639.70	639.70	639.70	639.70	639.70	639.70
Vapor Fraction	0.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Condensation Stream Report (3 of 3)

	S-422	S-425	S-426	S-507	S-520	S-601	S-602	S-603
Mass Flow (lb/hr)								
Sorbitol	0	0	526467	0	0	0	0	0
Para-Xylene	13713	41138	0	53820	53820	18807	18807	18807
Ortho-Xylene	254	763	0	3249	3249	2739	2739	2739
Meta-Xylene	28	85	0	5089	5089	5478	5478	5478
Methane	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0	0
N-Butane	2020	6059	0	0	0	2595	2595	2595
N-Pentane	7742	23225	0	0	0	15976	15976	15976
N-Hexane	10771	32312	0	0	0	0	0	0
Carbon Dioxide	0	0	0	0	0	0	0	0
Water	264302	792890	468556	0	0	0	0	0
Hydrogen	130	389	0	0	0	0	0	0
Glucose	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0
Ethylbenzene	141	424	0	835	835	548	548	548
Toluene	3029	9087	0	2374	2374	135120	135120	135120
Benzene	673	2019	0	0	0	19903	19903	19903
Napthalene	6732	20195	0	0	0	0	0	0
1,2,4-Trimethylbenzene	6732	20195	0	133	133	0	0	0
Isopropylbenzene	10098	30293	0	13174	13174	0	0	0
N-Heptane	2356	7068	0	0	0	0	0	0
1-Butene	324	972	0	0	0	384	384	384
1-Pentene	978	2934	0	0	0	1919	1919	1919
1-Hexene	1361	4081	0	0	0	0	0	0
1-Heptene	298	893	0	0	0	0	0	0
Air	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	15432	46295	28899	730	730	2281	2281	2281
Total Flow (lb/hr)	331681	995023	995023	78674	78674	203468	203468	203468
Total Flow (cuft/hr)	208897	937806	13777	1669	1603	185115	4867	4203
Temperature (°F)	505.98	122.00	206.67	282.70	226.67	850.00	348.63	182.00
Pressure (psia)	639.70	16.20	669.70	14.70	14.70	164.70	164.70	164.70
Vapor Fraction	1.00	0.05	0.00	0.00	0.00	1.00	0.00	0.00

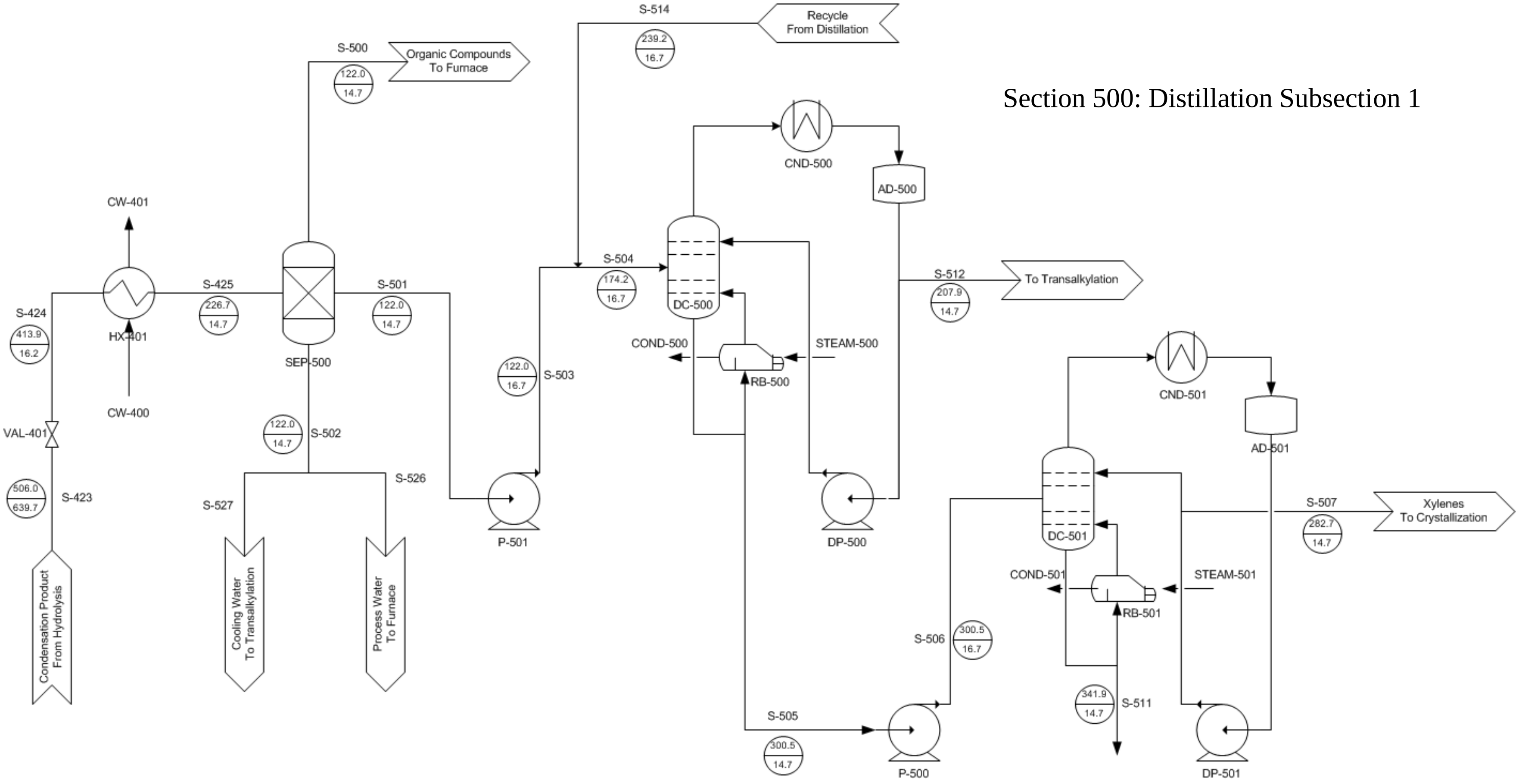
Section 500: Separations

Distillation Columns

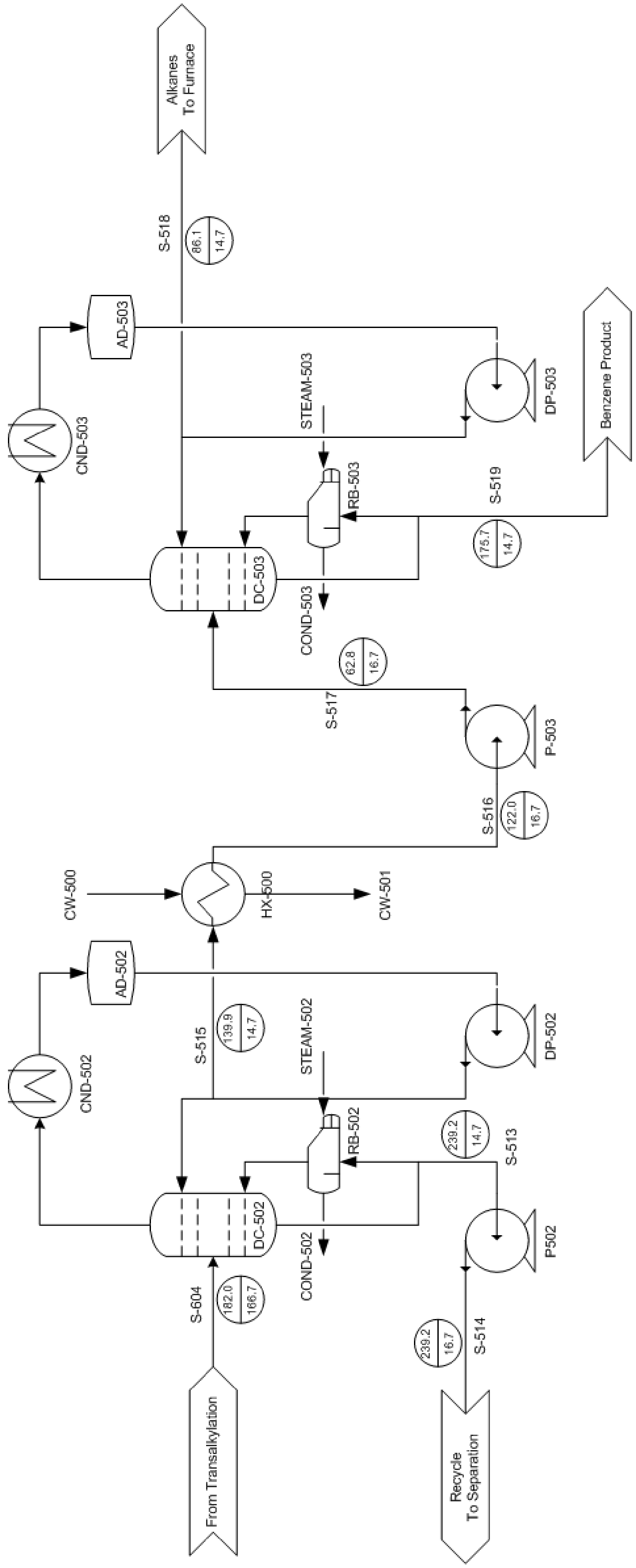
The separation scheme has four columns, DC-500, DC-501, DC-502, and DC-503. DC-500 and DC-501 follow the condensation, while DC-502 and DC-503 follow the transalkylation. DC-500 is a 30-tray separation between toluene and para-xylene. It's fed with a combination of effluent from the condensation reactor and a recycled stream of additional para-xylene and leftover toluene from DC-502 in the post-transalkylation separation. The distillate feeds the transalkylation reactor, while the bottoms product is sent to DC-501 for further separation. DC-501 then separates the xylene isomers, now the lightest components, from the other heavy components. The xylenes are sent for crystallization to isolate the para- isomer, and the heavy components are sent to the furnace to offset utilities. DC-502 follows the transalkylation, and separates benzene and lighter components from the heavier toluene and xylenes to be sent back DC-500. The distillate from DC-502 is then fed to DC-503, which separates lighter hydrocarbon side products, which can be burned to offset utilities, from valuable benzene, which can be sold for additional revenue. This scheme separates valuable components using the lowest possible number of distillation columns.

Columns were designed by modifying a McCabe-Thiele analysis. The McCabe-Thiele diagrams in Appendix B were generated by ignoring the presence of species that were neither the light nor heavy key. The columns were initially modeled after these diagrams. If ASPEN indicated a tendency for trays to dry out, the reflux ratio was increased in increments of 1 until the simulation successfully converged. Then, the distillate to feed ratio was adjusted to maximize light key recovery and minimize heavy key recovery. After achieving the desired separation, the idealized profile was translated into a more realistic set of trays and non-unity efficiencies using the O'Connell correlation. These calculations can be found in Appendix B. In all cases, these "real" columns performed separations that were nearly identical to their ideal counterparts.

Section 500: Distillation Subsection 1



Section 500: Distillation Subsection 2



Crystallization

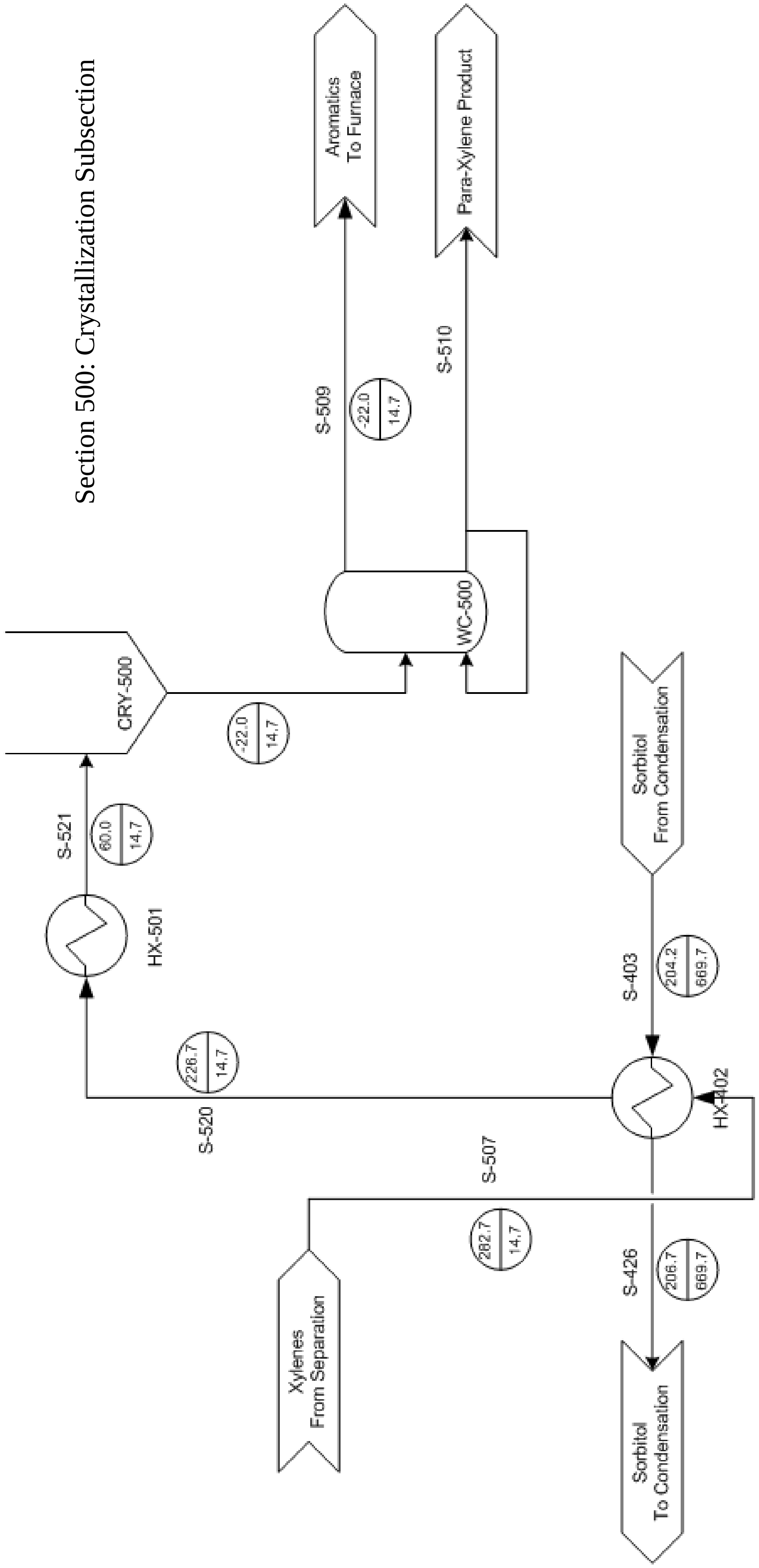
Crystallization is often used when para-xylene is mixed with other xylenes and ethylbenzene, but it can also be used for our scenario where there is a significant proportion of isopropylbenzene and toluene. As the freezing point of isopropylbenzene and toluene are considerably lower than meta-xylene and ortho-xylene (see Figure 6), it can be assumed that crystallization will work just as well, if not better at -30 °C, for a system including isopropylbenzene and toluene.

The xylenes product from the distillation columns is fed to a scraped surface crystallizer (SSC) with a cooling jacket. The SSC cools the solution of para-xylene, meta-xylene, ortho-xylene, isopropylbenzene, toluene, ethylbenzene and other aromatics to -30 °C which causes pure para-xylene crystals to form on the surface of the crystallizer. The scrapers, which rotate at 12 rpm, free the crystals and allow them to be fed into a washing column as a suspension in the mother liquor. The washing column consists of a piston with a filter attached to its face and a scraper at the bottom of the column. Washing takes place in four steps. In the first step, the piston is lifted to allow the crystal suspension to fill the column. The inlet is then shut off and an outlet above the piston is opened and the piston is forced downward, causing the mother liquor to flow through the filter on the piston. In the third step product purity para-xylene is fed through the bottom of the column, washing the crystals. For the final step the scraper is rotated as the piston continues to push downwards, grinding the crystals into smaller fragments that are carried through the bottom of the column and melt into the para-xylene product.

Figure 6

Compound	Normal Boiling Point (°C)	Freezing Point (°C)
Para-Xylene	138	13
Meta-Xylene	139	-48
Ortho-Xylene	144	-25.2
Ethylbenzene	136	-95
Isopropylbenzene	152	-96
Toluene	111	-95

Section 500: Crystallization Subsection



Separation Stream Report (1 of 2)

	CW-400	CW-401	S-423	S-424	S-425	S-500	S-501	S-502	S-503	S-504	S-505
Mass Flow (lb/hr)											
Sorbitol	0	0	0	0	0	0	0	0	0	0	0
Para-Xylene	0	0	41138	41138	41138	492	40646	0	40646	59451	53936
Ortho-Xylene	0	0	763	763	763	8	756	0	756	3495	3365
Meta-Xylene	0	0	85	85	85	1	84	0	84	5561	5103
Methane	0	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0	0	0	0	0
N-Butane	0	0	6059	6059	6059	3464	2595	0	2595	2595	0
N-Pentane	0	0	23225	23225	23225	7254	15971	0	15971	15976	0
N-Hexane	0	0	32312	32312	32312	4472	27840	0	27840	27840	0
Carbon Dioxide	0	0	0	0	0	0	0	0	0	0	0
Water	29651800	29651800	792890	792890	792890	978	1697	790215	1697	1697	0
Hydrogen	0	0	389	389	389	388	1	0	1	1	0
Glucose	0	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	424	424	424	6	418	0	418	966	836
Toluene	0	0	9087	9087	9087	295	8792	0	8792	135420	2374
Benzene	0	0	2019	2019	2019	200	1819	0	1819	2479	0
Napthalene	0	0	20195	20195	20195	16	20179	0	20179	20179	20179
1,2,4-Trimethylbenzene	0	0	20195	20195	20195	69	20126	0	20126	20126	20113
Isopropylbenzene	0	0	30293	30293	30293	222	30071	0	30071	30071	29739
N-Heptane	0	0	7068	7068	7068	391	6677	0	6677	6677	0
1-Butene	0	0	972	972	972	589	384	0	384	384	0
1-Pentene	0	0	2934	2934	2934	1016	1918	0	1918	1919	0
1-Hexene	0	0	4081	4081	4081	642	3440	0	3440	3440	0
1-Heptene	0	0	893	893	893	55	838	0	838	838	0
Air	0	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	1645920	1645920	46295	46295	46295	509	1922	43864	1922	3565	1194
Total Flow (lb/hr)	29651800	29651800	995023	995023	995023	20555	184252	790215	184252	339113	135645
Total Flow (cuft/hr)	481250	489452	626674	26662000	937806	213811	3797	13056	3797	6988	2814
Temperature (°F)	90.00	120.33	505.98	413.88	122.00	122.00	122.00	122.00	122.01	174.18	300.53
Pressure (psia)	16.20	16.20	639.70	16.20	16.20	14.70	14.70	14.70	16.70	16.70	14.70
Vapor Fraction	0.00	0.00	1.00	1.00	0.05	1.00	0.00	0.00	0.00	0.00	0.00

Separation Stream Report (2 of 2)

	S-506	S-507	S-508	S-510	S-511	S-512	S-514
Mass Flow (lb/hr)							
Sorbitol	0	0	0	0	0	0	0
Para-Xylene	53936	53820	53820	50322	116	5515	18805
Ortho-Xylene	3365	3249	3249	0	115	130	2739
Meta-Xylene	5103	5089	5089	0	15	458	5477
Methane	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0
N-Butane	0	0	0	0	0	2595	0
N-Pentane	0	0	0	0	0	15976	5
N-Hexane	0	0	0	0	0	27840	0
Carbon Dioxide	0	0	0	0	0	0	0
Water	0	0	0	0	0	1697	0
Hydrogen	0	0	0	0	0	1	0
Glucose	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0
Ethylbenzene	836	835	835	0	1	130	548
Toluene	2374	2374	2374	0	0	133046	126627
Benzene	0	0	0	0	0	2479	659
Napthalene	20179	0	0	0	20179	0	0
1,2,4-Trimethylbenzene	20113	133	133	0	19981	13	0
Isopropylbenzene	29739	13174	13174	0	16564	332	0
N-Heptane	0	0	0	0	0	6677	0
1-Butene	0	0	0	0	0	384	0
1-Pentene	0	0	0	0	0	1919	0
1-Hexene	0	0	0	0	0	3440	0
1-Heptene	0	0	0	0	0	838	0
Air	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	1194	730	730	474	464	2371	1642
Total Flow (lb/hr)	135645	78674	78674	50322	56971	203468	154861
Total Flow (cuft/hr)	2814	1669	1389	888	1157	1117480	3196
Temperature (°F)	300.54	282.70	-22.00	-22.00	341.89	207.92	239.18
Pressure (psia)	16.70	14.70	14.70	14.70	14.70	14.70	16.70
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	1.00	0.00

Distillation Stream Report (1 of 1)

	CW-500	CW-501	S-513	S-514	S-515	S-516	S-517	S-518	S-519	S-604
Mass Flow (lb/hr)										
Sorbitol	0	0	0	0	0	0	0	0	0	0
Para-Xylene	0	0	18805	18805	2	2	2	0	2	18807
Ortho-Xylene	0	0	2739	2739	0	0	0	0	0	2739
Meta-Xylene	0	0	5477	5477	1	1	1	0	1	5478
Methane	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0	0	0	0
N-Butane	0	0	0	0	2595	2595	2595	2590	5	2595
N-Pentane	0	0	5	5	15971	15971	15971	15041	930	15976
N-Hexane	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	0	0	0	0	0	0	0	0	0	0
Water	659777	659777	0	0	0	0	0	0	0	0
Hydrogen	0	0	0	0	0	0	0	0	0	0
Glucose	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	548	548	0	0	0	0	0	548
Toluene	0	0	126627	126627	8493	8493	8493	0	8493	135120
Benzene	0	0	659	659	19244	19244	19244	119	19125	19903
Napthalene	0	0	0	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0	0	0	0	0	0	0	0	0	0
Isopropylbenzene	0	0	0	0	0	0	0	0	0	0
N-Heptane	0	0	0	0	0	0	0	0	0	0
1-Butene	0	0	0	0	384	384	384	383	1	384
1-Pentene	0	0	0	0	1918	1918	1918	1828	90	1919
1-Hexene	0	0	0	0	0	0	0	0	0	0
1-Heptene	0	0	0	0	0	0	0	0	0	0
Air	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	36623	36623	1642	1642	639	639	639	287	351	2281
Total Flow (lb/hr)	659777	659777	154861	154861	48607	48607	48607	19960	28646	203468
Total Flow (cuft/hr)	10427	10499	3196	3196	270204	1036	1036	110213	573	4203
Temperature (°F)	40.00	53.18	239.17	239.18	139.86	62.80	62.82	86.09	175.69	182.01
Pressure (psia)	14.70	14.70	14.70	16.70	14.70	14.70	16.70	14.70	14.70	166.70
Vapor Fraction	0.00	0.00	0.00	0.00	1.00	0.00	0.00	1.00	0.00	0.00

Crystallization Stream Report (1 of 1)

	S-403	S-426	S-507	S-508	S-509	S-510	S-520	S-521
Mass Flow (lb/hr)								
Sorbitol	526467	526467	0	0	0	0	0	0
Para-Xylene	0	0	53820	53820	3498	50322	53820	53820
Ortho-Xylene	0	0	3249	3249	3249	0	3249	3249
Meta-Xylene	0	0	5089	5089	5089	0	5089	5089
Methane	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0	0
N-Butane	0	0	0	0	0	0	0	0
N-Pentane	0	0	0	0	0	0	0	0
N-Hexane	0	0	0	0	0	0	0	0
Carbon Dioxide	0	0	0	0	0	0	0	0
Water	468556	468556	0	0	0	0	0	0
Hydrogen	0	0	0	0	0	0	0	0
Glucose	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	835	835	835	0	835	835
Toluene	0	0	2374	2374	2374	0	2374	2374
Benzene	0	0	0	0	0	0	0	0
Napthalene	0	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0	0	133	133	133	0	133	133
Isopropylbenzene	0	0	13174	13174	13174	0	13174	13174
N-Heptane	0	0	0	0	0	0	0	0
1-Butene	0	0	0	0	0	0	0	0
1-Pentene	0	0	0	0	0	0	0	0
1-Hexene	0	0	0	0	0	0	0	0
1-Heptene	0	0	0	0	0	0	0	0
Air	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	28899	28899	730	730	256	474	730	730
Total Flow (lb/hr)	995023	995023	78674	78674	28352	50322	78674	78674
Total Flow (cuft/hr)	13758	13777	1669	1389	501	888	1603	1449
Temperature (°F)	204.16	206.67	282.70	-22.00	-22.00	-22.00	226.67	60.00
Pressure (psia)	669.70	669.70	14.70	14.70	14.70	14.70	14.70	14.70
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Section 600: Transalkylation

In transalkylation, side-products from the condensation reaction are converted into additional para-xylene. Because information on the possible products of condensation was limited, a large fraction of sorbitol was converted into undesired side-products. Transalkylation emerged as a way to recover some of this material, which would otherwise be burned or wasted. In addition, transalkylation simultaneously produced additional benzene, increasing benzene production to quantities significant enough to isolate and sell for additional revenue.

Of the available literature, US Patents 2011/0092756, 2005/0215839, and 6323381 provided the most complete and relevant information to the process at hand. This process's transalkylation was modeled after Example 2 on column 10 of US Patent 6323381 due the specific yields presented and because of the selective production of para-xylene over its isomers, which was necessary to maintain a high enough concentration of the para-xylene isomer for crystallization.

Toluene-rich distillate from the first post-condensation separation, with toluene as the light key and para-xylene as the heavy key, feeds the transalkylation. The products are then separated into hydrocarbons for burning, benzene for separate sale, and heavier products for recycle and recovery.

Pre-Heating

Before transalkylation, the 200,000 lb/hr feed is vaporized in HX-600 and brought to the appropriate temperature of 850 degrees Fahrenheit. These conditions are specified by US patent 6323381. The heat duty of 68 million BTU/hr is provided by the furnace R-700. The stream is then fed to the transalkylation reactor R-600.

Transalkylation

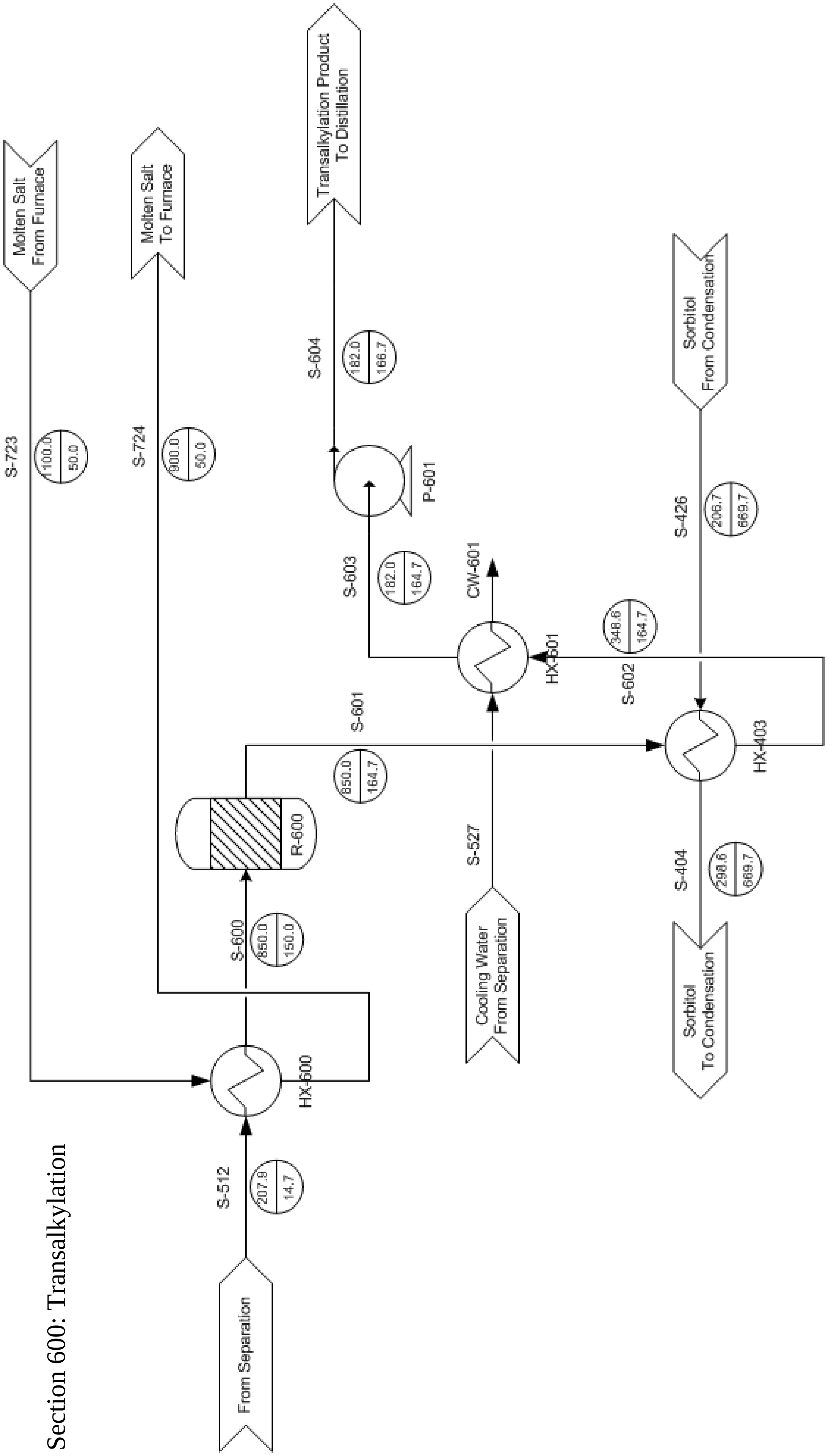
The heated feed is fed continuously as one stream to a packed bed reactor at 850 degrees Fahrenheit and atmospheric pressure, as specified in US Patent 6323381. The yields were estimated from data provided in Example 2 of the aforementioned patent, with yields scaled to compensate for the absence of species such as heavy aromatics and xylene isomers in the feed.

Transalkylation is catalyzed by zeolite catalyst, similar to the catalyzed condensation. In Example 2 of the aforementioned patent, a "selectivated large crystal HZSM-5 was used." Although no further specifics were given, the catalyst was assumed similar enough to the condensation catalyst that both could be ordered together in order to achieve economies of scale. Information and assumptions applied to pricing for the condensation catalyst were also applied to the transalkylation catalyst.

Cooling and Heat Recovery

After exiting the reactor, the effluent pass through heat exchanger HX-403, where it simultaneously preheats feed for the condensation reaction. Nearly 80 million BTU/hr are transferred between streams. The exchanger is configured to maximize heat transfer by achieving the minimum allowable temperature approach of 50 degrees Fahrenheit for streams over 300 degrees Fahrenheit. The effluent then flows through heat exchanger HX-601, where cooling water is used to bring the stream to 128 degrees Fahrenheit; the flow rate of cooling water was adjusted such that the water enters at 90 degrees Fahrenheit and exits at 120, consistent with industry heuristics. Finally, pump P-601 provides a 2 psi increase to combat frictional pressure losses. The cooled effluent is then returned to the separation section of the process at distillation column DC-502.

Section 600: Transalkylation



Transalkylation Stream Report (1 of 1)

	CW-600	CW-601	S-404	S-426	S-512	S-600	S-601	S-602	S-603	S-604
Mass Flow (lb/hr)										
Sorbitol	0	0	526467	526467	0	0	0	0	0	0
Para-Xylene	0	0	0	0	5515	5515	18807	18807	18807	18807
Ortho-Xylene	0	0	0	0	130	130	2739	2739	2739	2739
Meta-Xylene	0	0	0	0	458	458	5478	5478	5478	5478
Methane	0	0	0	0	0	0	0	0	0	0
Ethane	0	0	0	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0	0	0	0
N-Butane	0	0	0	0	2595	2595	2595	2595	2595	2595
N-Pentane	0	0	0	0	15976	15976	15976	15976	15976	15976
N-Hexane	0	0	0	0	27840	27840	0	0	0	0
Carbon Dioxide	0	0	0	0	0	0	0	0	0	0
Water	520883	520883	468556	468556	1697	1697	0	0	0	0
Hydrogen	0	0	0	0	1	1	0	0	0	0
Glucose	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0
Sodium Hydroxide	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	0	0	0	0	130	130	548	548	548	548
Toluene	0	0	0	0	133046	133046	135120	135120	135120	135120
Benzene	0	0	0	0	2479	2479	19903	19903	19903	19903
Napthalene	0	0	0	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0	0	0	0	13	13	0	0	0	0
Isopropylbenzene	0	0	0	0	332	332	0	0	0	0
N-Heptane	0	0	0	0	6677	6677	0	0	0	0
1-Butene	0	0	0	0	384	384	384	384	384	384
1-Pentene	0	0	0	0	1919	1919	1919	1919	1919	1919
1-Hexene	0	0	0	0	3440	3440	0	0	0	0
1-Heptene	0	0	0	0	838	838	0	0	0	0
Air	0	0	0	0	0	0	0	0	0	0
DowthermA	0	0	0	0	0	0	0	0	0	0
Total Flow (lbmol/hr)	28913	28913	28899	28899	2371	2371	2281	2281	2281	2281
Total Flow (lb/hr)	520883	520883	995023	995023	203468	203468	203468	203468	203468	203468
Total Flow (cuft/hr)	8454	8599	14561	13777	1117480	2258520	185115	4867	4203	4203
Temperature (°F)	90.00	120.61	298.62	206.67	207.92	850.00	850.00	348.63	182.00	182.01
Pressure (psia)	14.70	14.70	669.70	669.70	14.70	14.70	164.70	164.70	164.70	166.70
Vapor Fraction	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00

Section 700: Furnace & Heating Cycles

The process requires a great deal of heating due to the extreme conditions of several reactors and to the utility-intensive distillation columns. Fortunately, a large number of alkanes and other combustible hydrocarbons are made available for combustion by Section 300 (aqueous phase reforming) and by Section 500 (separations). In order to minimize utilities, these by-products are combusted for one of three purposes: boiling steam, vaporizing Dowtherm A, or heating Solar Salt. A quick sanity check (see SC-700) shows that the process provides well over 977 MBtu/h for production of steam, which exceeds the total heating and steam requirements of 912 MBtu/h (see Figure 24).

Molten Salt Furnace & Cycle

The transalkylation reaction in reactor R-600 occurs at 850^0F. Naturally, this requires extensive pre-heating of the feed (S-600) to the reactor. The most economical and environmentally-friendly material available at these temperatures is Solar Salt, a 60/40 mixture of sodium nitrate and potassium nitrate (other media considered are detailed in Table 18.1 of PPDP and in Mathur). Please see Section VIII and Appendix D for pricing and further materials specifications.

After exiting a cone-roof storage tank (ST-701), the Solar Salt is heated in FRN-700 and travels through heat exchanger (HX-600), cooling from 1100^0F to 900^0F. The sensible heat transfer increases the temperature of the S-512 to 850^0F.

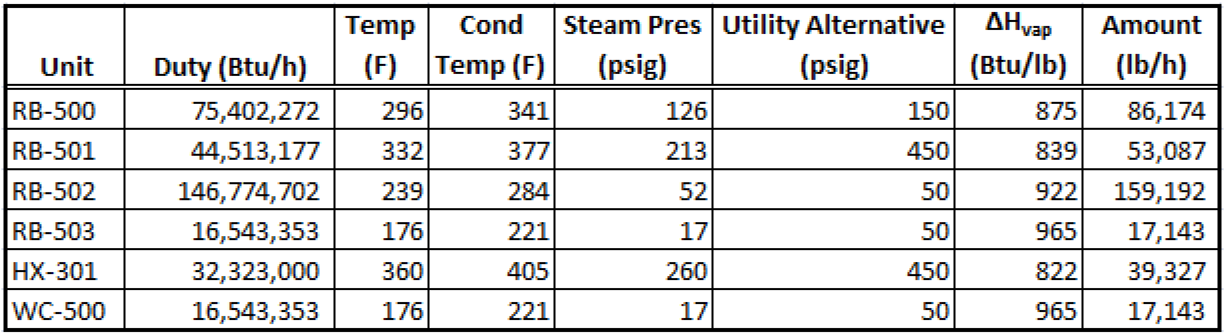
Dowtherm A Furnace & Cycle

Acid-catalyzed condensation (R-400 through R-403) occurs in this process at 698^0F - a temperature outside the reasonable reach of steam. Dowtherm A (product information in Appendix D) is sold by Dow Chemical Company, and is recommended for heating up to 750^0F (Table 18.1, PPDP). The Dowtherm A is stored in a spherical tank, ST-700. Due to the large amount required, the stream splits into two, each of which travels through a separate furnace (FRN-701 and FRN-702) before recombining as vapor and entering heat exchanger HX-404. The condensation of Dowtherm A provides the necessary heat to raise S-405 to the requisite 698^{0}F.

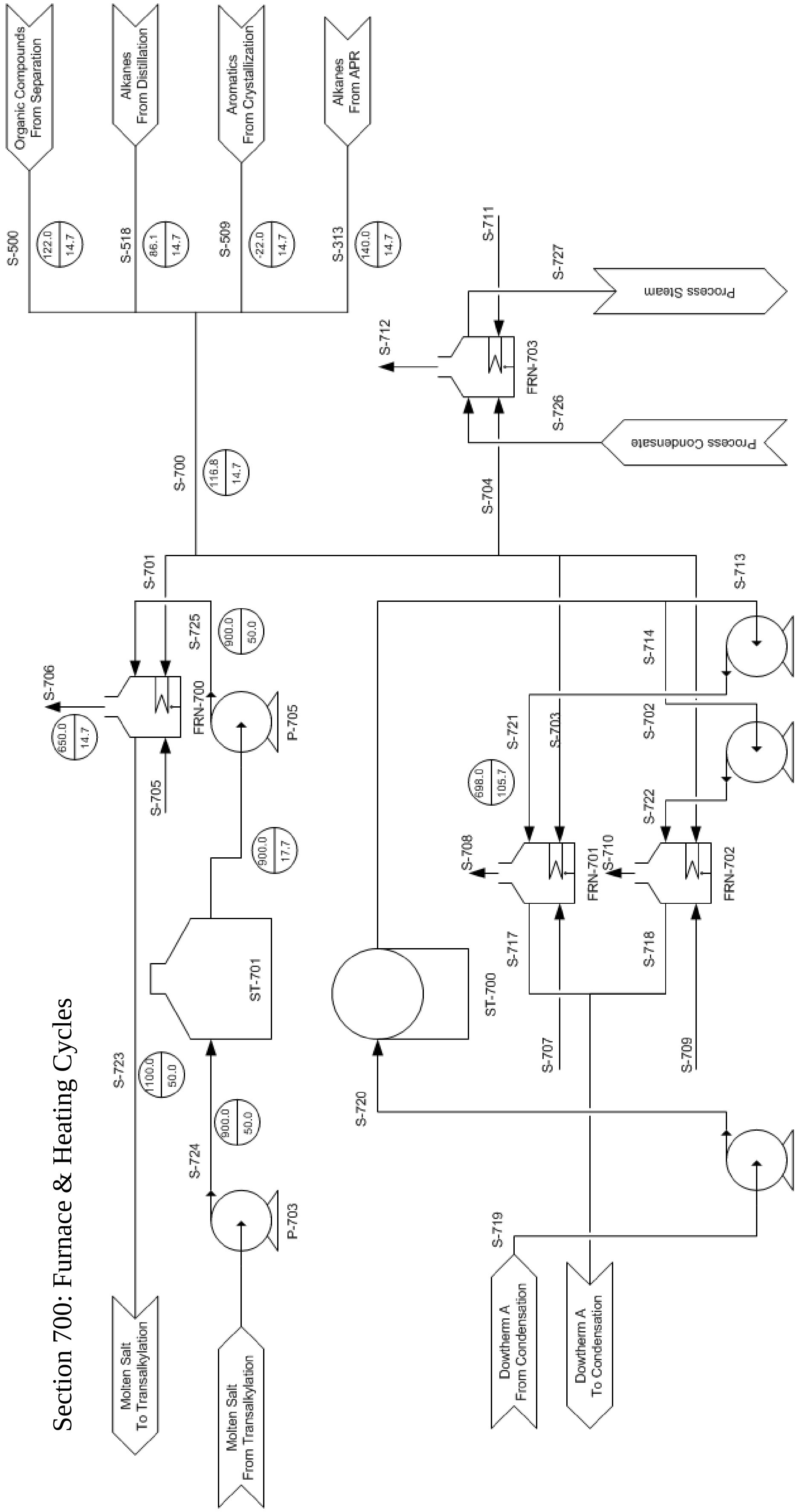
Fired Steam Boiler

The four distillation column reboilers (RB-500 through RB-503), the crystallizer apparatus (CRY-500 and WC-500), and heat exchanger HX-301 require steam heating. Rather than purchase it externally, the heat is supplied by vaporizing excess water (S-526) in a fired steam boiler (FRN-703). The steam output is split as necessary according to Figure 7, with valves employed to adjust each stream to the required pressure.

Figure 7



Unit	Duty (Btu/h)	Temp (F)	Cond Temp (F)	Steam Pres (psig)	Utility Alternative (psig)	ΔH_{vap} (Btu/lb)	Amount (lb/h)
RB-500	75,402,272	296	341	126	150	875	86,174
RB-501	44,513,177	332	377	213	450	839	53,087
RB-502	146,774,702	239	284	52	50	922	159,192
RB-503	16,543,353	176	221	17	50	965	17,143
HX-301	32,323,000	360	405	260	450	822	39,327
WC-500	16,543,353	176	221	17	50	965	17,143



Section 700: Furnace & Heating Cycles

Section IV

Energy Balance

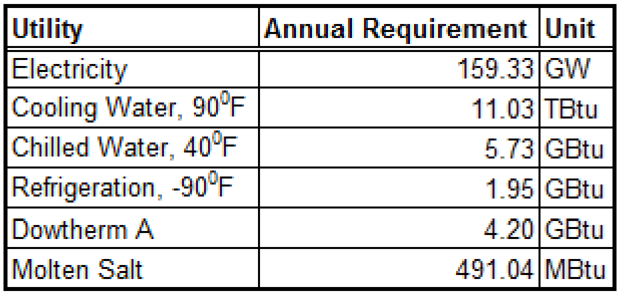
IV. ENERGY BALANCE & UTILITY REQUIREMENTS

An important specification of the project charter is to minimize utility usage and to ensure the project is “green.” This entails recycling as much water as possible, avoiding natural gases, and generally minimizing the carbon footprint. Regardless, the varied and at-times extreme conditions of the process require a variety of utilities for heating, cooling, and power. This section summarizes utility usage by type, describes assumptions and calculations, details cost-saving measures and their impact, and notes areas for further study.

Utility Requirements

Without integration or cost-saving measures, the process required electricity; steam at 50 psig, 150 psig, and 450 psig; cooling water; chilled water; refrigeration to -90^{0}F; Dowtherm A; and molten salts. Due to the excess heat generated by burning by-products, all of the process steam requirements were quickly substituted with boiler feed water. In the final process design, however, excess water from the three-phase separation in Section 500 is used in place of externally-purchased boiler feed water, as well as to offset some cooling water requirements. This resulted in overall utility requirements as summarized in Figure 8.

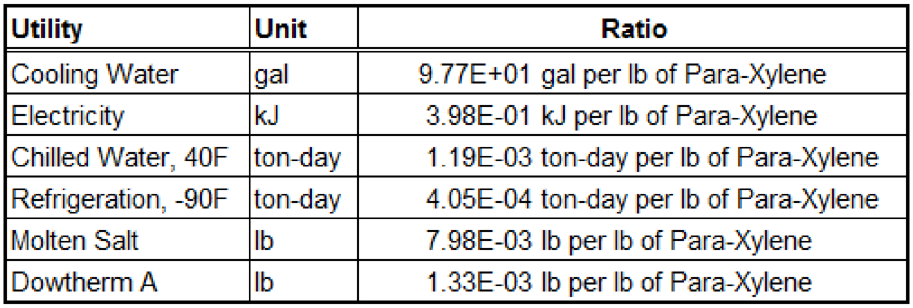
Figure 8



Utility	Annual Requirement	Unit
Electricity	159.33	GW
Cooling Water, 90^{0}F	11.03	TBtu
Chilled Water, 40^{0}F	5.73	GBtu
Refrigeration, -90^{0}F	1.95	GBtu
Dowtherm A	4.20	GBtu
Molten Salt	491.04	MBtu

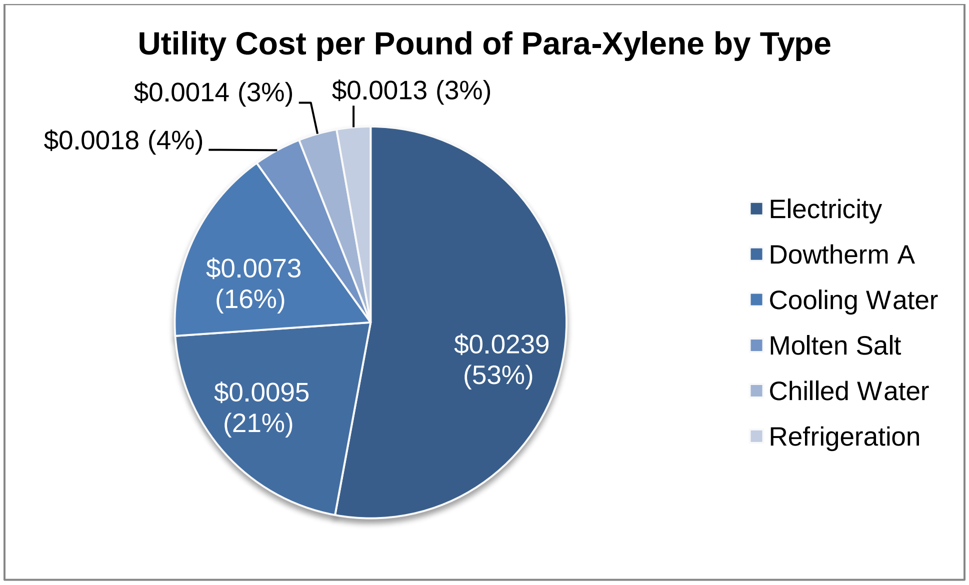
Amount and cost of utility are explored comparatively in Figure 9 and Figure 10.

Figure 9



Utility	Unit	Ratio
Cooling Water	gal	9.77E+01 gal per lb of Para-Xylene
Electricity	kJ	3.98E-01 kJ per lb of Para-Xylene
Chilled Water, 40F	ton-day	1.19E-03 ton-day per lb of Para-Xylene
Refrigeration, -90F	ton-day	4.05E-04 ton-day per lb of Para-Xylene
Molten Salt	lb	7.98E-03 lb per lb of Para-Xylene
Dowtherm A	lb	1.33E-03 lb per lb of Para-Xylene

Figure 10

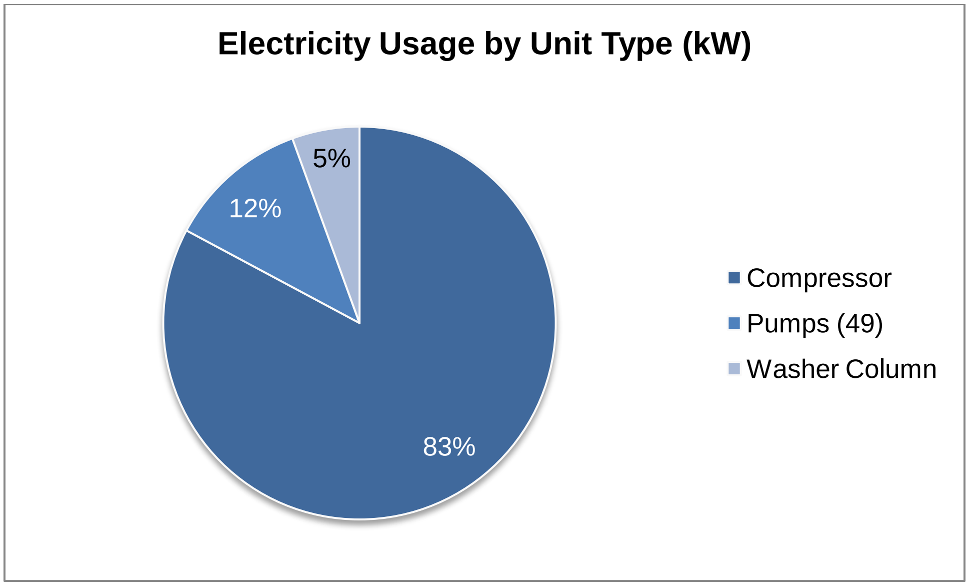


The utilities are examined by type in the following sections, but more detailed information on cost is available in the Process Economics segment Utility Requirements.

Electricity

Electricity is needed for pumps throughout the process, as well as for a compressor and a washer-column unit. These latter two units are by far the largest consumers of electricity on a per-unit basis, with 83% and 5% of the overall consumption, respectively. See Figure 11.

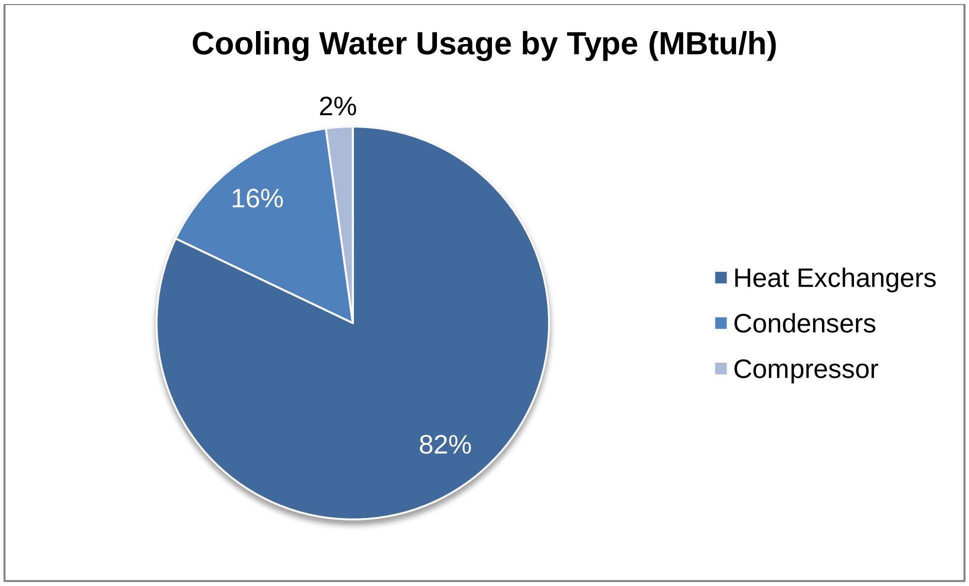
Figure 11



Cooling Water

Cooling water is procured at 90^{0}F for use in process heat exchangers, as well as distillation column condensers and in the multistage compressor's intercoolers. See the summary in Figure 12. In all cases, the full temperature range of heating (up to 120^{0}F) is used in order to minimize requirements while not violating Heuristic 27 (PPDP), which should prevent the worst of fouling. Note that one heat exchanger in particular, HX-401, is responsible for over 70% of the process cooling requirements. This unit should be further examined, as it represents a significant cost driver.

Figure 12



The total amount of cooling water used by this process, excluding HX-401 is 22,250 gpm, or about 10.5 billion gallons per year. Including HX-401, this increases dramatically to 82,250 gpm and 39.1 billion gallons per year.

Chilled Water

Chilled water is necessary to cool process streams to a minimum of 60^0F. It is used in HX-500 to pre-cool the DC-503 inlet stream to the requisite 62.8^0F (see Section 500). It is also used to minimize the amount of refrigeration required in block CRY-500, pre-cooling stream S-513. A total of 1,564 ton-day of chilled water is used. This equates to 2,650 gpm or 1.25 billion gallons per year.

Refrigeration

Refrigeration at -90^0F is used in CRY-500 to crystallize para-xylene at -22^0F. According to Table 18.1 of PPDP, vaporizing ethylene would be a more than adequate heat-transfer medium at this temperature range. The fluid is included in the overall purchase cost, according to the supplier.

Dowtherm A

Dowtherm A is a commonly employed heat source for temperatures outside the reasonable reach of steam, but not exceeding 750^0F. In order to meet the process heating requirements in this temperature range, about 532,000 pounds of Dowtherm A are required. Calculations are shown in SC-U00.

Molten Salt

Molten salts are employed to achieve temperatures up to 1,100^{0}F. The transalkylation reaction in R-600 takes place at 850^{0}F, and thus requires a medium like this. Solar Salt, detailed in Section -700 and in Appendix D is the molten salt used in this process. Given the residence time of six hours, around seven million pounds are necessary to achieve the required pre-heating of the feed. An example calculation is in SC-U00.

Cost-Saving Measures

Heat Integration

The process uses a multitude of heat exchangers in order to maximize energy efficiency. As a result, no externally-supplied steam or electric heating is required. See process overview and unit descriptions for m ore information.

Steam Generation

Excess process heat is used to vaporize water and produce steam for use in reboilers, HX-301, and SEP-500.

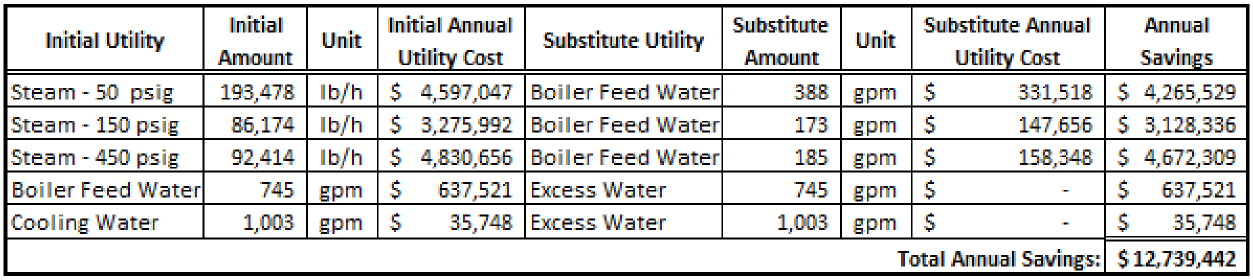
Excess Water Utilization

Both aqueous phase reforming (R-300) and condensation (R-40X) produce water, which is recovered after separations in streams S-324 and S-502, respectively. Both of these water supplies are extremely pure, but are at temperatures too high for use as cooling water. However, a portion of this water (S-527) is used in heat exchanger HX-601 to cool an inlet stream that exceeds 400^{0}F (p.471, PPDP). The remaining excess water (S-324 and S-526) is used as boiler feed, which replaces the need for any external purchase. Note that the amount of excess water available for use as boiler feed exceeds that needed to meet steam requirements.

Impact of Cost-Saving Measures

In total, these cost-saving measures reduced utilities by $12.7 million per year. Figure 13 summarizes the savings, and calculations are shown in SC-U01.

Figure 13



Initial Utility	Initial Amount	Unit	Initial Annual Utility Cost	Substitute Utility	Substitute Amount	Unit	Substitute Annual Utility Cost	Annual Savings
Steam - 50 psig	193,478	lb/h	$ 4,597,047	Boiler Feed Water	388	gpm	$ 331,518	$ 4,265,529
Steam - 150 psig	86,174	lb/h	$ 3,275,992	Boiler Feed Water	173	gpm	$ 147,656	$ 3,128,336
Steam - 450 psig	92,414	lb/h	$ 4,830,656	Boiler Feed Water	185	gpm	$ 158,348	$ 4,672,309
Boiler Feed Water	745	gpm	$ 637,521	Excess Water	745	gpm	$ -	$ 637,521
Cooling Water	1,003	gpm	$ 35,748	Excess Water	1,003	gpm	$ -	$ 35,748
							Total Annual Savings:	$ 12,739,442

Further Exploration

Excess Boiler Feed Water and Steam Turbines

Generation of electricity via steam turbines should be explored as a means of work-integration and cost saving. Streams S-324 and S-526 generate more steam than is needed for heating. The excess could be diverted to offset some power requirements. This was not explored in this analysis due to the expected limited impact in the face of extreme electricity requirements.

Cooling Efficiency of HX-401

The extreme amount of cooling water required for HX-401 represents a great cause for concern, and it is likely that a heat exchanger is not the most effective medium. Alternative cooling configurations such as a cooling tower should be explored before implementation.

Solar Heating

Solar Salt is traditionally heated in large solar fields. The current process uses a solar salt furnace as suggested by Table 22.32 of PPDP. If a solar heating setup is feasible given the conditions in Brazil, this would save construction of one furnace and allow for the combustion gases currently used in that furnace to be diverted elsewhere. The cost would be the construction of a second storage tank and other units needed for the solar heating process. More information can be found in Appendix D.

Section V

Unit Descriptions

V. UNIT DESCRIPTIONS

Section 000: Input Storage & Clarification

Storage Tanks
ST-000, ST-001, ST-002, ST-003, ST-004, ST-005, ST-006, ST-007, ST-008, ST-009, ST-010, ST-011, ST-012, ST-013, ST-014, ST-015
Base Purchase Cost: $1,906,800

At desired flow rate of 1.25 million pounds per hour of molasses, fifteen storage tanks are necessary to ensure that production can continue 330 days per year. Since the vapor pressure of molasses is extremely low, cone-roof tanks made of carbon steel were appropriate. The molasses is stored at ambient temperature, 77^0F, and atmospheric pressure, 14.7 psia. Each tank is 20,000,000 gallons, which is the upper limit of construction according (p.589, PPDP). The storage tanks are expected to operate at 76% capacity with a residence time of six days. For the nine months of the year that molasses produced, five tanks will be used to allow for deliveries once monthly. Since molasses is unavailable approximately 92 days per year, the remaining ten tanks will be filled as shortly as possible before end of season. Each tank empties on a rotating basis into stream S-000. See SC-000 for calculations.

Pumps
P-000
Base Purchase Cost: $84,300

This is a centrifugal cast iron pump that adds a driving force of 2 psi to the molasses feed, S-000, drawing it from the storage tank in operation and introducing it to the clarification process. This satisfies Heuristic 38 of PPDP, which allows for a 2 psi pressure drop across 100 ft of pipe. The electricity required is 2.23 kW. The pump head is 3.89 ft.

Other Equipment
C-000
Base Purchase Cost: $1,255,988

This unit is a clarifier vessel. Diluted molasses enters the clarifier to allow particles to settle. It handles 58,838 gallons per minute of liquid overflow. It has a settling area of 88,258 square feet and a diameter of 335 feet. It is made of concrete. It has a rotating rake to collect the sludge that accumulates at the bottom.

F-000
Base Purchase Cost: $129,978

This unit is a rotary drum filter. It removes 1500 pounds of filtrate per day per square foot. It has a surface area of 115 square feet.

Section 100: Hydrolysis

Pumps

P-100, P-101, P-102
Base Purchase Cost: $10,200

This is a centrifugal pump, of 304 stainless steel, that pumps the three identically split streams of input from SPT-100 to HX-100, HX-101, and HX-102. It operates at a rate of 5,610 ft^3/hr. The energy requirement for the pump is 14.13 HP. The pump operates at an efficiency of 0.74. The pump head is 50.1 ft. The pressure change across the pump is 1.75 atm.

P-103, P-104, P-105
Base Purchase Cost: $179,700

This is a centrifugal pump, of 304 stainless steel, that pumps the three identical streams from R-100, R-101, and R-102 to HX-200. It operates at a rate of 5,785 ft^3/hr. The energy requirement for the pump is 659.10 HP. The pump operates at an efficiency of 0.74. The pump head is 2,342.5 ft. The pressure change across the pump is 1167 psi.

Heat Exchangers

HX-100, HX-101, HX-102

Base Purchase Cost: $51,200

This is a heat exchanger that is used to heat the sucrose and water feed to R-100, R-101, and R-102 and cool the product from the condensation reaction. This is a floating head shell and tube heat exchanger. The streams exiting pumps P-100, P-101, and P-102 are passed through the heat exchangers at a flow rate of 5,610 ft^3/hr. The temperature of the cold inlet stream is increased from 77°F to 212°F (25°C to 100°C). The hot inlet stream from SPT-400 is passed through the heat exchangers at a flow rate of 276,000 ft^3/hr. The temperature of the hot inlet stream is decreased from 698°F to 506°F (370°C to 263.3°C). The heat duty of heat exchanger is 36,902,766 BTU/hr. The heat transfer area is 1,615 ft^2. Both the shell side and the tube side are made of 304 stainless steel.

Reactors

R-100, R-101, R-102

Base Purchase Cost: $175,600

This is a reactor used to convert the sucrose and water fed into it from P-100, P-101, and P-102 to glucose and water. The reactor is fed at 5,994 ft^3/hr. The reactor operates at 100°C and 1 atm. It is a 304 stainless steel fixed bed reactor loaded with catalyst. It has a capacity of 6,309 ft^3/hr. The weight of the catalyst needed per charge is 147,000,000 g, costing approximately $2,490,000 discounted to $0.621 million at 25%. The reactor is 23 feet tall and has a 6 ft diameter.

Catalyst

CAT-100

Base Purchase Cost, including Lifetime Recharge: 6,388,200

The catalyst used in hydrolysis is an HY-faujasite catalyst with an SI/Al ratio of 15. This is a zeolite catalyst much in the same sense as others that are needed later. This catalyst is used as a means to speed up the hydrolysis of sucrose in water which if just let to sit would take years to hydrolyze into glucose. To make up for the relatively rapid deactivation of the catalyst it possible to add a column of new catalyst to continuously pump catalyst into the reactor while filtering out older catalyst.

To create the catalyst H_4SiO_4 is fed into Na_2AlO_2 in a ratio of approximately 12 to 1. The catalyst is then steam-aged, for 2 hours at 500°C to create the stable faujasite crystals. Once the faujasite crystals have been obtained $(NH_4)_2SiF_6$ is added as desired until the specified Si/AL ratio is reached. The deactivation of this catalyst is estimated to be 13.29 grams of catalyst / lbmol of reactant fed, based on an estimate for a similar catalyst. This estimate may be a little high for the deactivation however seeing as the catalyst did not lose any activity in the 7 day period of testing (Moreau, 1999). It is also known that the catalyst can easily be regenerated a limited number of times by using a thermal technique of burning off the coked particles by passing a stream of hot (500°C) air through the catalyst.

To calculate the costs of the catalyst market pricing for H_4SiO_4, Na_2AlO_2, and $(NH_4)_2SiF_6$ were obtained. Once that was completed using data from Moreau, 1999, the weight hourly space velocity (WHSV) was calculated to be approximately 1.93 hr^{-1}. Using the value of the WHSV and the known amount of feed to the reactor, the amount of catalyst needed was determined to be 147,000,000 grams of catalyst per charge. From this it is known that to achieve a 15 to 1 ration of Si to Al that a ratio of 12:1:3 of H_4SiO_4: Na_2AlO_2: $(NH_4)_2SiF_6$ is needed to achieve this goal. So to determine the overall pricing of the catalyst 147,000,000 was multiplied by 12/16 and the market price of H_4SiO_4 per gram and added to 147,000,000 multiplied by 1/16 and the market price of Na_2AlO_2 per gram and 147,000,000 multiplied by 3/16 and the market price of $(NH_4)_2SiF_6$ per gram. This yields a value of $2.49 million per charge. It was then assumed to have a discount to 25% for bulk pricing options which gives a value of $0.62 million per charge.

The estimated deactivation of the catalyst, 13.29 grams/lbmol reactant was used to determine the deactivation of the catalyst. Since the flow rate of the reactant is known to determine the amount of deactivated catalyst in an hour the hourly lbmol flow rate is multiplied by 13.29. This yields a result of grams of deactivated catalyst per hour. The hourly deactivation of catalyst is 24,169 grams per hour. The price of the hourly deactivated catalyst is determined via the same process as before and this value is multiplied by 24 hours and 365 days to get a yearly cost. The cost was determined to be $3.52 million and with the discount 25% bulk pricing $0.88 million. See SC-C00 for calculations.

Section 200: Hydrogenation

Pumps

P-200, P-201, P-202, P-203, P-204, P-205
Base Purchase Cost: $6,500

This is a centrifugal pump, of 304 stainless steel, that pumps the six identically split streams from SPT-200 to R-200, R-201, R-202, R-203, R-204, and R-205. It operates at a rate of 2,828 ft^3/hr. The energy requirement for the pump is 0.61 HP. The pump operates at an efficiency of 0.68. The pump head is 3.9 ft. The pressure change across the pump is 2 psi.

P-206, P-207, P-208, P-209, P-210, P-211
Base Purchase Cost: $6,500

This is a centrifugal pump, of 304 stainless steel, that pumps the six identical streams from R-200, R-201, R-202, R-203, R-204, and R-205 to MIX-200. It operates at a rate of 2,841 ft^3/hr. The energy requirement for the pump is 0.61 HP. The pump operates at an efficiency of 0.68. The pump head is 3.9 ft. The pressure change across the pump is 2 psi.

Heat Exchangers

HX-200
Base Purchase Cost: $286,600

This is a heat exchanger that is used to cool the glucose and water stream going to SPT-200 by using cooling water. This is a floating head shell and tube heat exchanger. The stream exiting MIX-100 is passed through the heat exchanger at a flow rate of 17,739 ft^3/hr. The temperature of the hot inlet stream is decreased from 214.16°F to 173.75°F (101.2°C to 78.75°C). The cold inlet stream is passed through the heat exchangers at a flow rate of 20,654 ft^3/hr. The temperature of the cold inlet stream is increased from 90°F to 120°F (32.2°C to 48.9°C). The heat duty of heat exchanger is 40,777,165 BTU/hr. The heat transfer area is 9057 ft^2. Both the shell side and the tube side are made of 304 stainless steel.

Reactors

R-200, R-201, R-202, R-203, R-204, R-205
Base Purchase Cost: $191,300

This is a reactor used to convert the glucose fed into it from P-200, P-201, P-202, P-203, P-204, and P-205 to sorbitol. The reactor is fed at 2,828 ft^3/hr. The reactor operates at 353K and 80 bar. It is a Teflon coated stainless steel 316 trickle bed reactor loaded with catalyst. It is a Teflon coated reactor to prevent catalyst poisoning. It has a capacity of 211,083 lb/hr. The weight of the catalyst needed per charge is 24,202,200 g, costing approximately $47.5 million discounted to $11.9 million at 25%. The reactor is 18.5 feet tall and has a 5 ft diameter.

Catalyst

CAT-200
Purchase Cost, including Lifetime Recharge: $15,3.91,100

In typical glucose hydrogenation Ni used to be the preferred catalyst metal because of its high activity and low costs. Unfortunately Ni catalysts can leach and have their activity decreased rapidly and require possibly expensive separation processes to purify the product of the Ni particles. Ru catalysts however don't suffer from the same drawbacks as Ni which makes it much more appealing as a commercial catalyst. The catalyst which yielded the best result for glucose hydrogenation was a Ru05Ai catalyst.

The Ru05Ai catalyst creation process would be prepared by the impregnation of Al_2O_3 with Ruthenium (III) Acetylacetonate. The Al_2O_3 is used as the support metal for the activation of the ruthenium. To begin the preparation of the catalyst 73 g Al_2O_3 is mixed with 150 ml of toluene and stirred for 15 minutes. Once the Al_2O_3/toluene slurry is prepared, 2.907 g Ruthenium (III) Acetylacetonate is dissolved in a separate 150 ml of toluene and this solution is added to the slurry. This new slurry is stirred for one hour while being swirled occasionally to homogenize it. The toluene is also left to evaporate at room temperature at this time. The catalyst is then heated in by a helium stream within four hours to 250°C and held at this temperature for two more hours. To reduce the catalyst it is heated to 350°C within one hour by a hydrogen stream and held at this temperature for three more hours. (Kusserow, 2002) However based on the cost of buying of the raw materials needed and additional labor costs needed for creating the catalyst it was found to be much cheaper to purchase a catalyst that is believed to be similar from a supplier. Catalyst deactivation was assumed to be seven years because of Ruthenium's use as a precious metal. It was also assumed that the catalyst could be sold back to the supplier for half of the purchase price.

To estimate the cost of making the catalyst, the prices of Ruthenium (III) Acetyl Acetonate, Al_2O_3, and toluene were obtained. A scale up factor was determined based on the volumetric flow rate of the reactant feed and the volume of catalyst added. The scale up factor (SUF) is merely the volumetric flow rate of the limiting reactant feed needed divided by 0.04 L and 7.5 (a "volumetric hourly space velocity"). Based on a 300ml:73g:2.907g ratio of Toluene: Al_2O_3:Ruthenium (III) Acetyl Acetonate the price of the catalyst was determined to be \$229.7 million. With the discount to 25% it would cost \$57.4 million. Unfortunately these prices were too high so a similar catalyst that could be bought from a supplier was searched for. To determine the mass of the catalyst needed to be purchased the wt% of Ru in Ruthenium (III) Acetyl Acetonate was determined (approximately 25.4%). Using this value and the mass of Ruthenium (III) Acetyl Acetonate needed it was determined that 1.21 million grams of Ru would be needed. Using the catalyst specification of 5% Ru it was found that 24.2 million grams of catalyst is needed. To purchase this much catalyst from the supplier it was found to cost $47.5 million much less than the amount of money to produce it. Using the discount 25%, the price drops to $11.9 million. See calculation SC-C01.

Section 300: Aqueous Phase Reforming

Pumps

P-300
Base Purchase Cost: $8,500

This is a centrifugal pump, of 304 stainless steel, that pumps the heated sorbitol stream from HX-300 to HX-301. It operates at a rate of 4,859 ft^3/hr. The energy requirement for the pump is 3.39 HP. The pump operates at an efficiency of 0.73. The pump head is 14.4 ft. The pressure change across the pump is 7 psi.

P-301
Base Purchase Cost: $5,200

This is a centrifugal pump, of 304 stainless steel, that pumps the recycled sorbitol stream from F-300 to MIX-300. It operates at a rate of 1,390 ft^3/hr. The energy requirement for the pump is 0.34 HP. The pump operates at an efficiency of 0.60. The pump head is 4.5 ft. The pressure change across the pump is 2 psi.

P-302
Base Purchase Cost: $8,400

This is a centrifugal pump, of 304 stainless steel, that pumps the mixed sorbitol stream from MIX-300 to HX-300. It operates at a rate of 4,784 ft^3/hr. The energy requirement for the pump is

2.39 HP. The pump operates at an efficiency of 0.73. The pump head is 10.2 ft. The pressure change across the pump is 5 psi.

Heat Exchangers

HX-300

Base Purchase Cost: $56,000

This is a heat exchanger that is used to cool the hydrogen, carbon dioxide, alkane, and water stream from VAL-301, while heating the mixed sorbitol stream from P-302. This is a floating head shell and tube heat exchanger. The stream exiting VAL-301 is passed through the heat exchanger at a flow rate of 6,364,400 ft^3/hr. The temperature of the hot inlet stream is decreased from 338.74°F to 273.58°F (170.4°C to 134.2°C). The cold inlet stream is passed through the heat exchangers at a flow rate of 4784 ft^3/hr. The temperature of the cold inlet stream is increased from 227.58°F to 253.58°F (108.7°C to 123.1°C). The heat duty of heat exchanger is 7,700,625 BTU/hr. The heat transfer area is 2,422 ft^2. Both the shell side and the tube side are made of 304 stainless steel.

HX-301

Base Purchase Cost: $174,200

This is a heat exchanger that is used to heat the mix sorbitol stream from P-300 using some of the heat generated from the furnace. This is a floating head shell and tube heat exchanger. The stream exiting P-300 is passed through the heat exchanger at a flow rate of 4,858 ft^3/hr. The temperature of the cold inlet stream is increased from 253.59°F to 359.6°F (123.1°C to 182°C). The heat duty of heat exchanger is 32,547,633 BTU/hr. The heat transfer area is 8505 ft^2. Both the shell side and the tube side are made of 304 stainless steel.

HX-302

Base Purchase Cost: $16,000

This is a heat exchanger that is used to cool the hydrogen stream from HX-400 using cooling water. This is a floating head shell and tube heat exchanger. The stream exiting HX-400 is passed through the heat exchanger at a flow rate of 25,003 ft^3/hr. The temperature of the hot inlet stream is decreased from 254.16°F to 173.75°F (123.4°C to 78.75°C). The cold inlet stream is passed through the heat exchangers at a flow rate of 1003 ft^3/hr. The temperature of the cold inlet stream is increased from 90°F to 120°F (32.2°C to 48.9°C). The heat duty of heat exchanger is 2,014,133 BTU/hr. The heat transfer area is 157 ft^2. Both the shell side and the tube side are made of 304 stainless steel.

HX-303

Base Purchase Cost: $185,100

This is a heat exchanger that is used to cool the hydrogen, carbon dioxide, alkane, and water stream from HX-300 using chilled water. This is a floating head shell and tube heat exchanger. The stream exiting HX-300 is passed through the heat exchanger at a flow rate of 5,840,540 ft^3/hr. The temperature of the hot inlet stream is decreased from 273.58°F to 140°F (134.2°C to 60°C). The cold inlet stream is passed through the heat exchangers at a flow rate of 22,258 ft^3/hr. The temperature of the cold inlet stream is increased from 40°F to 120°F (4.4°C to 48.9°C). The heat duty of heat exchanger is 122,304,595BTU/hr. The heat transfer area is 12,179 ft^2. Both the shell side and the tube side are made of 304 stainless steel.

Reactors

R-300

Base Purchase Cost: $231,800

This is a reactor used to convert the sorbitol fed into it from HX-301 to hydrogen, alkanes, and carbon dioxide. The reactor is fed at 5,209 ft^3/hr. The reactor operates at 182°C and 50 bar. It is a 304 stainless steel trickle bed reactor loaded with catalyst. It has a capacity of 6,309 ft^3/hr. The weight of the catalyst needed per charge is 44,266,068 g, costing approximately $240.9 million discounted to $60.2 million at 25%. The reactor is 22 feet tall and has a 6 ft diameter.

Separators

SEP-300

Base Purchase Cost: $52,000

This is a separator used to separate hydrogen from carbon dioxide and alkanes. It utilizes pressure swing adsorption technology to create the separation. The separator is fed with 3,414,410 ft^3/hr. The separator is 12 ft tall and has a diameter of 11.5 ft. The separator has a heat duty of -14,767,649 BTU/hr. The separator is made of 304 stainless steel.

ST-300

Base Purchase Cost: $344,890

This unit is a horizontal pressure vessel for the storage of hydrogen gas. At 77 ^{0}F and 20 bar, the tank can hold 3393 cubic feet of hydrogen. The storage tank is constructed from carbon steel. It is 30 feet long and has a diameter of 12 feet.

ADS-300, ADS-301, ADS-302, ADS-303

Base Purchase Cost: $477,000

This unit is an adsorption column for pressure swing adsorption. It is 35 feet high and has a diameter of 8 feet. Gas feed enters the column at 20 bar. It is filled with 81,000 pounds of zeolite 13x.

F-300

Base Purchase Cost: $35,100

This is a separator used to separate sorbitol from hydrogen, carbon dioxide, and alkanes. It utilizes flash vaporization technology to create the separation. The separator is fed with 255,086 ft^3/hr. The separator is 13 ft tall and has a diameter of 6 ft. The separator has a heat duty of 77,018,428 BTU/hr. The separator operates at 359.6°F and 20 bar. The separator is made of 304 stainless steel.

F-301

Base Purchase Cost: $34,600

This is a separator used to separate water from hydrogen, carbon dioxide, and alkanes. It utilizes flash vaporization technology to create the separation. The separator is fed with 2,739,570 ft^3/hr. The separator is 12 ft tall and has a diameter of 9.5 ft. The separator has a heat duty of 5,106,795 BTU/hr. The separator operates at 140°F and 1 atm. The separator is made of 304 stainless steel.

Compressors

CMP-300

Base Purchase Cost: $10,132,800

This is a multi stage compressor, of 304 stainless steel, used to compress the hydrogen from SEP-300 to 80 bar. It operates at a rate of 1,612,640 ft^3/hr. The energy requirement for the compressor is 22,340 HP. The net cooling duty of the compressor is -30,562,822 BTU/hr. The pressure change across the compressor is 1149.6 psi.

Catalyst

CAT-300

Purchase Cost, including Lifetime Recharging: $77,995,500

The catalyst presentation in the patent was presented independent of the operating conditions discussion. The catalyst chosen is an RhReCe catalyst. The catalyst was made by adding 3.86g of Rhodium(III) Nitrate, 1.64g of Perrhenic acid, and 2.21g of Cerium(III) Nitrate hexahydrate to 12 ml of deionized water in the presence of titania modified carbon and dried overnight under a vacuum at 100°C. The titania modified carbon was created by adding 1.95g of Titanium n-butoxide to 12 ml of anhydrous isopropanol in the presence of 10g of activated carbon. However due to the high costs of Rhodium (III) Nitrate it was assumed that the metals were purchased at market price and could be sold back to the supplier after deactivation for half the purchase price to be regenerated. It was also assumed that because rhodium is a precious metal the deactivation would take place over 7 years.

To calculate the price of this catalyst the prices of Rhodium (III) Nitrate, Perrhenic acid, and Cerium (III) Nitrate were obtained. It necessary that 175,659 lb of sorbitol is fed to the APR reactor per hour and from the specified WHSV of 1.8 (WO 2007/075476) it was determined that 97,588 lb (or 44.27 million grams) of catalyst is needed. Since 17.985 g is needed per batch the number of batches needed to be made is 2.46 million. The price of each material per batch was determined by the mass needed of each per batch and the price of the material. These prices were multiplied by the number of batches needed and summed together. This returns a value of $686 million which is entirely unreasonable. So to combat this issue the market prices of the metals themselves was obtained and the weight of each metal needed per batch was determined using weight percents. The price of each metal was converted to a per gram basis and the value of a single batch was determined to be $72.25 for 13.28 grams. The mass of catalyst needed was divided by the 13.28 and multiplied the $72.25 to determine the value of the catalyst needed by metal market pricing. This returned a more reasonable, although still very expensive, $240.9 million per charge. Using the discount to 25%, the price becomes $60.2 million. See calculation SC-C02.

Section 400: Condensation

Pumps

P-400

FOB Cost: $119,300

This unit is a centrifugal pump made of carbon steel. It pumps sorbitol from heat exchanger HX-400 to heat exchanger HX-402. It operates at a temperature of 204 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 1727 gallons per minute with a density of 72.33 lb/ft^3. The pump head is 3.98 feet. The pump uses 1.86kW of electricity and generates 2.5hp of brake power operating at 80.8% efficiency. These properties were determined using ASPEN for the specified 2psi pressure increase.

P-401
FOB Cost: $272,300

This unit is a centrifugal pump made of carbon steel. It pumps sorbitol from heat exchanger HX-404 the splitter SPT-400. It operates at a temperature of 698 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 2818 gallons per minute with a density of 44.33 lb/ft^3. The pump head is 6.5 feet. The pump uses 2.94kW of electricity and generates 3.94hp of brake power operating at 83.5% efficiency. These properties were determined using ASPEN for the specified 2psi pressure increase.

P-402
FOB Cost: $121,400

This unit is a centrifugal pump made of carbon steel. It pumps sorbitol from heat exchanger HX-404 the heat exchanger HX-404. It operates at a temperature of 302 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 1832 gallons per minute with a density of 68.18 lb/ft^3. The pump head is 4.33 feet. The pump uses 1.96kW of electricity and generates 2.63hp of brake power operating at 81.1% efficiency. These properties were determined using ASPEN for the specified 2psi pressure increase.

Heat Exchangers:
HX-400
FOB Cost: $764,100

This is a shell and tube heat exchanger made of carbon steel on the tube side and 304 stainless steel on the shell side. It performs heat recovery by heating 1 million lb/hr sorbitol from 177 to 204 degrees Fahrenheit and cooling 7420lb/hr hydrogen from 1150 to 254 degrees Fahrenheit. It transfers a heat duty of 23.23 million BTU/hr over 1340 ft^2 of heat transfer area and was designed assuming an overall heat coefficient of 50 BTU/hr-ft^2-^{o}F. It is 20ft long. The above was calculated by ASPEN based on the assumed overall heat transfer coefficient, a specified minimum temperature approach of 50 degrees Fahrenheit, and a specified hot/cold outlet temperature approach of 50 degrees Fahrenheit to reasonably maximize heat transfer.

HX-401
FOB Cost: $1,375,300

This is a shell and tube heat exchanger made of carbon steel on the tube side and 304 stainless steel on the shell side. It performs heat recovery by cooling 1 million lb/hr condensation product from 414 to 122 degrees Fahrenheit and using 29.652 million lb/hr cooling water heated from 90 to 120 degrees Fahrenheit. It transfers a heat duty of 978.49 million BTU/hr over 55,302 ft^2 of heat transfer area and was designed assuming an overall heat coefficient of 150 BTU/hr-ft^2-^oF. It is 20ft long. The above was calculated by ASPEN based on the assumed overall heat transfer coefficient, a specified minimum temperature approach of 20 degrees Fahrenheit, and a specified hot stream outlet temperature 122 degrees Fahrenheit as required for the three-phase separation.

HX-402
FOB Cost: $1,375,300

This is a shell and tube heat exchanger made of carbon steel on the tube side and 304 stainless steel on the shell side. It performs heat recovery by heating 1 million lb/hr condensation product from 204 to 206 degrees Fahrenheit and cooling 74508 lb/hr xylenes from 276 to 226 degrees Fahrenheit. It transfers a heat duty of 1.805 million BTU/hr over 1084 ft^2 of heat transfer area and was designed assuming an overall heat coefficient of 40 BTU/hr-ft^2-^oF. It is 20ft long. The above was calculated by ASPEN based on the assumed overall heat transfer coefficient, a specified minimum temperature approach of 20 degrees Fahrenheit, and a specified hot/cold outlet temperature approach of 20 degrees Fahrenheit in order to reasonably assure maximum heat transfer.

HX-403
FOB Cost: $762,600

This is a shell and tube heat exchanger made of carbon steel. It performs heat recovery by heating 1 million lb/hr of sorbitol solution from 207 to 302 degrees Fahrenheit and cooling 214929 lb/hr of transalkylation product from 850 to 352 degrees Fahrenheit. It transfers a heat duty of 83.72 million BTU/hr over 6890 ft^2 of heat transfer area and was designed assuming an overall heat coefficient of 40 BTU/hr-ft^2-^oF. It is 20ft long. The above was calculated by ASPEN based on the assumed overall heat transfer coefficient, a specified minimum temperature approach of 50 degrees Fahrenheit, and a specified hot/cold outlet temperature approach of 50 degrees Fahrenheit in order to reasonably assure maximum heat transfer.

HX-404
FOB Cost: $11,854,500

This is a shell and tube heat exchanger made of carbon steel. It heats 1 million lb/hr sorbitol solution from 640 to 698 degrees Fahrenheit using hot Dowtherm A. It transfers a heat duty of 527.76 million BTU/hr over 2858 ft^2 of heat transfer area. It is 20ft long. The above was calculated by ASPEN based on the specified outlet temperature of the sorbitol necessary for condensation.

Reactors

R-400, R-401, R-402, R-403
FOB Cost: $460,500 each

These are packed bed reactors made of carbon steel responsible for the catalyzed condensation reactor that convert sorbitol into para-xylene and other aromatics. Four identical reactors are used due to size limitations. Each reactor handles 250480 pounds of sorbitol solution per hour and operates at a temperature of 698 degrees Fahrenheit. Each has a volume of 4759.2 gallons, of which 3331 is working volume. Each is 22.5 feet high and 6 feet in diameter.

CAT-400

Purchase Cost, including Lifetime Reloading: $11,745,000

An activated *zeolite* or *aluminosilicate* catalyst, normally *pentasil* (more commonly called ZSM-5), facilitates the reaction. Zeolites have a porous structure that can accommodate a wide variety of cations. The cations are loosely held and exchange easily with cations in the contacted solution. Similar catalysts are used in the aqueous phase reforming and transalkylation portions of this process, and information on their manufacture and properties can be found in US patent 2008/0300435 A1. For the condensation of sorbitol to produce para-xylene, ZSM-5, with a thirty-to-one silicon dioxide to aluminum oxide ratio, is treated with a gallium nitrate solution, dried overnight in a vacuum oven, and subsequently calcined in flowing air at 400 degrees Celsius to effect 1.2% loading by weight of gallium (Example 46 in the patent). The WHSV is specified in the patent as 2 hr^{-1}. To make up for the relatively rapid deactivation of the catalyst it possible to add a column of new catalyst to continuously pump catalyst into the reactor while filtering out older catalyst.

To calculate the same costs of the catalyst market pricing for H_4SiO_4 and Na_2AlO_2were used. Using the value of the specified WHSV and the known amount of feed to the reactor, the amount of catalyst needed was determined to be 120.2 million grams of catalyst per charge. From this, it is known that to achieve a 30 to 1 ration of Si to Al which implies that a ratio of 30:1 of H_4SiO_4: Na_2AlO_2 is needed to achieve this goal. So to determine the overall pricing of the catalyst, 120.2 million was multiplied by 30/31 and the market price of H_4SiO_4 per gram and added to 120.2 million multiplied by 1/31 and the market price of Na_2AlO_2 per gram. This yields a value of $2.41 million per charge. It was then assumed to have a discount to 25% for bulk pricing options which gives a value of $0.60 million per charge.

The estimated deactivation of the catalyst, 13.29 grams/lbmol reactant was used to determine the deactivation of the catalyst. Since the flow rate of the reactant is known to determine the amount of deactivated catalyst in an hour the hourly lbmol flow rate is multiplied by 13.29. This yields a result of grams of deactivated catalyst per hour. The hourly deactivation of catalyst is 38,674 grams per hour. The price of the hourly deactivated catalyst is determined via the same process as before and this value is multiplied by 24 hours and 365 days to get a yearly cost. The cost was determined to be $6.80 million and with the discount 25% bulk pricing $1.70 million. See calculation SC-C03.

Section 500: Separations

P-500
FOB Cost: $45,200

This unit is a centrifugal pump made of carbon steel. It pumps bottoms product from column DC-500 to column DC-501. It operates at a temperature of 346 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 407 gallons per minute with a specific gravity of 0.773. The pump head is 5.98 feet. The pump operates at 68.4% efficiency, uses 0.47kW of electricity and generates 0.63hp of brake power. These properties were determined using ASPEN for the specified 2psi pressure increase.

DP-500
FOB Cost: $9,900

This unit is a centrifugal pump made of carbon steel. It pumps distillate from DC-500 back into the column DC-500 or out. It operates at a temperature of 259 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 494 gallons per minute with a specific gravity of 0.773. The pump operates at 70% efficiency. These properties were determined automatically by ASPEN as part of the RADFRAC subroutine.

P-501
FOB Cost: $53,600

This unit is a centrifugal pump made of carbon steel. It pumps organic condensation product from the three phase separator (SEP-500) to the first column (DC-500). It operates at a temperature of 250 degrees Fahrenheit. It moves 524 gallons per minute with a specific gravity of 0.777. The pump head is 5.98 feet. The pump operates at 70.9% efficiency, uses 0.585kW of electricity and generates 0.78hp of brake power. These properties were determined using ASPEN for the specified 2psi pressure increase.

DP-501
FOB Cost: $13,600

This unit is a centrifugal pump made of carbon steel. It pumps distillate from DC-501 back into the column or out. It operates at a temperature of 326 degrees Fahrenheit. It moves 864 gallons per minute with a specific gravity of 0.758. The pump operates at 70% efficiency. These properties were determined automatically by ASPEN as part of the RADFRAC subroutine.

P-502
FOB Cost: $53,500

This unit is a centrifugal pump made of carbon steel. It pumps bottoms product from column DC-502 in a recycle loop back to column DC-500. It operates at a temperature of 289 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 489 gallons per minute with a specific gravity of 0.776. The pump head is 5.95 feet. The pump operates at 70.2% efficiency, uses 0.55kW of electricity and generates 0.74hp of brake power. These properties were determined using ASPEN for the specified 2psi pressure increase.

DP-502
FOB Cost: $26,600

This unit is a centrifugal pump made of carbon steel. It pumps distillate from DC-502 back into the column or out. It operates at a temperature of 250 degrees Fahrenheit. It moves 2105 gallons per minute with a specific gravity of 0.776. The pump operates at 70% efficiency. These properties were determined automatically by ASPEN as part of the RADFRAC subroutine.

P-503
FOB Cost: $34,000

This unit is a centrifugal pump made of carbon steel. It pumps distillate from column DC-502 to column DC-503. It operates at a temperature of 70 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 176 gallons per minute with a specific gravity of 0.775. The pump head is 5.96 feet. The pump operates at 59.3% efficiency, uses 0.23kW of electricity and generates 0.31hp of brake power. These properties were determined using ASPEN for the specified 2psi pressure increase.

DP-503
FOB Cost: $6,200

This unit is a centrifugal pump made of carbon steel. It pumps distillate from DC-503 back into the column or out. It operates at a temperature of 250 degrees Fahrenheit. It moves 183 gallons per minute with a specific gravity of 0.812. The pump operates at 70% efficiency. These properties were determined automatically by ASPEN as part of the RADFRAC subroutine.

Heat Exchangers:
RB-500
FOB Cost: $381,200

This is a shell and tube heat exchanger made of carbon steel which heat and boil fractions of the bottoms product of its respective distillation columns so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It have heat transfer area of 18984 ft^{2}and heat duty of 75.4 million BTU/hr.

RB-501
FOB Cost: $238,100

This is a shell and tube heat exchanger made of carbon steel which heat and boil fractions of the bottoms product of its respective distillation columns so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It have heat transfer area of 11149 ft^{2}and heat duty of 44.5 million BTU/hr.

RB-502
FOB Cost: $313,700

This is a shell and tube heat exchanger made of carbon steel which heat and boil fractions of the bottoms product of its respective distillation columns so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It have heat transfer area of 15247 ft^{2}and heat duty of 146.8 million BTU/hr.

RB-503
FOB Cost: $29,600

This is a shell and tube heat exchanger made of carbon steel which heat and boil fractions of the bottoms product of its respective distillation columns so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It have heat transfer area of 998 ft^{2}and heat duty of 16.5 million BTU/hr..

CND-500

This is a shell and tube heat exchanger made of carbon steel which condenses fractions of the distillate of its respective distillation column so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It has heat transfer area of 1639 ft^2.

CND-501

This is a shell and tube heat exchanger made of carbon steel which condenses fractions of the distillate of its respective distillation column so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It has heat transfer area of 1585 ft^2.

CND-502

This is a shell and tube heat exchanger made of carbon steel which condenses fractions of the distillate of its respective distillation column so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It has heat transfer area of 13760 ft^2.

CND-503

This is a shell and tube heat exchanger made of carbon steel which condenses fractions of the distillate of its respective distillation column so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It has heat transfer area of 18473 ft^2.

Columns

DC-500

FOB Cost: $528,900

This is a distillation tower separating toluene in the light key from para-xylene in the heavy key. The distillate is sent to transalkylation for further conversion, while the bottoms is further distilled to isolate xylenes. The tower has tangent-to-tangent height 68 feet and diameter 16.5 feet, in included 28 trays spaced 2 feet apart. The column operates with a reflux ratio of 0.809, is fed on tray 15, and has an average tray efficiency 0.58. The operating temperature is 296 degrees Fahrenheit. 96% of the light key and 8% of the heavy key were recovered in the distillate.

DC-501

FOB Cost: $458,000

This is a distillation tower separating xylenes in the light key from isopropylbenzene in the heavy key. The distillate is sent to crystallization for further para-xylene isolation, while the bottoms is burned in the furnace. The tower has tangent-to-tangent height 94 feet and diameter 12.5 feet, in included 41 trays spaced 2 feet apart. The column operates with a reflux ratio of 3.0, is fed on tray 16, and has an average tray efficiency 0.64. The operating temperature is 332 degrees Fahrenheit. 96% of the light key and 17% of the light key were recovered in the distillate.

DC-502
FOB Cost: $580,000

This is a distillation tower separating benzene in the light key from toluene in the heavy key. The distillate is sent to column DC-503 to isolate benzene, while the bottoms is recycled for further recovery of xylenes. The tower has tangent-to-tangent height 48 feet and diameter 22.5 feet, in included 18 trays spaced 2 feet apart. The column operates with a reflux ratio of 12, is fed on stage 15, and has an average tray efficiency 0.56. The operating temperature is 239 degrees Fahrenheit. 98% of the light key and 1% of the heavy key were recovered in the distillate.

DC-503
FOB Cost: $117,600

This is a distillation tower separating alkanes in the light key from benzene in the heavy key. The distillate is burned in the furnace, while the bottoms sold for profit. The tower has tangent-to-tangent height 48 feet and diameter 22.5 feet, in included 18 trays spaced 2 feet apart. The column operates with a reflux ratio of 3, is fed on stage 16, and has an average tray efficiency 0.49. The operating temperature is 176 degrees Fahrenheit. 99% of the light key and 4% of the light key were recovered in the distillate.

Drums:

AD-500
FOB Cost: $27,700

This is a carbon steel horizontal drum which handles the accumulated condensate from the condenser of the column. It has a volume of 3022 gallons and diameter of 17 feet.

AD-501
FOB Cost: $35,100

This is a carbon steel horizontal drum which handles the accumulated condensate from the condenser of the column. It has a volume of 5089 gallons and diameter of 20.5 feet.

AD-502

FOB Cost: $51,600

This is a carbon steel horizontal drum which handles the accumulated condensate from the condenser of the column. It has a volume of 13326 gallons and diameter of 28 feet.

AD-503

FOB Cost: $18,700

This is a carbon steel horizontal drum which handles the accumulated condensate from the condenser of the column. It has a volume of 1128 gallons and diameter of 12 feet.

Section 600: Transalkylation

Pumps

P-601

FOB Cost: $54,200

This is a centrifugal carbon steel pump which pumps sorbitol solution from heat exchanger HX-601 to mixer MIX-502. It operates at 182 degrees Fahrenheit and moves 85780 lb/hrr of fluid with density 48.5 lb/ft^3. The pump generates a pressure increase of 2psi to combat frictional losses. The pump head is 5.9 feet. The pump uses 0.67kW of electricity and generates 0.89hp of brake power operating at 72.2% efficiency. These properties were determined using ASPEN for the specified 2psi pressure increase.

Heat Exchangers

HX-600

FOB Cost: $541,900

This is a shell and tube heat exchanger made of 304 stainless steel. It heats 214922 lb/hr of toluene-rich distillate from DC-500 from 209 to 850 degrees Fahrenheit using molten salt. It transfers a heat duty of 71.35 million BTU/hr. It is 20ft long. The above was calculated by ASPEN based on the specified outlet temperature of the sorbitol necessary for condensation.

HX-601

FOB Cost: $119,400

This is a shell and tube heat exchanger made of carbon steel. It cools 2406 lb/hr transalkylation product from 352 to 182 degrees Fahrenheit using 568330 lb/hr of cooling water heated from 90 to 120 Fahrenheit. It transfers a heat duty of 18.59 million BTU/hr over 1536 ft^2 of heat transfer area and was designed assuming an overall heat coefficient of 80 BTU/hr-ft^2-^oF. It is 20ft long. The above was calculated by ASPEN based on the assumed overall heat transfer coefficient, a specified minimum temperature approach of 50 degrees Fahrenheit, and a specified hot stream outlet temperature of 182 degrees Fahrenheit, suitable for entry into DC-502.

Reactors

R-600

FOB Cost: $567,800

This is a low alloy steel packed-bed catalytic reactor that hosts the transalkylation reaction, converting toluene into saleable para-xylene and benzene. The reactor handles 214922 pounds of feed per hour and operates at a temperature of 850 degrees Fahrenheit. It has a volume of 9254 gallons, of which 6477 gallons is working volume. It is 28 feet tall and 7.5 feet in diameter.

CAT-600

Purchase Cost, including Lifetime Reloading: $6,065,700

Transalkylation is catalyzed by zeolite catalyst, similar to the catalyzed condensation. In Example 2 of US Patent 6323381, a “selectivated large crystal HZSM-5 was used.” This catalyst has a Si/Al ratio of 70 to 1. Although no further specifics were given, the catalyst was assumed similar enough to the condensation catalyst that both could be ordered together in order to achieve economies of scale. Information and assumptions applied to pricing for the condensation catalyst were also applied to the transalkylation catalyst. To make up for the relatively rapid deactivation of the catalyst it possible to add a column of new catalyst to continuously pump catalyst into the reactor while filtering out older catalyst.

To calculate the same costs of the catalyst market pricing for H_4SiO_4 and Na_2AlO_2were used. Using the data given in the patent, and the assumption that the feed was 100% toluene a WHSV of 5.2 hr^{-1} was determined. Using this value for WHSV and the known amount of feed to the reactor, the amount of catalyst needed was determined to be 12.6 million grams of catalyst per charge. From this, it is known that to achieve a 30 to 1 ration of Si to Al which implies that a ratio of 70:1 of H_4SiO_4: Na_2AlO_2 is needed to achieve this goal. So to determine the overall pricing of the catalyst, 12.6 million was multiplied by 70/71 and the market price of H_4SiO_4 per gram and added to 12.6 million multiplied by 1/71 and the market price of Na_2AlO_2 per gram. This yields a value of $0.25 million per charge. It was then assumed to have a discount to 25% for bulk pricing options which gives a value of $0.06 million per charge.

The estimated deactivation of the catalyst, 13.29 grams/lbmol reactant was used to determine the deactivation of the catalyst. Since the flow rate of the reactant is known to determine the amount of deactivated catalyst in an hour the hourly lbmol flow rate is multiplied by 13.29. This yields a result of grams of deactivated catalyst per hour. The hourly deactivation of catalyst is 20,883 grams per hour. The price of the hourly deactivated catalyst is determined via the same process as before and this value is multiplied by 24 hours and 365 days to get a yearly cost. The cost was determined to be $3.67 million and with the discount 25% bulk pricing $0.92 million. See calculation SC-C04.

Section 700: Furnace & Heating Cycles

Storage Tanks

ST-700

FOB Cost: $719,833

ST-700 is a spherical pressure vessel for the storage of Dowtherm A, as part of the Dowtherm A heating cycle. To store 532,000 pounds of Dowtherm A with a residence time of six minutes and a capacity usage of 70%, a tank volume of 124,000 gallons is required. Low-alloy steel is an appropriate material since the heating fluid is stored saturated at 698^0F and 93.69 psia. See SC-701 for volume and pricing calculations for storage vessels.

ST-701
FOB Cost: $658,751

This unit is a cone-roof tank for the storage of Solar Salt, as part of the molten salt heating cycle. With a suggested residence time of six hours and capacity usage of 70%, the tank has a volume of 639,300 gallons. The heating fluid is stored at 900^0F and 3 psig. Due to the high operating temperature, the tank must be constructed from stainless steel. See SC-701 for calculations.

Furnaces
FRN-700
FOB Cost: $3,253,196

This unit is a stainless steel molten salt fired heater, which provides the heat for the molten salt heating cycle. An inlet stream of molten salt, S-723, absorbs 62 MBtu/h from this furnace and increases 200 degrees in temperature to 1100^0F. This temperature rise is suggested by the materials specifications for Solar Salt (Appendix D) and 900^0F is selected as the lower bound because it is the lowest temperature that does not violate the requirements of HX-600. Heuristic 26 of PPDP suggests a minimum approach temperature for fired heaters of flue temperature 250^0F above inlet. Therefore, the air intake (S-705) is adjusted to 26,000 lbmol/h such that the flue gas (S-706) exits at 1150^0F. Fortunately, this temperature is below the maximum and above the minimum suggested by PPDP Heuristic 30, which allows complete combustion and avoids any condensation. However, the extreme conditions require stainless steel, rather than carbon steel. The furnace operates at atmospheric pressure. See SC-702 for pricing calculations.

FRN -701, FRN -702
FOB Cost: $5,186,584

About 532 MBtu/h of Dowtherm A latent heat is required to heat the condensation inlet stream, S-405, to 698^{0}F. Since the upper limit of heat transfer on commercial fired heaters is 340 MBtu/h (p.482, PPDP), two Dowtherm A furnaces are required for this phase-change process. Although close to the upper limit, carbon steel furnaces are acceptable in this range of operating temperatures (Appendix 23, PPDP). Again following Heuristic 26 of PPDP, an air intake of about 135,000 lbmol/h is specified to ensure the flue gas leaves at 1000^{0}F. The furnaces operate at atmospheric pressure. See SC-702 for pricing calculations.

FRN -703
FOB Cost: $1,495,615

This carbon steel steam boiler provides the steam for heating units RB-500, RB-501, RB-502, RB-503, HX-301, and WC-500. The total energy required from this steam is 319 MBtu/h, and it is provided by evaporating and condensing water from stream S-526. The furnace operates at 405^{0}F and 260 psig in order to provide steam at the pressure required for HX-301, which is the maximum. An air flow rate of 290,000 lbmol/h sets the flue gas exit temperature at about 500^{0}F, which satisfies Heuristic 26 (PPDP). See SC-702 for pricing calculations.

Pumps
P-700, P-701
FOB Cost: $481,700

This is a centrifugal pump Dowtherm A loop that operates at a rate of 8517 gpm. The energy required is 7.84 kW, given an efficiency of 0.859. This provides 79.13 ft of head with a pressure increase of 23.5 psi. This pressure increase was specified to satisfy Heuristic 38, which allows for a pressure drop due to liquid flow through 100 ft of pipe; and Heuristic 31, which dictates a 20 psi allowance for drop through a furnace and a 1.5 psi drop for phase changes in a heat exchanger (PPDP).

P-702
FOB Cost: $854,100

This is a centrifugal pump in the Dowtherm A loop that operates at a rate of 16111 gpm. The energy required is 29.65 kW, given an efficiency of 0.859. This provides 12.74 ft of head with a pressure increase of 4 psi. This pressure increase was specified to satisfy Heuristic 38 (PPDP), which allows for a pressure drop due to liquid flow through 100 ft of each of two pipes, after splitting.

P-703

FOB Cost: $114,000

This is a centrifugal pump in the molten salt loop that operates at a rate of 2599 gpm. The energy required is 60.98 kW, given an efficiency of 0.826. This provides 163.80 ft of head with a pressure increase of 70.5 psi. This pressure increase was specified to satisfy Heuristics 31 and 38 (PPDP), while also increasing the flow to operating pressure of 50 psig from 3 psig. Note that molten salts are not available in ASPEN and this pump was sized using milk as an estimate since the viscosities of milk and Solar Salt are within a few millipoise of each other.

P-704

FOB Cost: $94,100

This is a centrifugal pump in the molten salt loop that operates at a rate of 2560 gpm. The energy required is 2.49 kW, given an efficiency of 0.826. This provides 4.65 ft of head with a pressure increase of 2 psi. This pressure increase was specified to satisfy Heuristic 38 (PPDP). Note that molten salts are not available in ASPEN and this pump was sized using milk as an estimate since the viscosities of milk and Solar Salt are within a few millipoise of each other.

P-705(IN), P-705(IN)-2

FOB Cost: $4,500

This is a centrifugal pump in the HX-301 steam loop that operates at a rate of 88 gpm. The energy required is 0.14 (0.21) kW, given an efficiency of 0.506. This provides 4.68 (7.02) ft of head with a pressure increase of 2 psi (3 psi). This pressure increase was specified to satisfy Heuristics 31 and 38 (PPDP).

P-706(IN)

FOB Cost: $5,200

This is a centrifugal pump in the RB-500 steam loop that operates at a rate of 192 gpm. The energy required is 0.25 (0.38) kW, given an efficiency of 0.604. This provides 4.68 (7.02) ft of head with a pressure increase of 2 psi (3 psi). This pressure increase was specified to satisfy Heuristics 31 and 38 (PPDP).

P-707(IN)

FOB Cost: $4,700

This is a centrifugal pump in the RB-501 steam loop that operates at a rate of 118 gpm. The energy required is 0.17 (0.26) kW, given an efficiency of 0.545. This provides 4.68 (7.02) ft of head with a pressure increase of 2 psi (3 psi). This pressure increase was specified to satisfy Heuristics 31 and 38 (PPDP).

P-708(IN)

FOB Cost: $6,300

This is a centrifugal pump in the RB-502 steam loop that operates at a rate of 354 gpm. The energy required is 0.47 (0.63) kW, given an efficiency of 0.671. This provides 4.68 (7.02) ft of head with a pressure increase of 2 psi (3 psi). This pressure increase was specified to satisfy Heuristics 31 and 38 (PPDP).

P-709(IN)

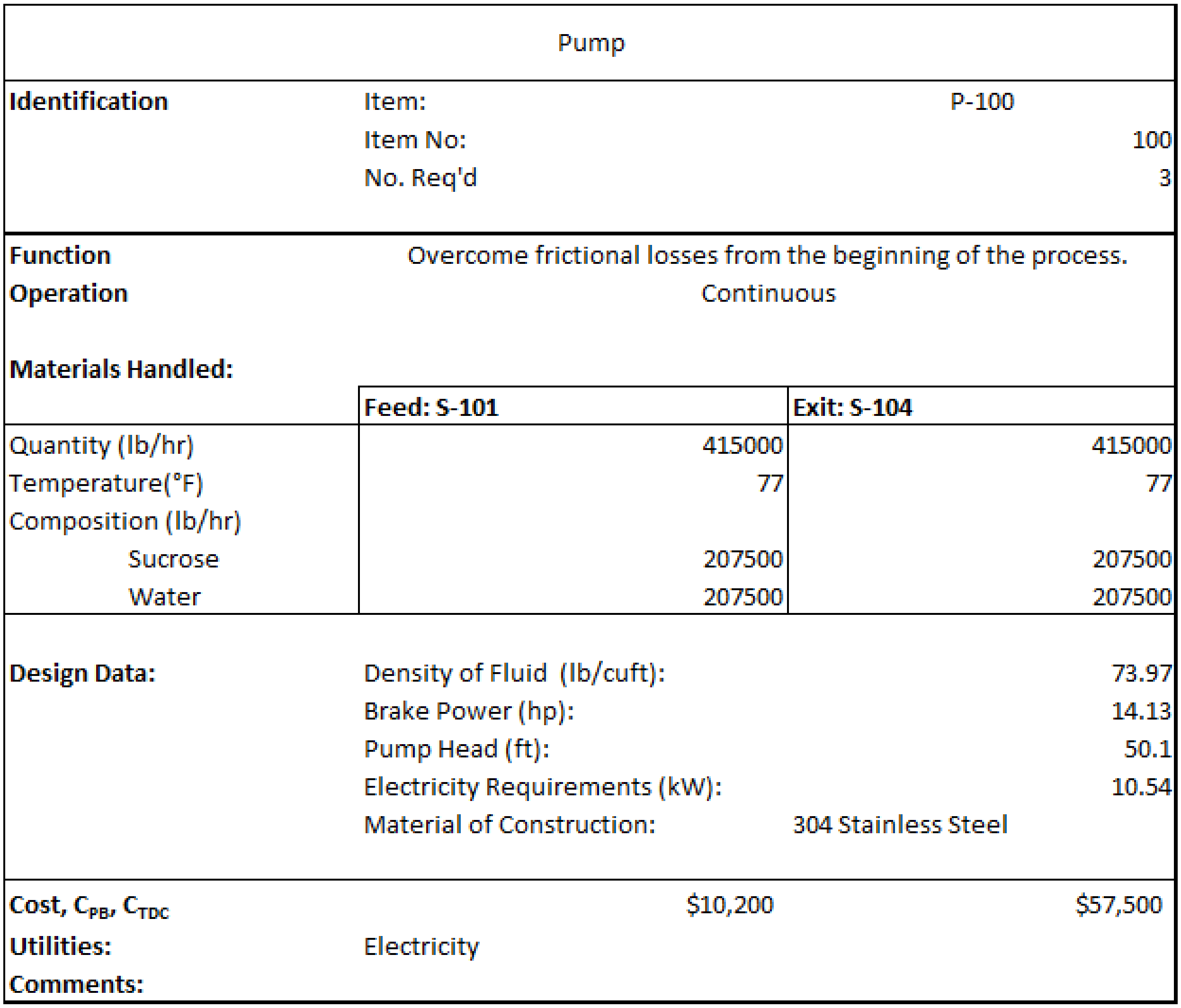
FOB Cost: $4,300

This is a centrifugal pump in the RB-503 steam loop that operates at a rate of 38 gpm. The energy required is 0.08 (0.12) kW, given an efficiency of 0.385. This provides 4.68 (7.02) ft of head with a pressure increase of 2 psi (3 psi). This pressure increase was specified to satisfy Heuristics 31 and 38 (PPDP).

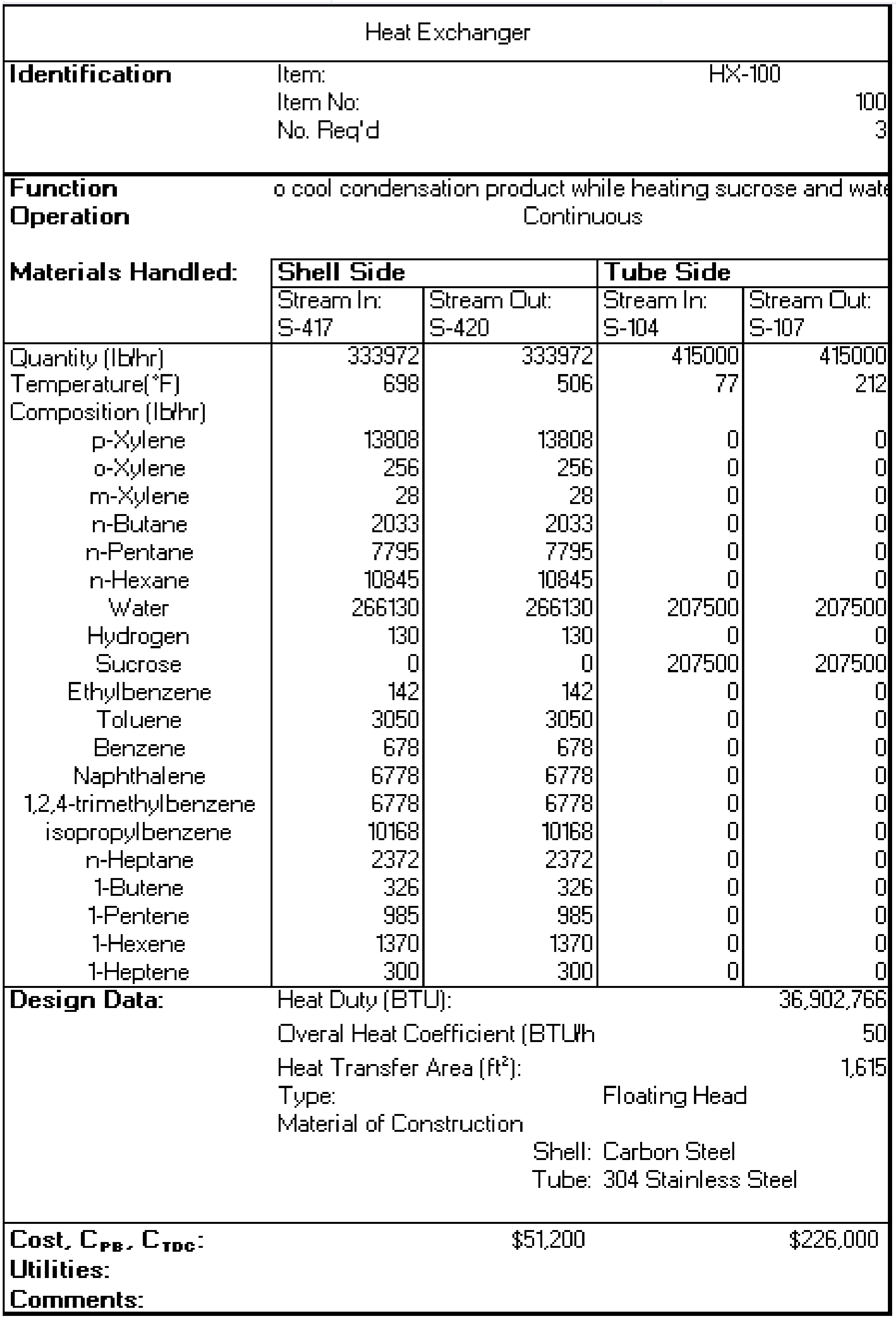
Section VI

Specification Sheets

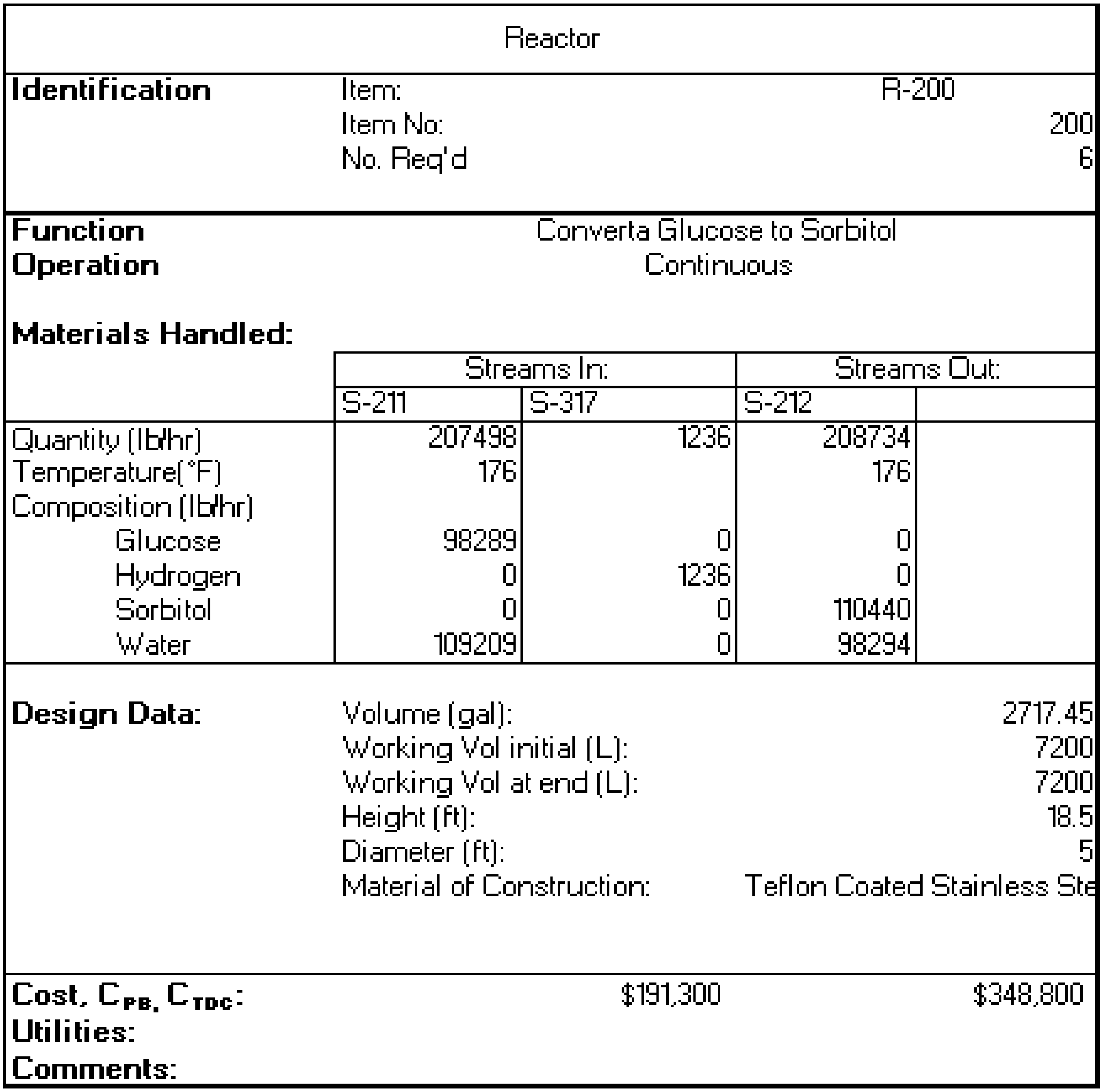
VI. SPECIFICATION SHEETS



	Pump	
Identification	Item:	P-100
	Item No:	100
	No. Req'd	3
Function	Overcome frictional losses from the beginning of the process.	
Operation	Continuous	
Materials Handled:		
	Feed: S-101	**Exit: S-104**
Quantity (lb/hr)	415000	415000
Temperature(°F)	77	77
Composition (lb/hr)		
Sucrose	207500	207500
Water	207500	207500
Design Data:	Density of Fluid (lb/cuft):	73.97
	Brake Power (hp):	14.13
	Pump Head (ft):	50.1
	Electricity Requirements (kW):	10.54
	Material of Construction:	304 Stainless Steel
Cost, C_{PB}, C_{TDC}	$10,200	$57,500
Utilities:	Electricity	
Comments:		



		Heat Exchanger		
Identification	Item:		HX-100	
	Item No:			100
	No. Req'd			3
Function	o cool condensation product while heating sucrose and wat			
Operation		Continuous		
Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In: S-417	Stream Out: S-420	Stream In: S-104	Stream Out: S-107
Quantity (lb/hr)	333972	333972	415000	415000
Temperature(°F)	698	506	77	212
Composition (lb/hr)				
p-Xylene	13808	13808	0	0
o-Xylene	256	256	0	0
m-Xylene	28	28	0	0
n-Butane	2033	2033	0	0
n-Pentane	7795	7795	0	0
n-Hexane	10845	10845	0	0
Water	266130	266130	207500	207500
Hydrogen	130	130	0	0
Sucrose	0	0	207500	207500
Ethylbenzene	142	142	0	0
Toluene	3050	3050	0	0
Benzene	678	678	0	0
Naphthalene	6778	6778	0	0
1,2,4-trimethylbenzene	6778	6778	0	0
isopropylbenzene	10168	10168	0	0
n-Heptane	2372	2372	0	0
1-Butene	326	326	0	0
1-Pentene	985	985	0	0
1-Hexene	1370	1370	0	0
1-Heptene	300	300	0	0
Design Data:	Heat Duty (BTU):			36,902,766
	Overal Heat Coefficient (BTU/h			50
	Heat Transfer Area (ft^2):			1,615
	Type:		Floating Head	
	Material of Construction			
		Shell:	Carbon Steel	
		Tube:	304 Stainless Steel	
Cost, C_{PB}, C_{TDC}:		$51,200		$226,000
Utilities:				
Comments:				



Reactor

Identification
Item: R-200
Item No: 200
No. Req'd 6

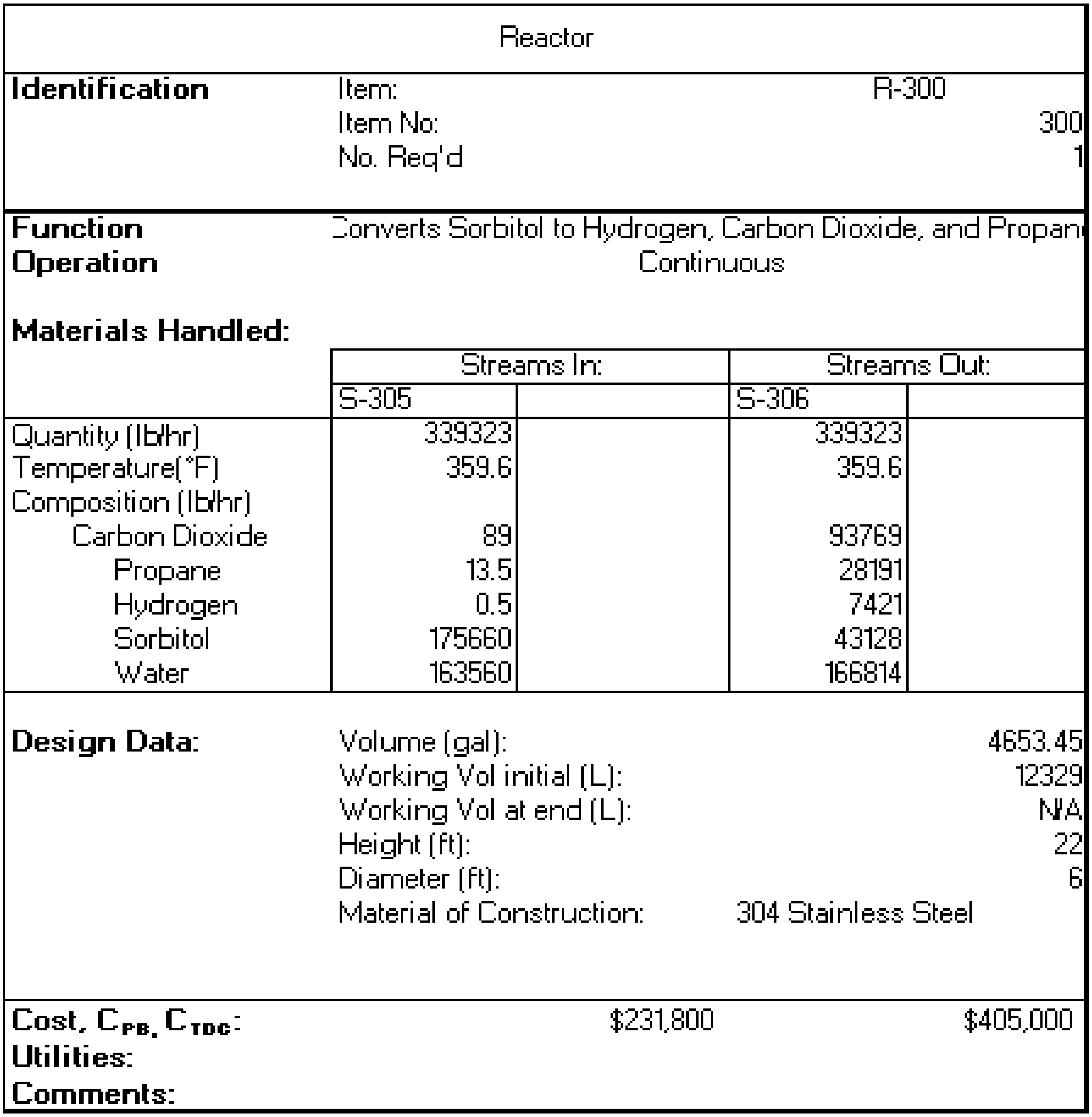
Function Converta Glucose to Sorbitol
Operation Continuous

Materials Handled:

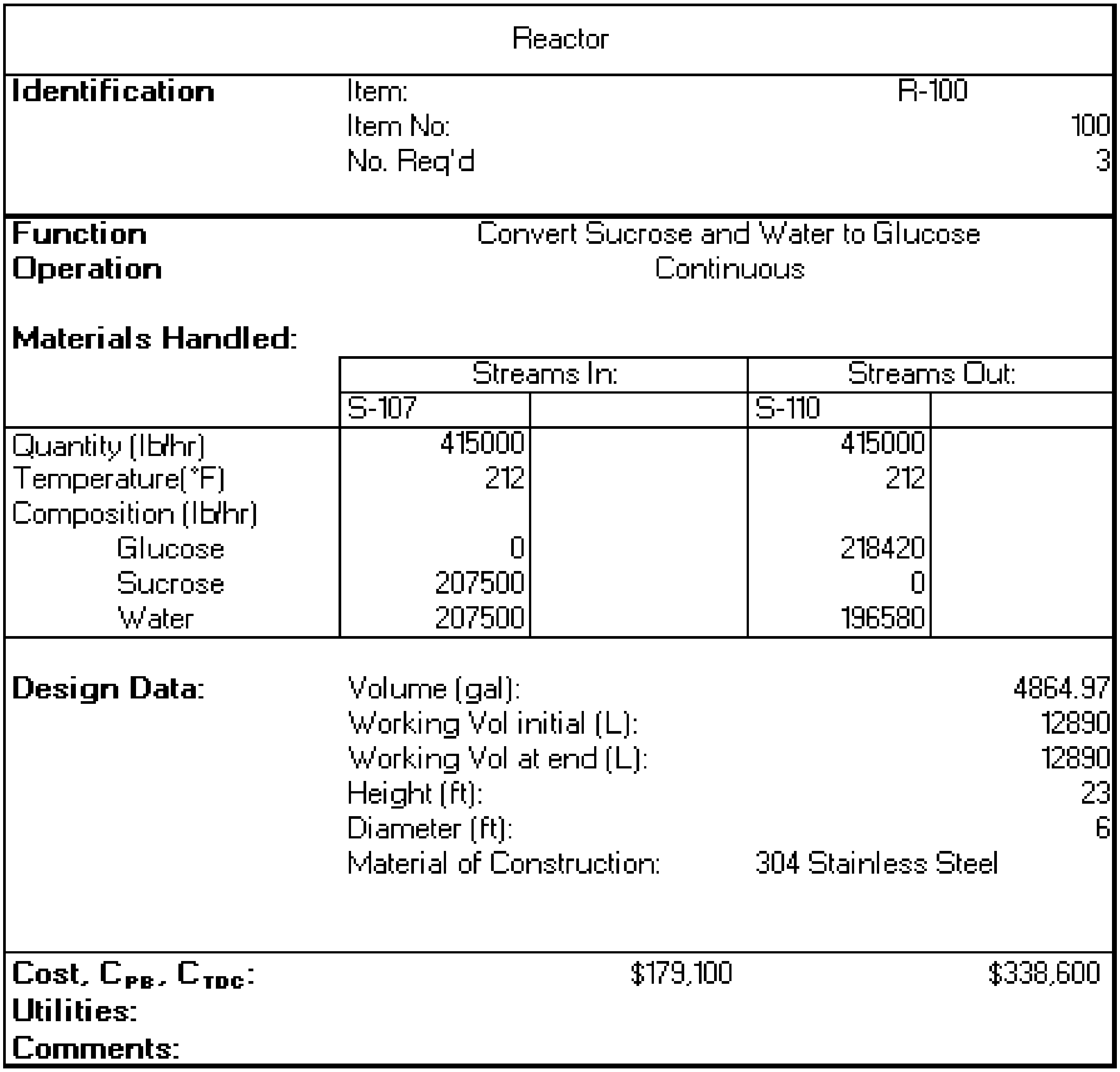
	Streams In:		Streams Out:	
	S-211	S-317	S-212	
Quantity (lb/hr)	207498	1236	208734	
Temperature(°F)	176		176	
Composition (lb/hr)				
Glucose	98289	0	0	
Hydrogen	0	1236	0	
Sorbitol	0	0	110440	
Water	109209	0	98294	

Design Data:
Volume (gal): 2717.45
Working Vol initial (L): 7200
Working Vol at end (L): 7200
Height (ft): 18.5
Diameter (ft): 5
Material of Construction: Teflon Coated Stainless Ste

Cost, C_{PB}, C_{TDC}: $191,300 $348,800
Utilities:
Comments:



		Reactor		
Identification	Item:		R-300	
	Item No:			300
	No. Req'd			1
Function	Converts Sorbitol to Hydrogen, Carbon Dioxide, and Propan			
Operation		Continuous		
Materials Handled:				
	Streams In:		Streams Out:	
	S-305		S-306	
Quantity (lb/hr)	339323		339323	
Temperature(°F)	359.6		359.6	
Composition (lb/hr)				
Carbon Dioxide	89		93769	
Propane	13.5		28191	
Hydrogen	0.5		7421	
Sorbitol	175660		43128	
Water	163560		166814	
Design Data:	Volume (gal):			4653.45
	Working Vol initial (L):			12329
	Working Vol at end (L):			N/A
	Height (ft):			22
	Diameter (ft):			6
	Material of Construction:		304 Stainless Steel	
Cost, C_{PB}, C_{TDC}:		$231,800		$405,000
Utilities:				
Comments:				



Reactor

Identification	Item:	R-100
	Item No:	100
	No. Req'd	3

Function Convert Sucrose and Water to Glucose

Operation Continuous

Materials Handled:

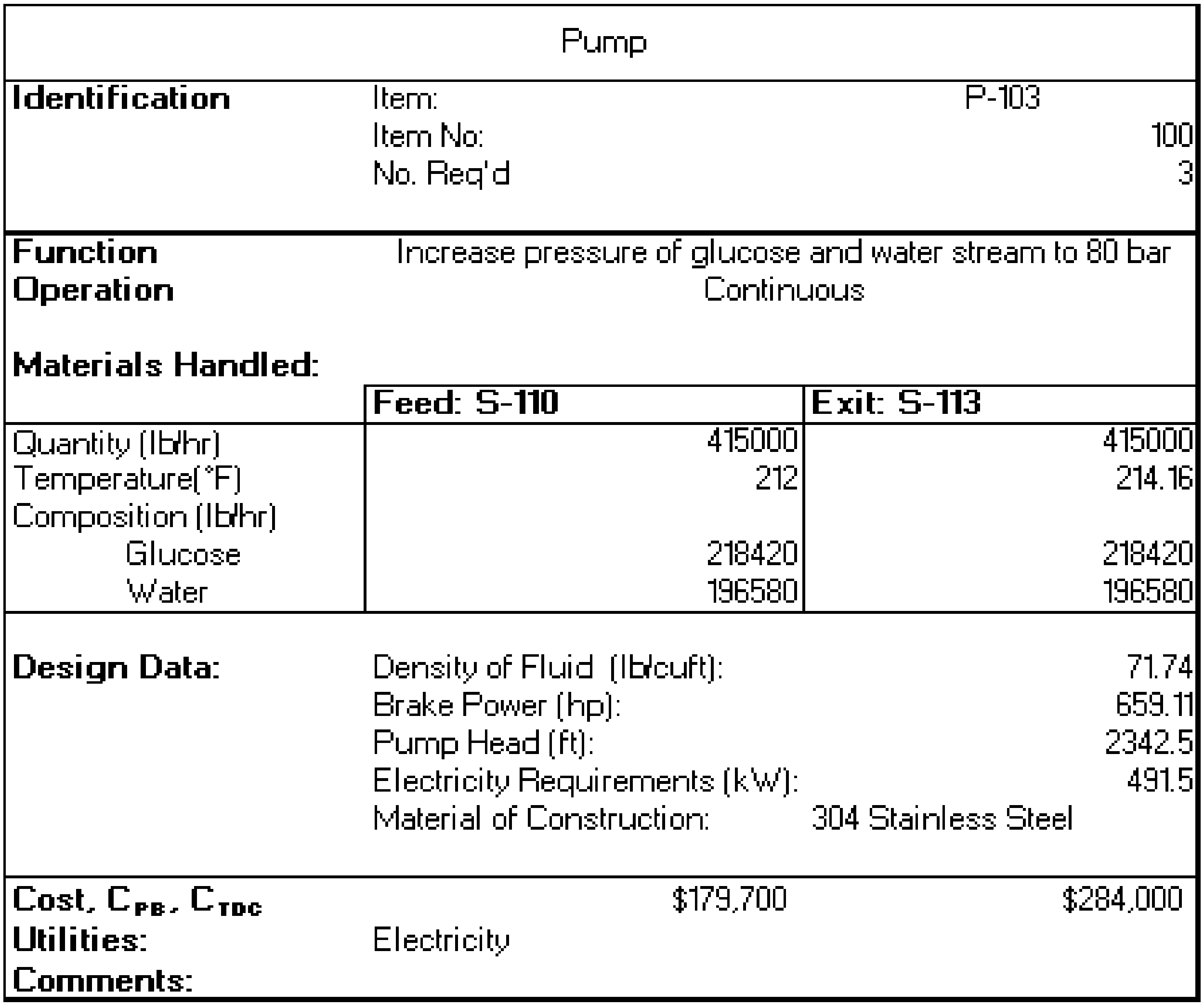
	Streams In:		Streams Out:	
	S-107		S-110	
Quantity (lb/hr)	415000		415000	
Temperature(°F)	212		212	
Composition (lb/hr)				
Glucose	0		218420	
Sucrose	207500		0	
Water	207500		196580	

Design Data:	Volume (gal):	4864.97
	Working Vol initial (L):	12890
	Working Vol at end (L):	12890
	Height (ft):	23
	Diameter (ft):	6
	Material of Construction:	304 Stainless Steel

Cost, C_{PB}, C_{TDC}: $179,100 $338,600

Utilities:

Comments:



	Pump	
Identification	Item:	P-103
	Item No:	100
	No. Req'd	3
Function	Increase pressure of glucose and water stream to 80 bar	
Operation	Continuous	
Materials Handled:		
	Feed: S-110	**Exit: S-113**
Quantity (lb/hr)	415000	415000
Temperature(°F)	212	214.16
Composition (lb/hr)		
Glucose	218420	218420
Water	196580	196580
Design Data:	Density of Fluid (lb/cuft):	71.74
	Brake Power (hp):	659.11
	Pump Head (ft):	2342.5
	Electricity Requirements (kW):	491.5
	Material of Construction:	304 Stainless Steel
Cost, C_{PB}, C_{TDC}	$179,700	$284,000
Utilities:	Electricity	
Comments:		

	Pump	
Identification	Item:	P-200
	Item No:	200
	No. Req'd	6
Function	ring the glucose and water stream to the hydrogenation rea	
Operation	Continuous	
Materials Handled:	**Feed: S-200**	**Exit: S-211**
Quantity (lb/hr)	207498	207498
Temperature(°F)	173.75	173.754
Composition (lb/hr)		
Glucose	109209	109209
Water	98289	98289
Design Data:	Density of Fluid (lb/cuft):	73.37
	Brake Power (hp):	0.61
	Pump Head (ft):	3.9
	Electricity Requirements (kW):	0.45
	Material of Construction:	304 Stainless Steel
Cost, C_{PB}, C_{TDC}	$6,500	$52,800
Utilities:	Electricity	
Comments:		

	Pump	
Identification	Item:	P-206
	Item No:	206
	No. Req'd	6
Function	To bring the sorbitol and water stream to the stream mixer.	
Operation	Continuous	
Materials Handled:	**Feed: S-212**	**Exit: S-218**
Quantity (lb/hr)	208734	207296
Temperature(°F)	173.75	173.754
Composition (lb/hr)		
Sorbitol	110440	109680
Water	98294	97616
Design Data:	Density of Fluid (lb/cuft):	73.47
	Brake Power (hp):	0.61
	Pump Head (ft):	3.9
	Electricity Requirements (kW):	0.45
	Material of Construction:	304 Stainless Steel
Cost, C_{PB}, C_{TDC}	$6,500	$52,800
Utilities:	Electricity	
Comments:		

	Pump	
Identification	Item:	P-300
	Item No:	300
	No. Req'd	1
Function	bring the mixed sorbitol stream to a heat exchanger for heat	
Operation	Continuous	
Materials Handled:		
	Feed: S-303	**Exit: S-304**
Quantity (lb/hr)	339323	339323
Temperature(°F)	253.57	253.59
Composition (lb/hr)	339323	339323
Sorbitol	175660	175660
Hydrogen	0.5	0.5
Carbon Dioxide	89	89
Propane	13.5	13.5
Water	163560	163560
Design Data:	Density of Fluid (lb/cuft):	69.84
	Brake Power (hp):	3.39
	Pump Head (ft):	14.4
	Electricity Requirements (kW):	2.53
	Material of Construction:	304 Stainless Steel
Cost, C_{PB}, C_{TDC}	$8,500	$57,900
Utilities:	Electricity	
Comments:		

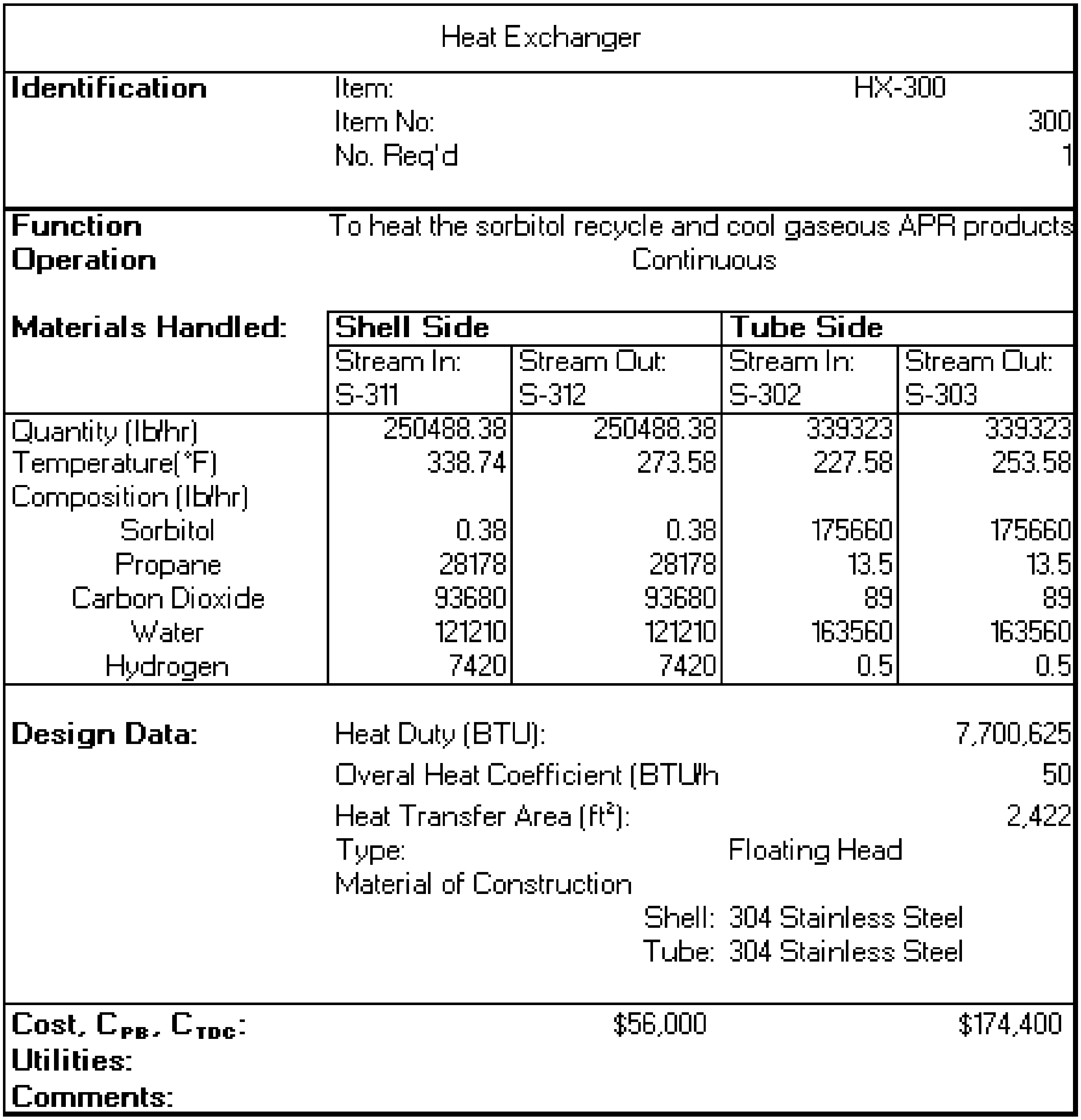
	Pump	
Identification	Item:	P-301
	Item No:	301
	No. Req'd	1
Function	To bring the sorbitol recycle to the sorbitol mixer.	
Operation	Continuous	
Materials Handled:		
	Feed: S-308	**Exit: S-309**
Quantity (lb/hr)	88840	88840
Temperature(°F)	359.6	359.61
Composition (lb/hr)		
Sorbitol	43128	43128
Hydrogen	0.5	0.5
Carbon Dioxide	89	89
Propane	13.5	13.5
Water	45609	45609
Design Data:	Density of Fluid (lb/cuft):	63.92
	Brake Power (hp):	0.34
	Pump Head (ft):	4.5
	Electricity Requirements (kW):	0.25
	Material of Construction:	304 Stainless Steel
Cost, C_{PB}, C_{TDC}	$5,200	$39,500
Utilities:	Electricity	
Comments:		

Pump

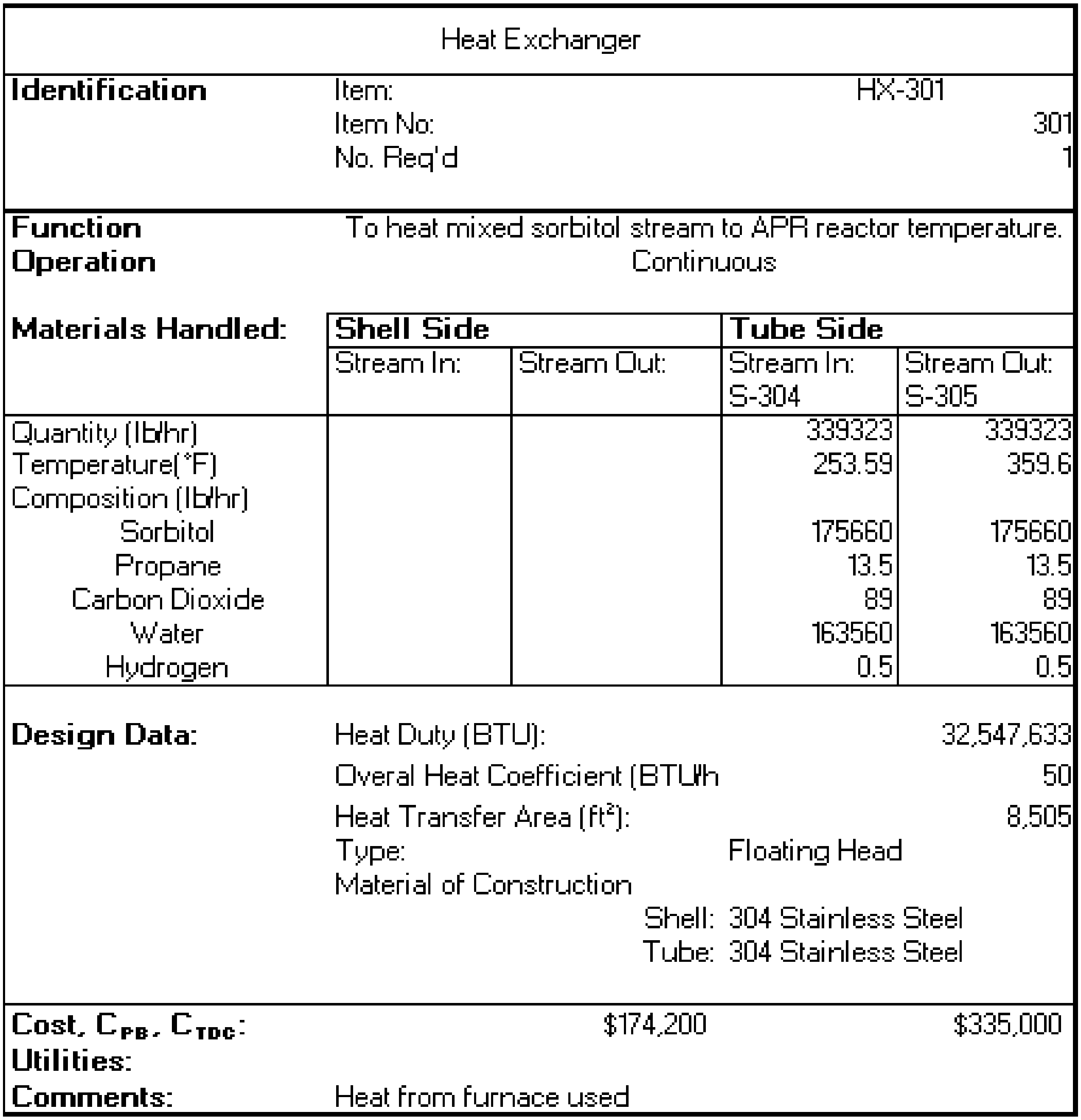
Identification	Item:		P-302
	Item No:		302
	No. Req'd		1
Function	bring the mixed sorbitol stream to a heat exchanger for heat		
Operation	Continuous		
Materials Handled:		**Feed: S-301**	**Exit: S-302**
Quantity (lb/hr)		339323	339323
Temperature(°F)		227.58	227.59
Composition (lb/hr)			
Sorbitol		175660	175660
Hydrogen		0.5	0.5
Carbon Dioxide		89	89
Propane		13.5	13.5
Water		163560	163560
Design Data:	Density of Fluid (lb/cuft):		70.93
	Brake Power (hp):		2.39
	Pump Head (ft):		10.2
	Electricity Requirements (kW):		1.78
	Material of Construction:	304 Stainless Steel	
Cost, C_{PB}, C_{TDC}		$8,400	$57,700
Utilities:	Electricity		
Comments:			

Heat Exchanger

Identification	Item:		HX-200	
	Item No:			200
	No. Req'd			1
Function	cool glucose and water to hydrogenation reactor temperatu			
Operation	Continuous			
Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In: S-119	Stream Out: S-226	Stream In: CW-100	Stream Out: CW-101
Quantity (lb/hr)	1245000	1245000	1272600	1272600
Temperature(°F)	214.16	175.73	90	120
Composition (lb/hr)				
Water	589730	589730	1272600	1272600
Glucose	655270	655270	0	0
Design Data:	Heat Duty (BTU):			40,777,165
	Overal Heat Coefficient (BTU/h			50
	Heat Transfer Area (ft^2):			9,057
	Type:		Floating Head	
	Material of Construction			
		Shell:	304 Stainless Steel	
		Tube:	304 Stainless Steel	
Cost, C_{PB}, C_{TDC}:		$286,600		$485,300
Utilities:	Cooling Water			
Comments:				



Heat Exchanger				
Identification	Item:		HX-300	
	Item No:			300
	No. Req'd			1
Function	To heat the sorbitol recycle and cool gaseous APR products			
Operation	Continuous			
Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In: S-311	Stream Out: S-312	Stream In: S-302	Stream Out: S-303
Quantity (lb/hr)	250488.38	250488.38	339323	339323
Temperature(°F)	338.74	273.58	227.58	253.58
Composition (lb/hr)				
Sorbitol	0.38	0.38	175660	175660
Propane	28178	28178	13.5	13.5
Carbon Dioxide	93680	93680	89	89
Water	121210	121210	163560	163560
Hydrogen	7420	7420	0.5	0.5
Design Data:	Heat Duty (BTU):			7,700,625
	Overal Heat Coefficient (BTU/h			50
	Heat Transfer Area (ft^2):			2,422
	Type:		Floating Head	
	Material of Construction			
		Shell:	304 Stainless Steel	
		Tube:	304 Stainless Steel	
Cost, C_{PB}, C_{TDC}:		$56,000		$174,400
Utilities:				
Comments:				



Heat Exchanger

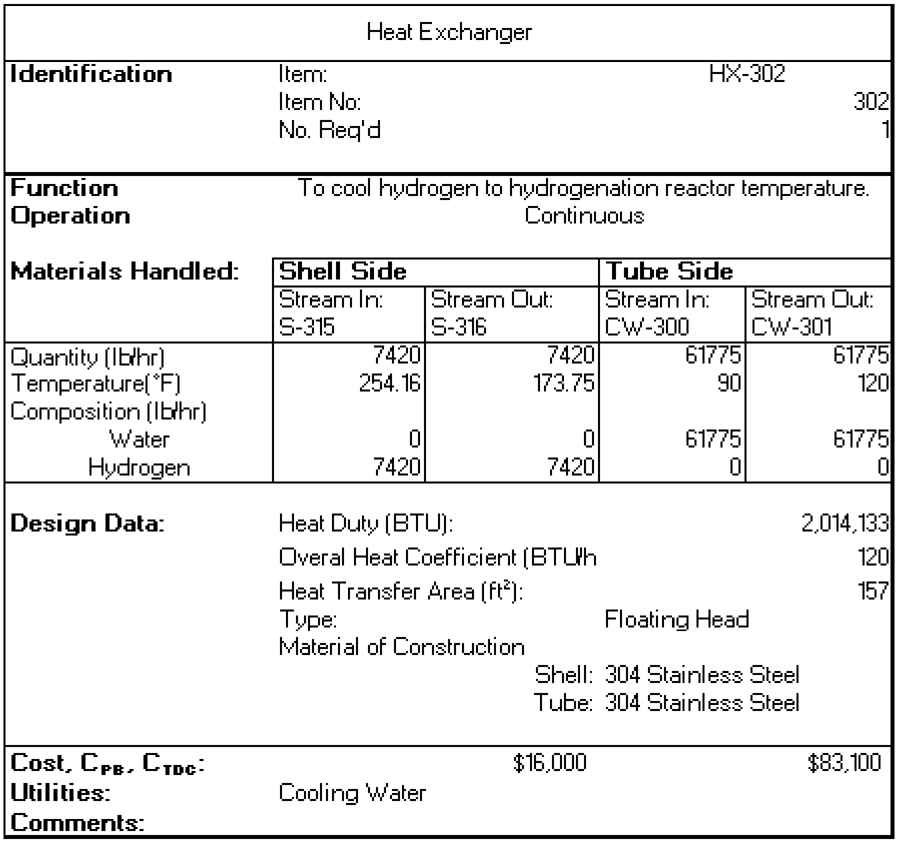
Identification	Item:	HX-301
	Item No:	301
	No. Req'd	1
Function	To heat mixed sorbitol stream to APR reactor temperature.	
Operation	Continuous	

Materials Handled:

	Shell Side		Tube Side	
	Stream In:	Stream Out:	Stream In: S-304	Stream Out: S-305
Quantity (lb/hr)			339323	339323
Temperature(°F)			253.59	359.6
Composition (lb/hr)				
Sorbitol			175660	175660
Propane			13.5	13.5
Carbon Dioxide			89	89
Water			163560	163560
Hydrogen			0.5	0.5

Design Data:	Heat Duty (BTU):	32,547,633
	Overal Heat Coefficient (BTU/h	50
	Heat Transfer Area (ft²):	8,505
	Type:	Floating Head
	Material of Construction	
	Shell:	304 Stainless Steel
	Tube:	304 Stainless Steel

Cost, C_{PB}, C_{TDC}:	$174,200	$335,000
Utilities:		
Comments:	Heat from furnace used	



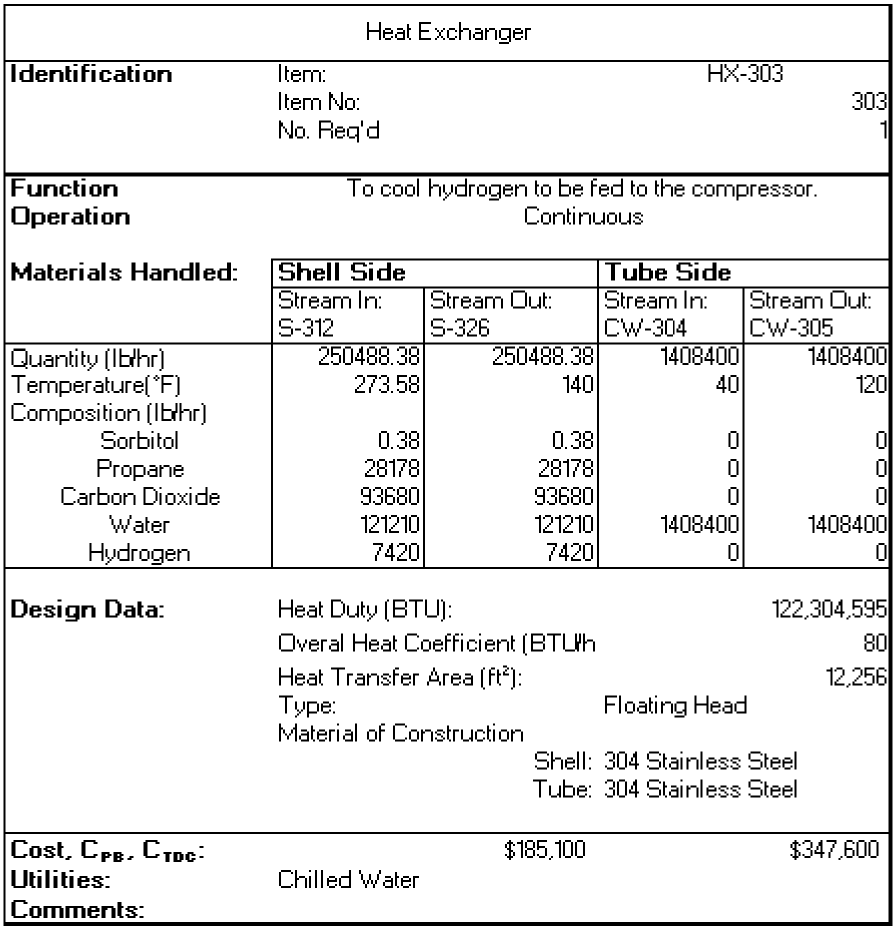
Heat Exchanger

Identification	Item:	HX-302
	Item No:	302
	No. Req'd	1
Function	To cool hydrogen to hydrogenation reactor temperature.	
Operation	Continuous	

Materials Handled:

	Shell Side		Tube Side	
	Stream In: S-315	Stream Out: S-316	Stream In: CW-300	Stream Out: CW-301
Quantity (lb/hr)	7420	7420	61775	61775
Temperature(°F)	254.16	173.75	90	120
Composition (lb/hr)				
Water	0	0	61775	61775
Hydrogen	7420	7420	0	0

Design Data:	Heat Duty (BTU):	2,014,133
	Overal Heat Coefficient (BTU/h	120
	Heat Transfer Area (ft^2):	157
	Type:	Floating Head
	Material of Construction	
	Shell:	304 Stainless Steel
	Tube:	304 Stainless Steel
Cost, C_{PB}, C_{TDC}:	$16,000	$83,100
Utilities:	Cooling Water	
Comments:		



Heat Exchanger

Identification	Item:	HX-303
	Item No:	303
	No. Req'd	1
Function	To cool hydrogen to be fed to the compressor.	
Operation	Continuous	

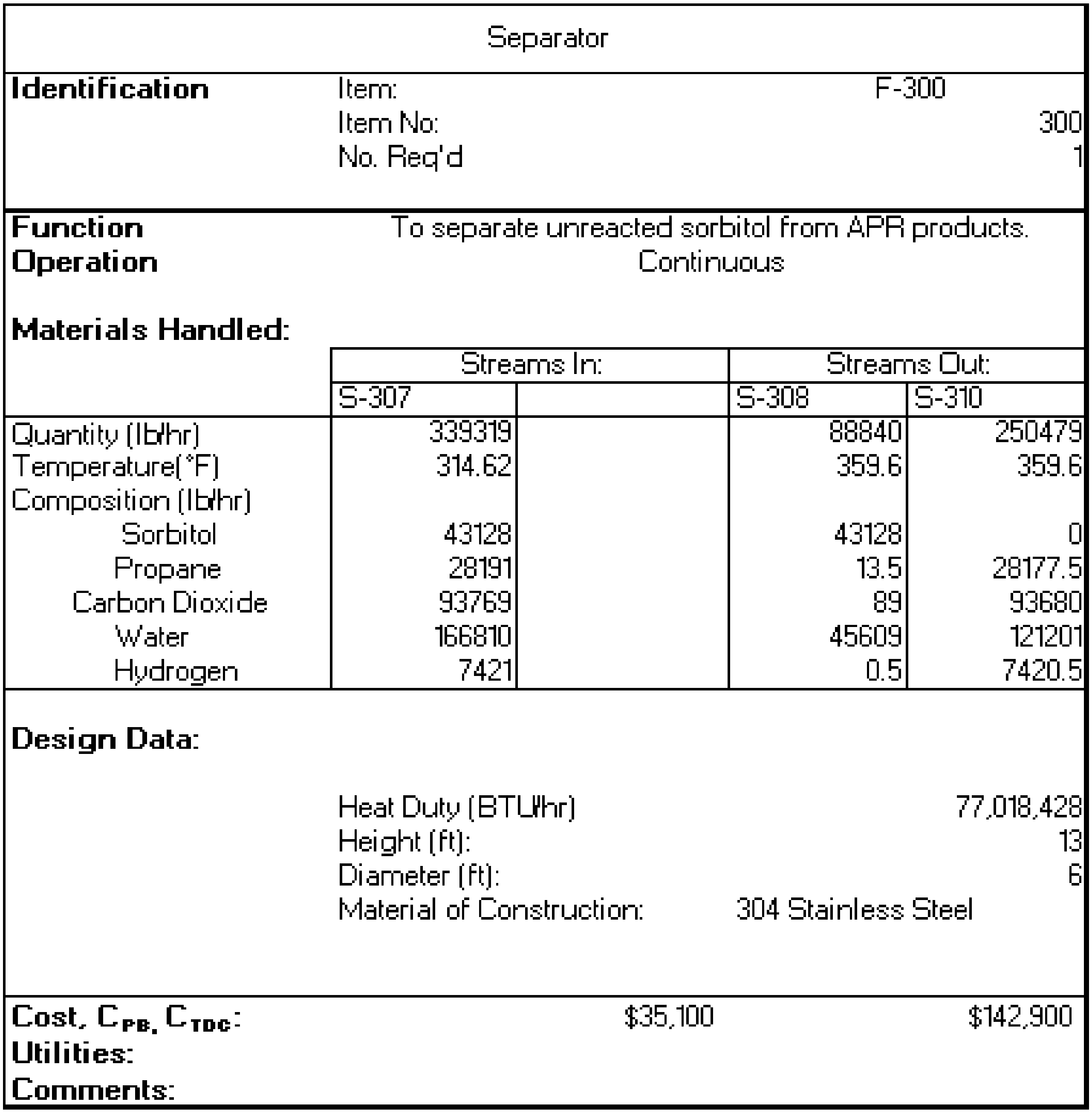
Materials Handled:

	Shell Side		Tube Side	
	Stream In: S-312	Stream Out: S-326	Stream In: CW-304	Stream Out: CW-305
Quantity (lb/hr)	250488.38	250488.38	1408400	1408400
Temperature(°F)	273.58	140	40	120
Composition (lb/hr)				
Sorbitol	0.38	0.38	0	0
Propane	28178	28178	0	0
Carbon Dioxide	93680	93680	0	0
Water	121210	121210	1408400	1408400
Hydrogen	7420	7420	0	0

Design Data:	Heat Duty (BTU):	122,304,595
	Overal Heat Coefficient (BTU/h	80
	Heat Transfer Area (ft^2):	12,256
	Type:	Floating Head
	Material of Construction	
	Shell:	304 Stainless Steel
	Tube:	304 Stainless Steel
Cost, C_{PB}, C_{TDC}:	$185,100	$347,600
Utilities:	Chilled Water	
Comments:		

Compressor		
Identification	Item:	CMP-300
	Item No:	300
	No. Req'd	1
Function	Compress hydrogen to hydrogenation reactor pressure.	
Operation	Continuous	
Materials Handled:		
	Feed: S-325	**Exit: S-314**
Quantity (lb/hr)	7420	7420
Temperature(°F)	140	1150
Composition (lb/hr)		
Hydrogen	7420	7420
Design Data:	Density of Fluid (lb/cuft):	0.0046014
	Total Work (hp):	22340
	Outlet Pressure (psia):	1164.3
	Net Cooling Duty (BTU/hr):	-30,562,822
	Material of Construction:	304 Stainless Steel
Cost, C_{PB}, C_{TDC}	$10,132,800	$10,868,300
Utilities:	Electricity	Cooling Water
Comments:		

Separator				
Identification	Item:			SEP-300
	Item No:			300
	No. Req'd			1
Function	essure swing adsorption to remove hydrogen from other gas			
Operation	Continuous			
Materials Handled:				
	Streams In:		Streams Out:	
	S-323		S-313	S-325
Quantity (lb/hr)	407409		399989	7420
Temperature(°F)	140		140	140
Composition (lb/hr)				
Propane	281770		281770	0
Carbon Dioxide	93678		93678	0
Water	24541		24541	0
Hydrogen	7420		0	7420
Design Data:				
	Heat Duty (BTU/hr)			-14,767,649
	Height (ft):			12
	Diameter (ft):			11.5
	Material of Construction:		304 Stainless Steel	
Cost, C_{PB}, C_{TDC}:	$52,000		$202,700	
Utilities:				
Comments:				



Separator

Identification	Item:	F-300
	Item No:	300
	No. Req'd	1

Function To separate unreacted sorbitol from APR products.

Operation Continuous

Materials Handled:

	Streams In:		Streams Out:	
	S-307		S-308	S-310
Quantity (lb/hr)	339319		88840	250479
Temperature(°F)	314.62		359.6	359.6
Composition (lb/hr)				
Sorbitol	43128		43128	0
Propane	28191		13.5	28177.5
Carbon Dioxide	93769		89	93680
Water	166810		45609	121201
Hydrogen	7421		0.5	7420.5

Design Data:

Heat Duty (BTU/hr)	77,018,428
Height (ft):	13
Diameter (ft):	6
Material of Construction:	304 Stainless Steel

Cost, C_{PB}, C_{TDC}:	$35,100	$142,900
Utilities:		
Comments:		

Separator

Identification	Item:	F-301
	Item No:	301
	No. Req'd	1

Function	To separate water from the APR products to be fed into PSA
Operation	Continuous

Materials Handled:

	Streams In:		Streams Out:	
	S-326		S-324	S-323
Quantity (lb/hr)	250488.38		96666.38	153822
Temperature(°F)	140		140	140
Composition (lb/hr)				
Sorbitol	0.38		0.38	0
Propane	28178		0	28178
Carbon Dioxide	93680		1	93679
Water	121210		96665	24545
Hydrogen	7420		0	7420

Design Data:

	Heat Duty (BTU/hr)	5,106,795
	Height (ft):	12
	Diameter (ft):	9.5
	Material of Construction:	304 Stainless Steel

Cost, C_{PB}, C_{TDC}:	$34,600	$157,400
Utilities:		
Comments:		

Pump

Identification	Item:	P-400
	Item No:	400
	No. Req'd	1

Function	To pump the sorbitol water stream from HX-400 to HX-402.
Operation	Continuous

Materials Handled:

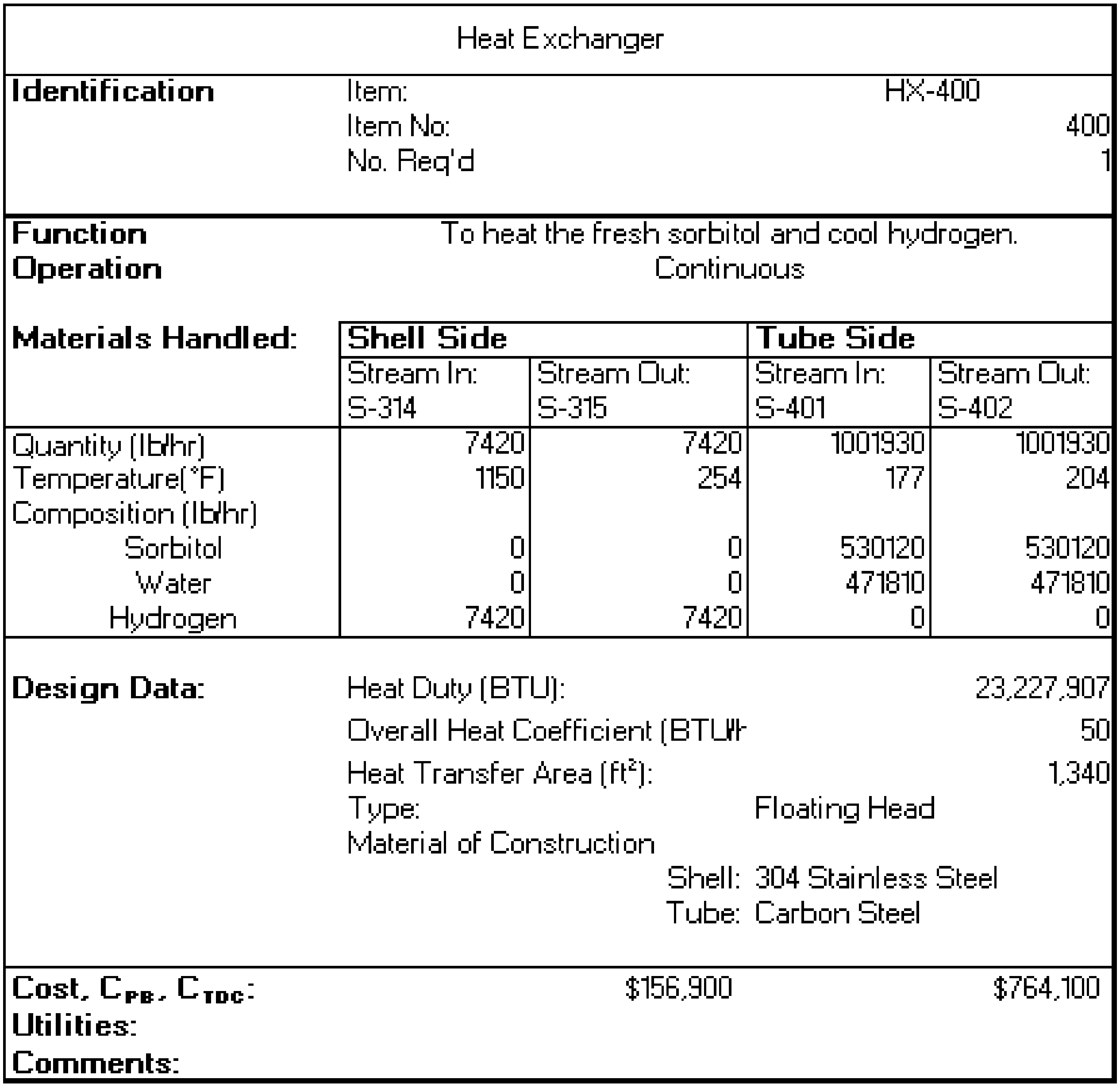
	Feed: S-402	**Exit: S-403**
Quantity (lb/hr)	1001930	1001930
Temperature(°F)	204	204
Composition (lb/hr)		
Sorbitol	530120	530120
Water	471810	471810

Design Data:	Density of Fluid (lb/cuft):	72.33
	Brake Power (hp):	2.5
	Pump Head (ft):	3.98
	Electricity Requirements (kW):	1.86
	Material of Construction:	Carbon Steel

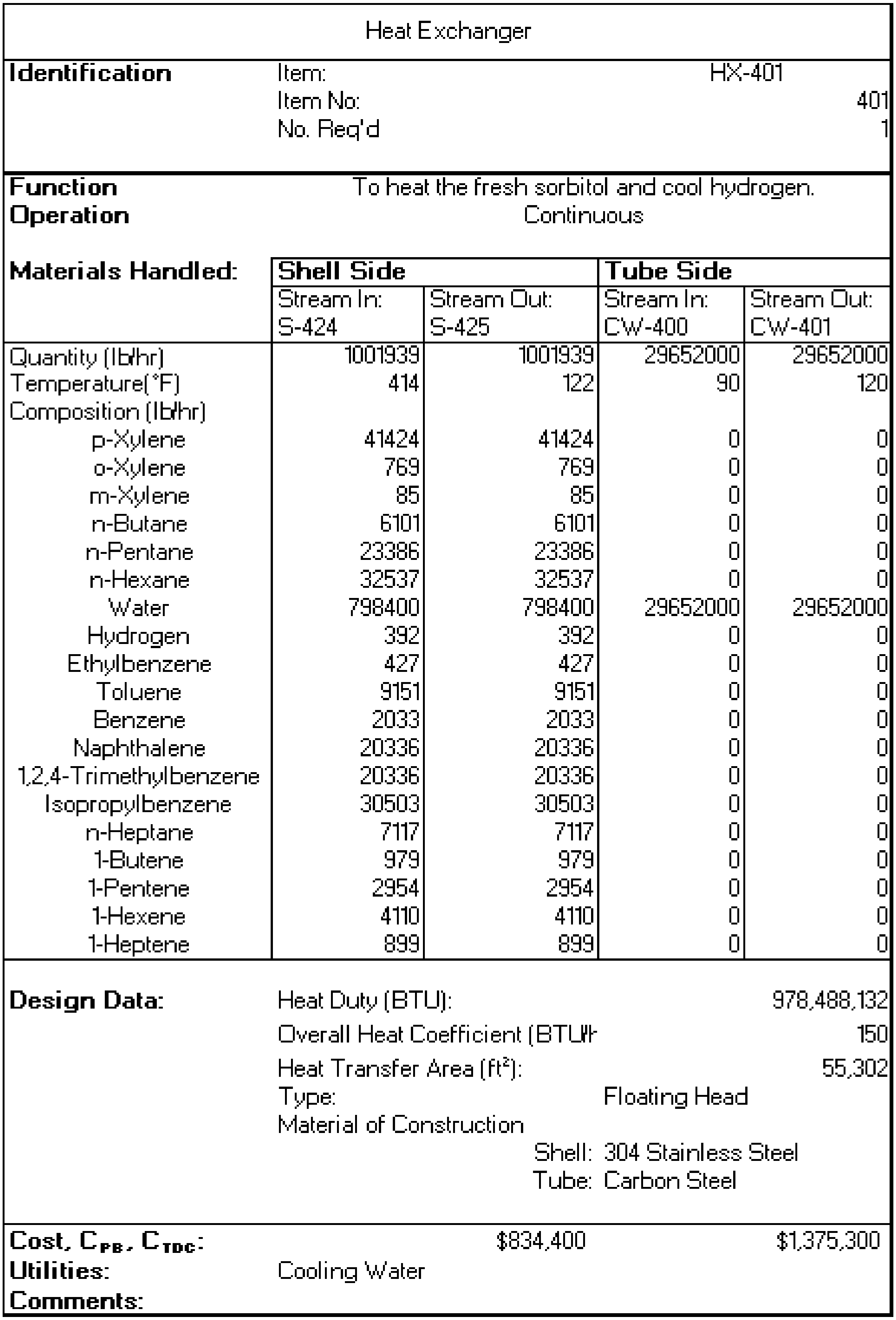
Cost, C_{PB}, C_{TDC}	$10,600	$119,300
Utilities:	Electricity	
Comments:		

	Pump	
Identification	Item:	P-401
	Item No:	401
	No. Req'd	1
Function	To pump the sorbitol water stream from HX-404 to SPT-400.	
Operation	Continuous	
Materials Handled:		
	Feed: S-406	**Exit: S-407**
Quantity (lb/hr)	1001930	1001930
Temperature(°F)	698.1	698.15
Composition (lb/hr)		
Sorbitol	530120	530120
Water	471810	471810
Design Data:	Density of Fluid (lb/cuft):	44.33
	Brake Power (hp):	3.94
	Pump Head (ft):	6.5
	Electricity Requirements (kW):	2.94
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$13,400	$272,300
Utilities:	Electricity	
Comments:		

	Pump	
Identification	Item:	P-402
	Item No:	402
	No. Req'd	1
Function	To pump the sorbitol water stream from HX-403 to HX-404.	
Operation	Continuous	
Materials Handled:		
	Feed: S-404	**Exit: S-405**
Quantity (lb/hr)	1001930	1001930
Temperature(°F)	302	302
Composition (lb/hr)		
Sorbitol	530120	530120
Water	471810	471810
Design Data:	Density of Fluid (lb/cuft):	68.18
	Brake Power (hp):	2.63
	Pump Head (ft):	4.33
	Electricity Requirements (kW):	1.96
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$11,000	$121,400
Utilities:	Electricity	
Comments:		



Heat Exchanger				
Identification	Item:		HX-400	
	Item No:			400
	No. Req'd			1
Function	To heat the fresh sorbitol and cool hydrogen.			
Operation	Continuous			
Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In: S-314	Stream Out: S-315	Stream In: S-401	Stream Out: S-402
Quantity (lb/hr)	7420	7420	1001930	1001930
Temperature(°F)	1150	254	177	204
Composition (lb/hr)				
Sorbitol	0	0	530120	530120
Water	0	0	471810	471810
Hydrogen	7420	7420	0	0
Design Data:	Heat Duty (BTU):			23,227,907
	Overall Heat Coefficient (BTU/h			50
	Heat Transfer Area (ft^2):			1,340
	Type:		Floating Head	
	Material of Construction			
		Shell:	304 Stainless Steel	
		Tube:	Carbon Steel	
Cost, C_{PB}, C_{TDC}:		$156,900		$764,100
Utilities:				
Comments:				



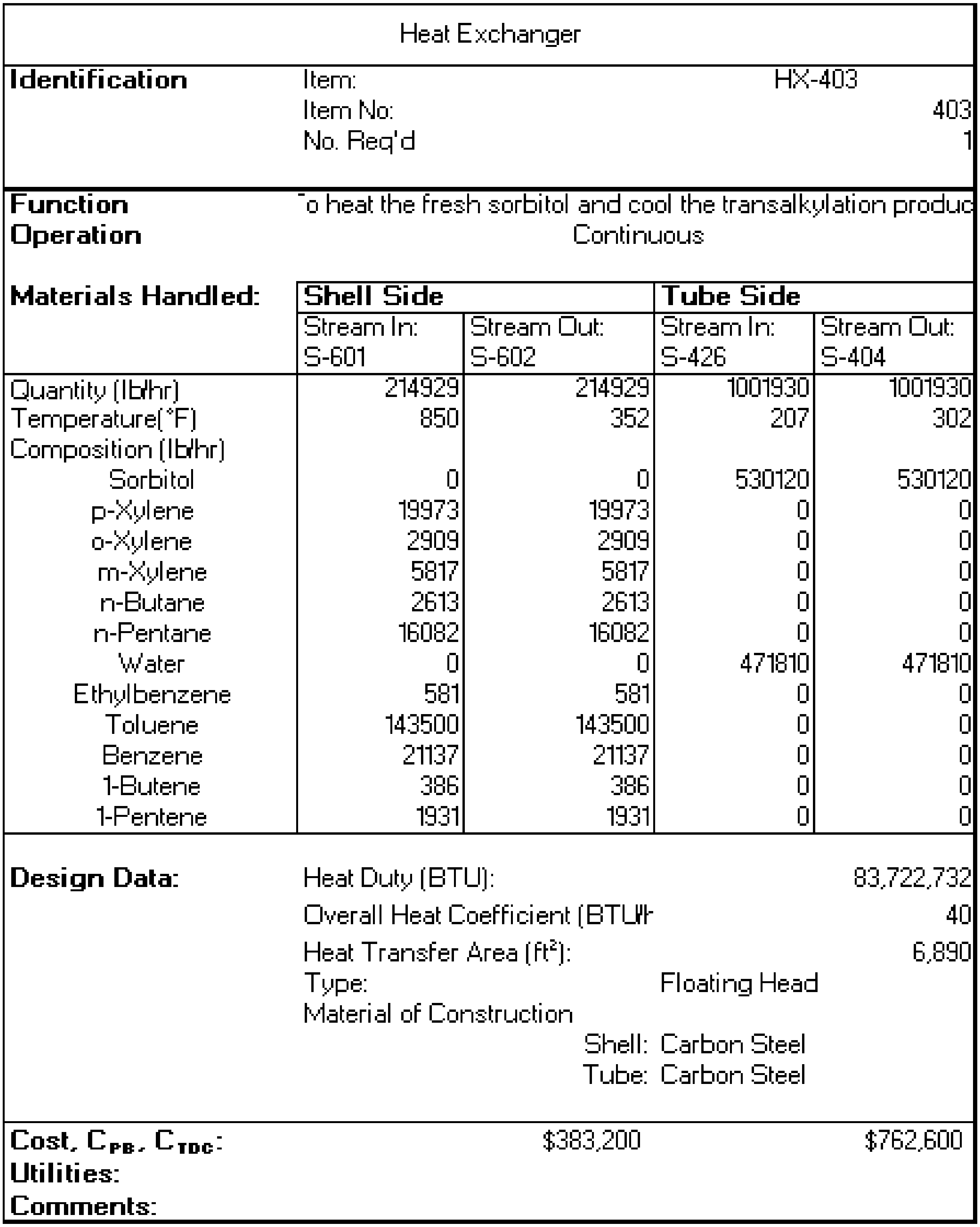
Heat Exchanger

Identification	Item:	HX-401
	Item No:	401
	No. Req'd	1
Function	To heat the fresh sorbitol and cool hydrogen.	
Operation	Continuous	

Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In: S-424	Stream Out: S-425	Stream In: CW-400	Stream Out: CW-401
Quantity (lb/hr)	1001939	1001939	29652000	29652000
Temperature(°F)	414	122	90	120
Composition (lb/hr)				
p-Xylene	41424	41424	0	0
o-Xylene	769	769	0	0
m-Xylene	85	85	0	0
n-Butane	6101	6101	0	0
n-Pentane	23386	23386	0	0
n-Hexane	32537	32537	0	0
Water	798400	798400	29652000	29652000
Hydrogen	392	392	0	0
Ethylbenzene	427	427	0	0
Toluene	9151	9151	0	0
Benzene	2033	2033	0	0
Naphthalene	20336	20336	0	0
1,2,4-Trimethylbenzene	20336	20336	0	0
Isopropylbenzene	30503	30503	0	0
n-Heptane	7117	7117	0	0
1-Butene	979	979	0	0
1-Pentene	2954	2954	0	0
1-Hexene	4110	4110	0	0
1-Heptene	899	899	0	0

Design Data:	Heat Duty (BTU):		978,488,132
	Overall Heat Coefficient (BTU/h		150
	Heat Transfer Area (ft^2):		55,302
	Type:	Floating Head	
	Material of Construction		
	Shell:	304 Stainless Steel	
	Tube:	Carbon Steel	
Cost, C_{PB}, C_{TDC}:		$834,400	$1,375,300
Utilities:	Cooling Water		
Comments:			

Heat Exchanger				
Identification	Item:		HX-402	
	Item No:			402
	No. Req'd			1
Function	o heat the fresh sorbitol and to cool the pre crystallizer strear			
Operation	Continuous			
Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In: S-507	Stream Out: S-520	Stream In: S-403	Stream Out: S-426
Quantity (lb/hr)	74508	74508	1001930	1001930
Temperature(°F)	276	226	204	206
Composition (lb/hr)				
Sorbitol	0	0	530120	530120
p-Xylene	53936	53936	0	0
o-Xylene	2490	2490	0	0
m-Xylene	5216	5216	0	0
Water	0	0	471810	471810
Ethylbenzene	877	877	0	0
Toluene	6745	6745	0	0
1,2,4-Trimethylbenzene	60	60	0	0
Isopropylbenzene	5184	5184	0	0
Design Data:	Heat Duty (BTU):			1,804,692
	Overall Heat Coefficient (BTU/h			40
	Heat Transfer Area (ft^2):			1,084
	Type:		Floating Head	
	Material of Construction			
		Shell:	Carbon Steel	
		Tube:	Carbon Steel	
Cost, C_{PB}, C_{TDC}:		$39,400		$136,400
Utilities:				
Comments:				



Heat Exchanger				
Identification	Item:		HX-403	
	Item No:			403
	No. Req'd			1
Function	o heat the fresh sorbitol and cool the transalkylation produc			
Operation		Continuous		
Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In: S-601	Stream Out: S-602	Stream In: S-426	Stream Out: S-404
Quantity (lb/hr)	214929	214929	1001930	1001930
Temperature(°F)	850	352	207	302
Composition (lb/hr)				
Sorbitol	0	0	530120	530120
p-Xylene	19973	19973	0	0
o-Xylene	2909	2909	0	0
m-Xylene	5817	5817	0	0
n-Butane	2613	2613	0	0
n-Pentane	16082	16082	0	0
Water	0	0	471810	471810
Ethylbenzene	581	581	0	0
Toluene	143500	143500	0	0
Benzene	21137	21137	0	0
1-Butene	386	386	0	0
1-Pentene	1931	1931	0	0
Design Data:	Heat Duty (BTU):			83,722,732
	Overall Heat Coefficient (BTU/h			40
	Heat Transfer Area (ft^2):			6,890
	Type:		Floating Head	
	Material of Construction			
		Shell:	Carbon Steel	
		Tube:	Carbon Steel	
Cost, C_{PB}, C_{TDC}:		$383,200		$762,600
Utilities:				
Comments:				

Heat Exchanger

Identification	Item:		HX-404	
	Item No:			404
	No. Req'd			1
Function	heat fresh sorbitol stream to condensation reactor temperatu			
Operation	Continuous			
Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In:	Stream Out:	Stream In: S-405	Stream Out: S-406
Quantity (lb/hr)			1001930	1001930
Temperature(°F)			253.59	359.6
Composition (lb/hr)				
Sorbitol			530120	530120
Water			471810	471810
Design Data:	Heat Duty (BTU):			527,756,123
	Overal Heat Coefficient (BTU/h			50
	Heat Transfer Area (ft^2):			138,719
	Type:		Floating Head	
	Material of Construction			
		Shell:	Carbon Steel	
		Tube:	Carbon Steel	
Cost, C_{PB}, C_{TDC}:		$3,568,600		$11,854,500
Utilities:				
Comments:				

Reactor				
Identification	Item:		R-400	
	Item No:			400
	No. Req'd			4
Function	Convert Sorbitol to Aromatics and other Hydrocarbons			
Operation	Continuous			
Materials Handled:	Streams In:		Streams Out:	
	S-408		S-412	
Quantity (lb/hr)	250480		250480	
Temperature(°F)	698		698	
Composition (lb/hr)				
Sorbitol	132530		0	
p-Xylene	0		10357	
o-Xylene	0		193	
m-Xylene	0		22	
n-Butane	0		1526	
n-Pentane	0		5847	
n-Hexane	0		8135	
Water	117950		199604	
Hydrogen	0		98	
Ethylbenzene	0		107	
Toluene	0		2288	
Benzene	0		508	
Naphthalene	0		5085	
1,2,4-Trimethylbenzene	0		5085	
Isopropylbenzene	0		7627	
n-Heptane	0		1780	
1-Butene	0		225	
1-Pentene	0		740	
1-Hexene	0		1028	
1-Heptene	0		225	
Design Data:	Volume (gal):			4759.21
	Working Vol initial (L):			12610
	Working Vol at end (L):			12610
	Height (ft):			22.5
	Diameter (ft):			6
	Material of Construction:		Carbon Steel	
Cost, C_{PB}, C_{TDC}:		$233,300		$460,500
Utilities:				
Comments:				

Pump

Identification	Item:	P-500
	Item No:	500
	No. Req'd	1

Function	Pumps bottoms from DC-500 as feed for DC-501.
Operation	Continuous

Materials Handled:

	Feed: S-505	**S-506**
Quantity (lb/hr)	29976	29976
Temperature(˚F)	296	296
Composition (lb/hr)		
p-Xylene	56067	56067
o-Xylene	3549	3549
m-Xylene	5484	5484
Ethylbenzene	890	890
Toluene	6745	6745
Naphthalene	20320	20320
1,2,4-Trimethylbenzene	20254	20254
Isopropylbenzene	29976	29976

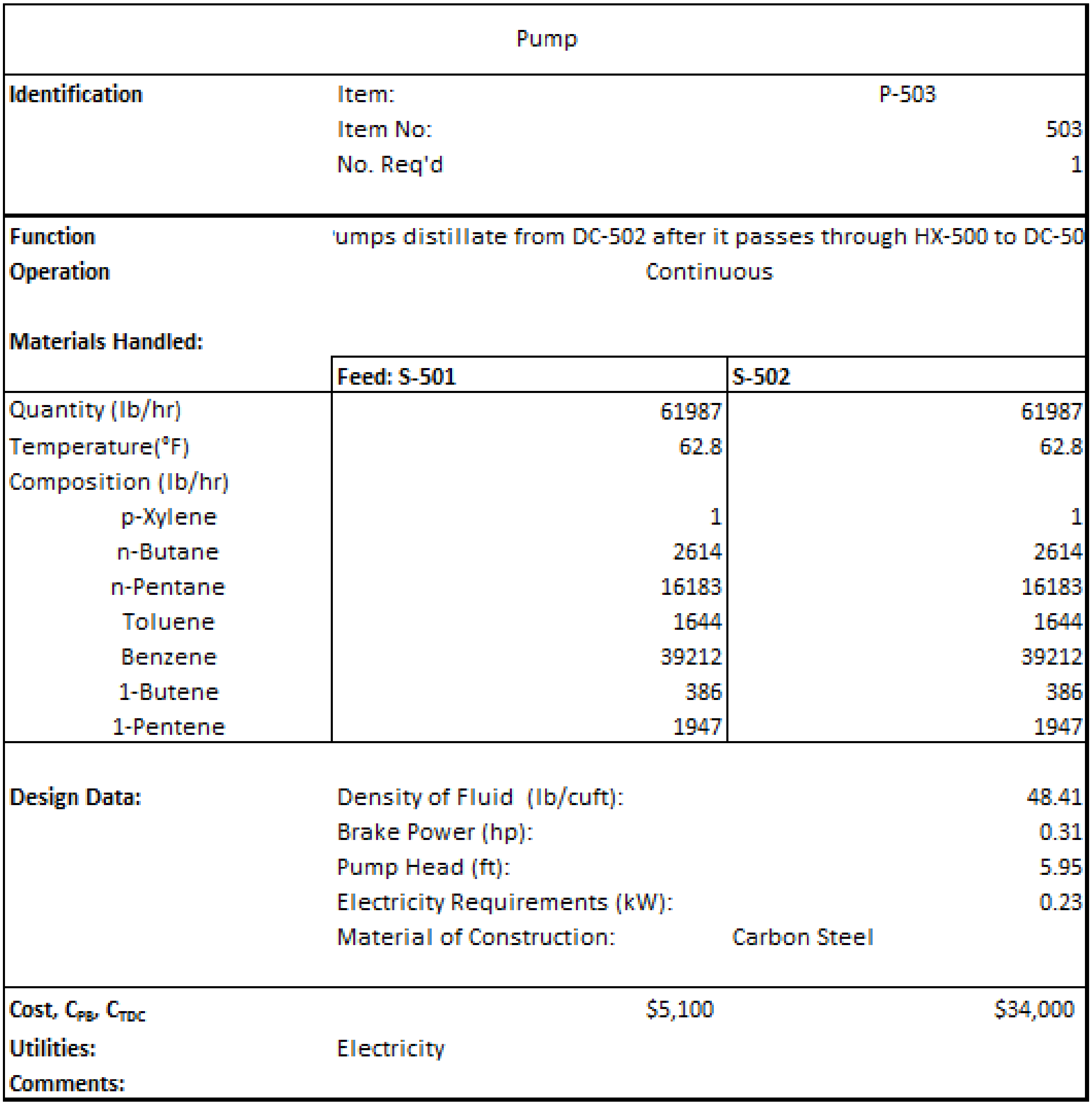
Design Data:	Density of Fluid (lb/cuft):	48.25
	Brake Power (hp):	0.63
	Pump Head (ft):	5.97
	Electricity Requirements (kW):	0.47
	Material of Construction:	Carbon Steel

Cost, C_{PB}, C_{TDC}	$6,600	$45,200
Utilities:	Electricity	
Comments:		

	Pump	
Identification	Item:	P-501
	Item No:	501
	No. Req'd	1
Function	Pumps hydrocarbons from SEP-500 to MIX-500.	
Operation	Continuous	
Materials Handled:		
	Feed: S-501	**S-502**
Quantity (lb/hr)	29976	29976
Temperature(°F)	122	122
Composition (lb/hr)		
p-Xylene	56067	56067
o-Xylene	3549	3549
m-Xylene	5484	5484
n-Butane		
n-Pentane		
n-Hexane		
Water		
Hydrogen		
Ethylbenzene	890	890
Toluene	6745	6745
Naphthalene	20320	20320
1,2,4-Trimethylbenzene	20254	20254
Isopropylbenzene		
	29976	29976
Design Data:	Density of Fluid (lb/cuft):	61.61
	Brake Power (hp):	0.78
	Pump Head (ft):	5.93
	Electricity Requirements (kW):	0.59
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$6,600	$45,200
Utilities:	Electricity	
Comments:		

Pump

Identification	Item:	P-502
	Item No:	502
	No. Req'd	1
Function	Pumps bottoms from DC-502 to MIX-500.	
Operation	Continuous	
Materials Handled:		
	Feed: S-513	**S-514**
Quantity (lb/hr)	172681	172681
Temperature(°F)	239	239
Composition (lb/hr)		
p-Xylene	19973	19973
o-Xylene	2909	2909
n-Hexane	5817	5817
Ethylbenzene	582	582
Toluene	142675	142675
Benzene	725	725
Design Data:	Density of Fluid (lb/cuft):	45.46
	Brake Power (hp):	0.74
	Pump Head (ft):	5.94
	Electricity Requirements (kW):	0.55
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$7,200	$53,500
Utilities:	Electricity	
Comments:		



Pump		
Identification	Item:	P-503
	Item No:	503
	No. Req'd	1
Function	umps distillate from DC-502 after it passes through HX-500 to DC-50	
Operation	Continuous	
Materials Handled:		
	Feed: S-501	**S-502**
Quantity (lb/hr)	61987	61987
Temperature(°F)	62.8	62.8
Composition (lb/hr)		
p-Xylene	1	1
n-Butane	2614	2614
n-Pentane	16183	16183
Toluene	1644	1644
Benzene	39212	39212
1-Butene	386	386
1-Pentene	1947	1947
Design Data:	Density of Fluid (lb/cuft):	48.41
	Brake Power (hp):	0.31
	Pump Head (ft):	5.95
	Electricity Requirements (kW):	0.23
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$5,100	$34,000
Utilities:	Electricity	
Comments:		

Distillation Column

Identification	Item:	DC-500
	Item No:	500
	No. Req'd	1

Function Separates "light" hydrocarbons from "heavy" hydrocarbons.

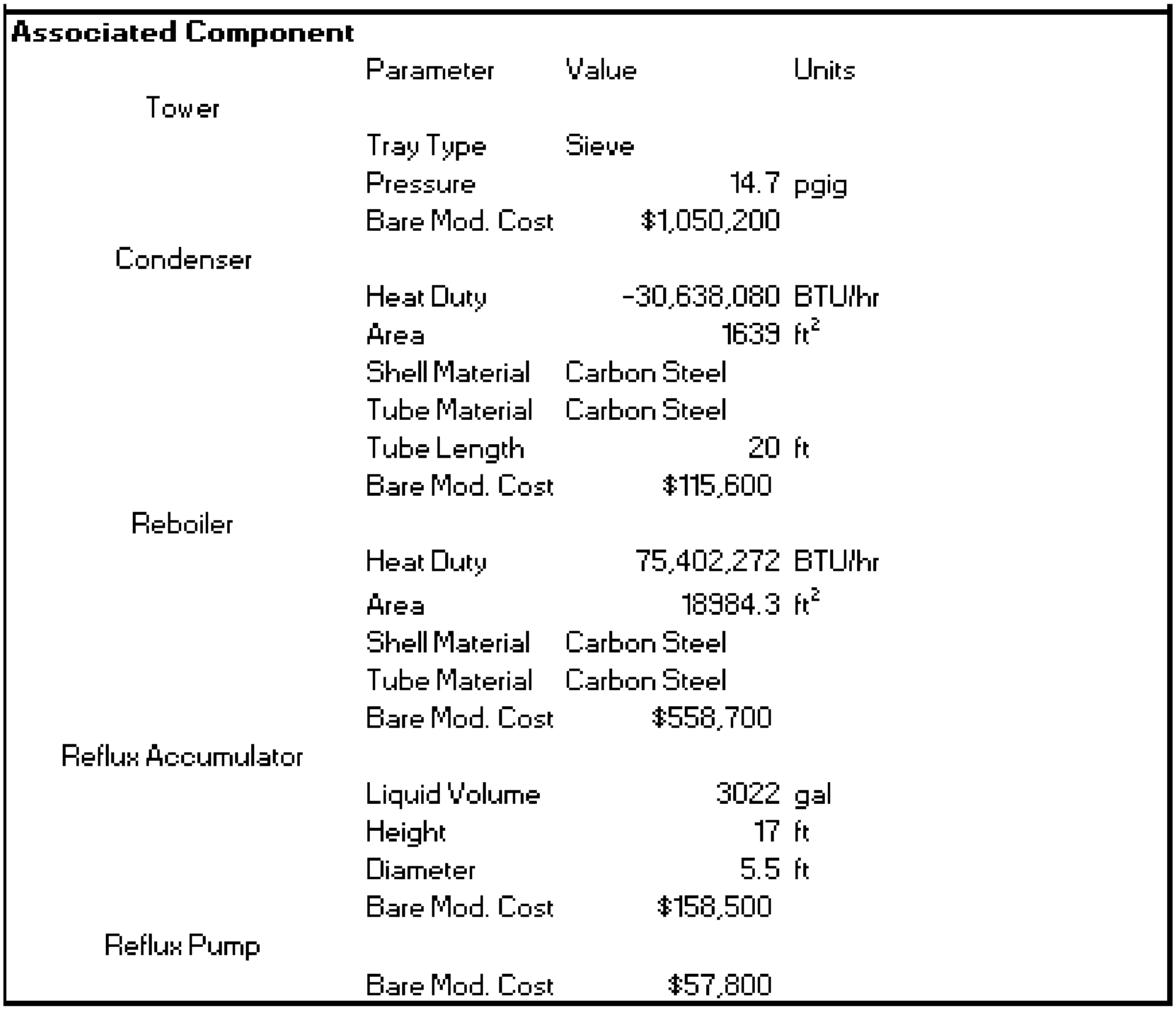
Operation Continuous

Materials Handled:

	Feed: S-504	**S-505**	**S-512**
Quantity (lb/hr)	358214	143285	214929
Temperature(°F)	177	296	209
Composition (lb/hr)			
p-Xylene	60901	56067	4834
o-Xylene	3670	3549	121
m-Xylene	5902	5484	418
n-Butane	2613	0	2613
n-Pentane	16082	0	16082
n-Hexane	28033	0	28033
Water	1709	0	1709
Hydrogen	1	0	1
Ethylbenzene	1003	890	113
Toluene	151529	6745	144784
Benzene	2557	0	2557
Naphthalene	20320	20320	0
1,2,4-Trimethylbenzene	20266	20254	12
Isopropylbenzene	30280	29976	304
n-Heptane	6724	0	6724
1-Butene	386	0	386
1-Pentene	1931	0	1931
1-Hexene	3463	0	3463
1-Heptene	844	0	844

Design Data:	Stages:	30
	Feed Stage:	12
	Reflux Ratio:	0.86
	Height (ft):	68
	Diameter (ft):	16.5
	Material of Construction:	Carbon Steel

Cost, C_{PB}, C_{TDC}	$981,500	$1,940,800
Utilities:	Electricity	Steam
Comments:		



Associated Component

	Parameter	Value	Units
Tower			
	Tray Type	Sieve	
	Pressure	14.7	pgig
	Bare Mod. Cost	$1,050,200	
Condenser			
	Heat Duty	-30,638,080	BTU/hr
	Area	1639	ft^2
	Shell Material	Carbon Steel	
	Tube Material	Carbon Steel	
	Tube Length	20	ft
	Bare Mod. Cost	$115,600	
Reboiler			
	Heat Duty	75,402,272	BTU/hr
	Area	18984.3	ft^2
	Shell Material	Carbon Steel	
	Tube Material	Carbon Steel	
	Bare Mod. Cost	$558,700	
Reflux Accumulator			
	Liquid Volume	3022	gal
	Height	17	ft
	Diameter	5.5	ft
	Bare Mod. Cost	$158,500	
Reflux Pump			
	Bare Mod. Cost	$57,800	

Distillation Column

Identification	Item:	DC-501	
	Item No:		501
	No. Req'd		1
Function	eparates heavy hydrocarbons from xylenes and similar compound		
Operation	Continuous		
Materials Handled:			
	Feed: S-506	**S-507**	**S-511**
Quantity (lb/hr)	143285	143285	
Temperature(°F)	296	276	332
Composition (lb/hr)			
p-Xylene	56067	53936	2131
o-Xylene	3549	2490	1059
m-Xylene	5484	5216	268
Ethylbenzene	890	877	13
Toluene	6745	6745	0
Naphthalene	20320	0	20320
1,2,4-Trimethylbenzene	20254	59.7	20194.3
Isopropylbenzene	29976	5184	24792
Design Data:	Stages:		43
	Feed Stage:		16
	Reflux Ratio:		3
	Height (ft):		94
	Diameter (ft):		12.5
	Material of Construction:	Carbon Steel	
Cost, C_{PB}, C_{TDC}	$775,800		$1,631,800
Utilities:	Electricity	Steam	
Comments:			

Associated Component			
	Parameter	Value	Units
Tower			
	Tray Type	Sieve	
	Pressure	14.7	pgig
	Bare Mod. Cost	$898,800	
Condenser			
	Heat Duty	-44,015,182	BTU/hr
	Area	1585	ft^2
	Shell Material	Carbon Steel	
	Tube Material	Carbon Steel	
	Tube Length	20	ft
	Bare Mod. Cost	$113,300	
Reboiler			
	Heat Duty	44,513,177	BTU/hr
	Area	11149.4	ft^2
	Shell Material	Carbon Steel	
	Tube Material	Carbon Steel	
	Bare Mod. Cost	$371,900	
Reflux Accumulator			
	Liquid Volume	5089	gal
	Height	20.5	ft
	Diameter	6.5	ft
	Bare Mod. Cost	$180,600	
Reflux Pump			
	Bare Mod. Cost	$67,200	

Distillation Column			
Identification	Item:	DC-502	
	Item No:		502
	No. Req'd		1
Function	Separates "light" hydrocarbons from "heavy" hydrocarbons.		
Operation	Continuous		
Materials Handled:	**Feed: S-524**	**S-515**	**S-513**
Quantity (lb/hr)	234767	61986	172781
Temperature(˚F)	177	142	239
Composition (lb/hr)			
p-Xylene	19974	1	19973
o-Xylene	2909	0	2909
m-Xylene	5917	0	5917
n-Butane	2614	2614	0
n-Pentane	16182	16182	0
Ethylbenzene	582	0	582
Toluene	144319	1644	142675
Benzene	39937	39212	725
1-Butene	386	386	0
1-Pentene	1947	1947	0
Design Data:	Stages:		20
	Feed Stage:		15
	Reflux Ratio:		12
	Height (ft):		48
	Diameter (ft):		22.5
	Material of Construction:	Carbon Steel	
Cost, C_{PB}, C_{TDC}	$981,500		$2,485,600
Utilities:	Electricity	Steam	
Comments:			

Associated Component	Parameter	Value	Units
Tower			
	Tray Type	Sieve	
	Pressure	14.7	pgig
	Bare Mod. Cost	$1,279,600	
Condenser			
	Heat Duty	-133,428,352	BTU/hr
	Area	13760	ft^2
	Shell Material	Carbon Steel	
	Tube Material	Carbon Steel	
	Tube Length	20	ft
	Bare Mod. Cost	$380,300	
Reboiler			
	Heat Duty	146,774,702	BTU/hr
	Area	15246.5	ft^2
	Shell Material	Carbon Steel	
	Tube Material	Carbon Steel	
	Bare Mod. Cost	$522,000	
Reflux Accumulator			
	Liquid Volume	13326	gal
	Height	28	ft
	Diameter	9	ft
	Bare Mod. Cost	$199,500	
Reflux Pump			
	Bare Mod. Cost	$104,200	

Distillation Column

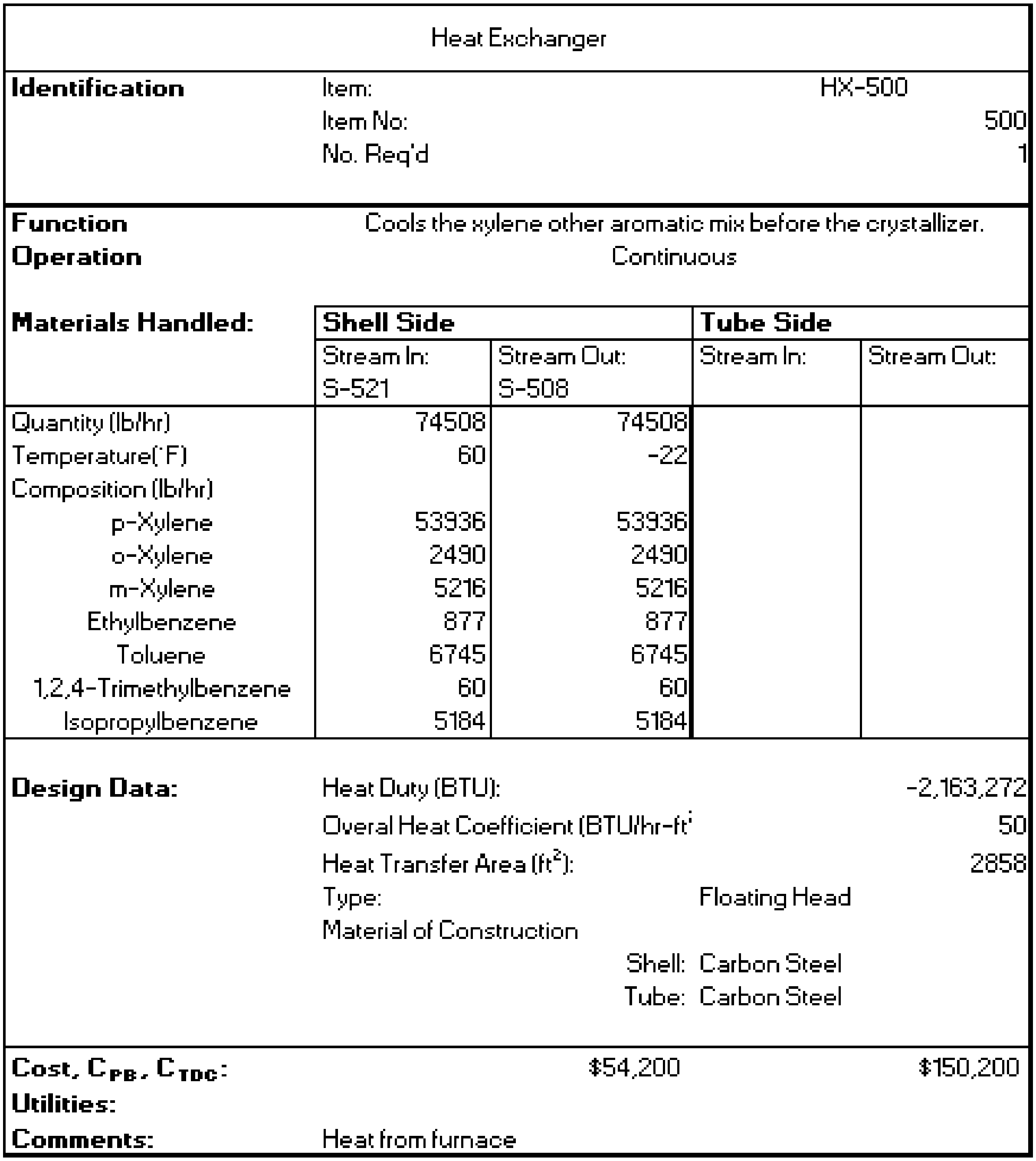
Identification	Item:	DC-503	
	Item No:		503
	No. Req'd		1
Function	Separates Toluene from other hydrocarbons for transalkylation.		
Operation	Continuous		

Materials Handled:

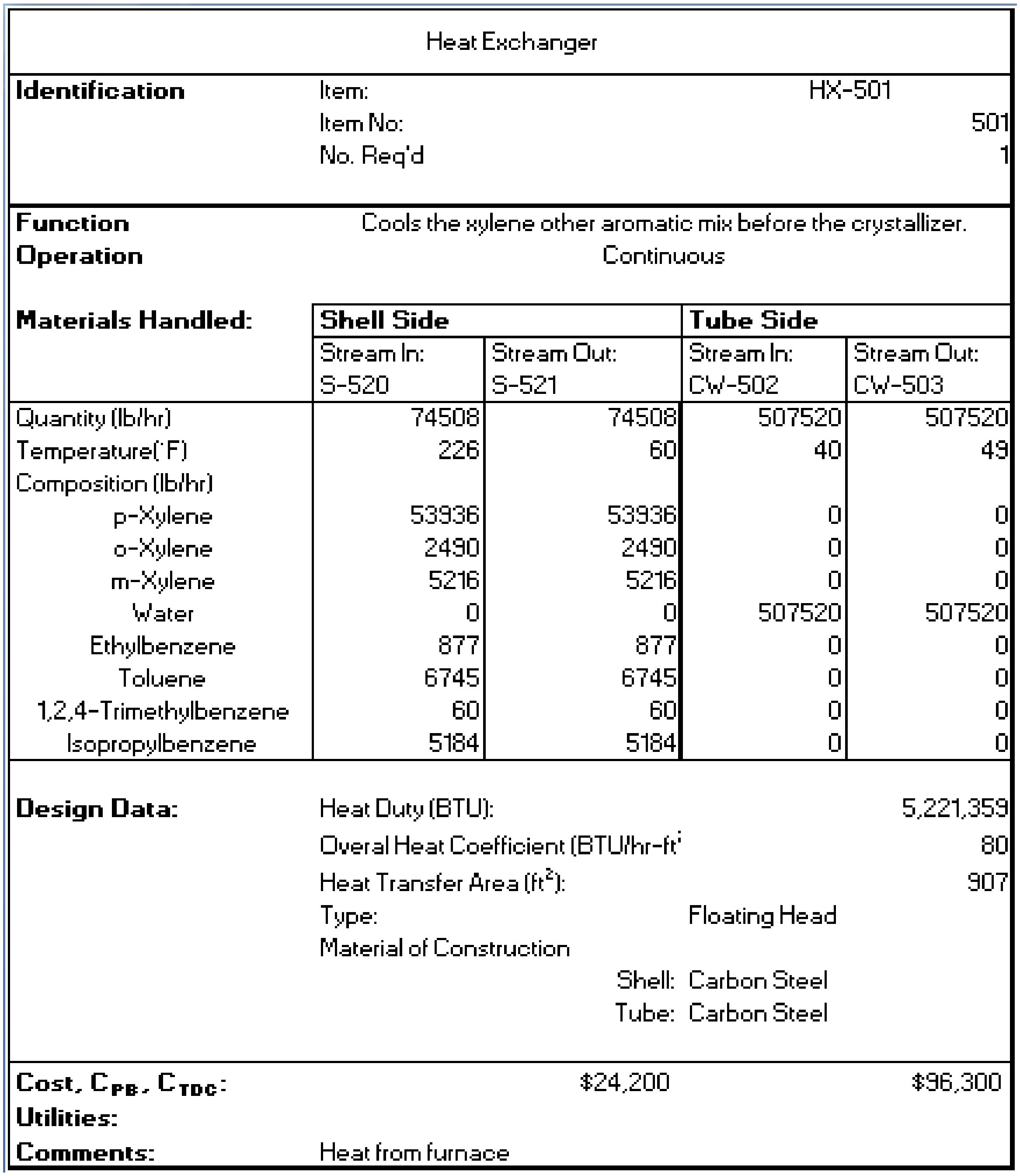
	Feed: S-517	**S-519**	**S-518**
Quantity (lb/hr)	61986	39480	22506
Temperature(°F)	63	176	91
Composition (lb/hr)			
p-Xylene	1	1	0
n-Butane	2614	3	2611
n-Pentane	16182	202	15980
Toluene	1644	1644	0
Benzene	39212	37599	1613
1-Butene	386	0	386
1-Pentene	1947	31	1916

Design Data:	Stages:		17
	Feed Stage:		145
	Reflux Ratio:		3
	Height (ft):		42
	Diameter (ft):		7
	Material of Construction:	Carbon Steel	
Cost, C_{PB}, C_{TDC}	$438,200		$1,010,900
Utilities:	Electricity	Steam	
Comments:			

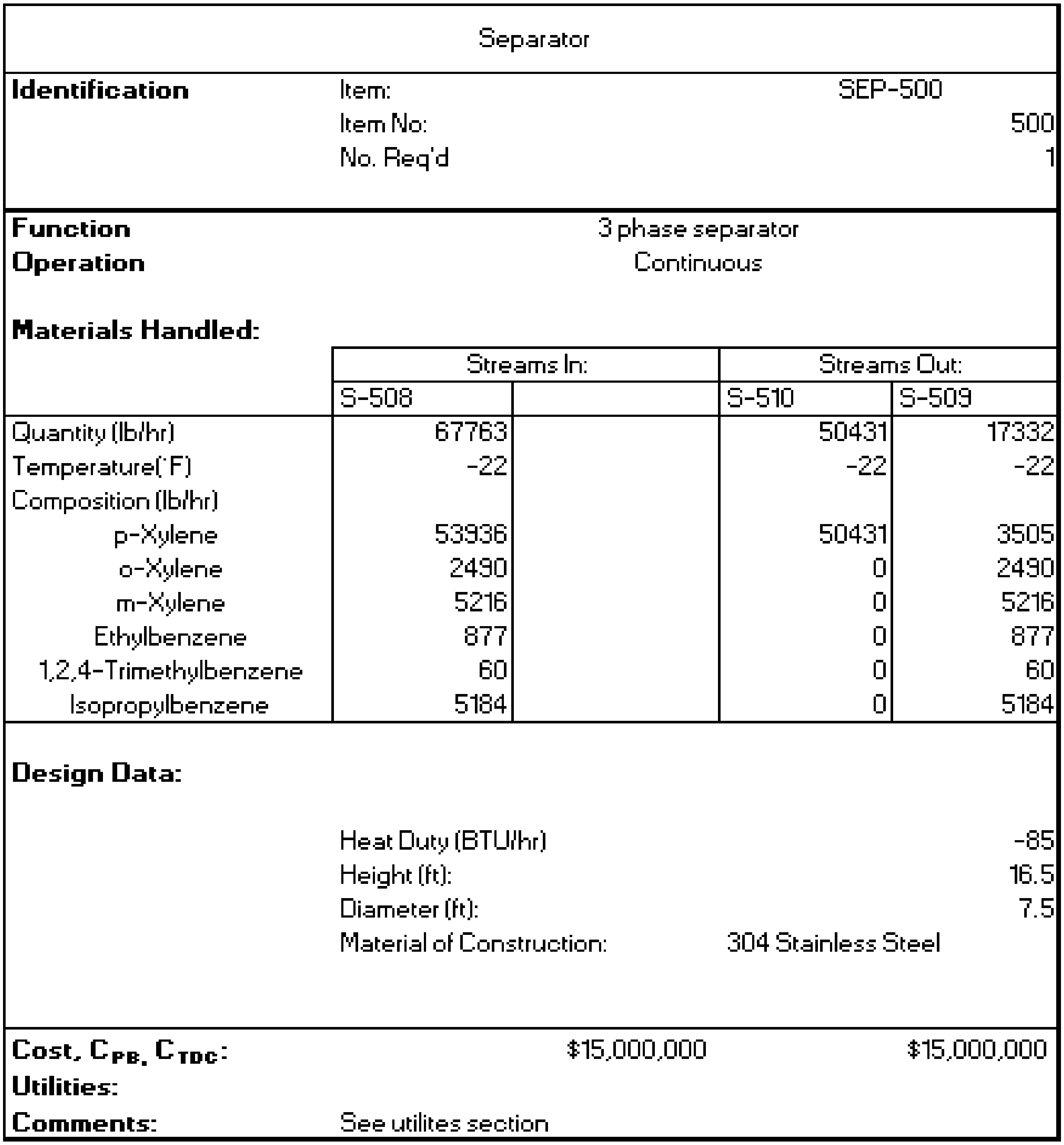
Associated Component	Parameter	Value	Units
Tower			
	Tray Type	Sieve	
	Pressure	14.7	pgig
	Bare Mod. Cost	$330,800	
Condenser			
	Heat Duty	-11,088,679	BTU/hr
	Area	18423	ft^2
	Shell Material	Carbon Steel	
	Tube Material	Carbon Steel	
	Tube Length	20	ft
	Bare Mod. Cost	$421,600	
Reboiler			
	Heat Duty	16,543,353	BTU/hr
	Area	998	ft^2
	Shell Material	Carbon Steel	
	Tube Material	Carbon Steel	
	Bare Mod. Cost	$113,500	
Reflux Accumulator			
	Liquid Volume	1128	gal
	Height	12	ft
	Diameter	4	ft
	Bare Mod. Cost	$106,000	
Reflux Pump			
	Bare Mod. Cost	$39,000	



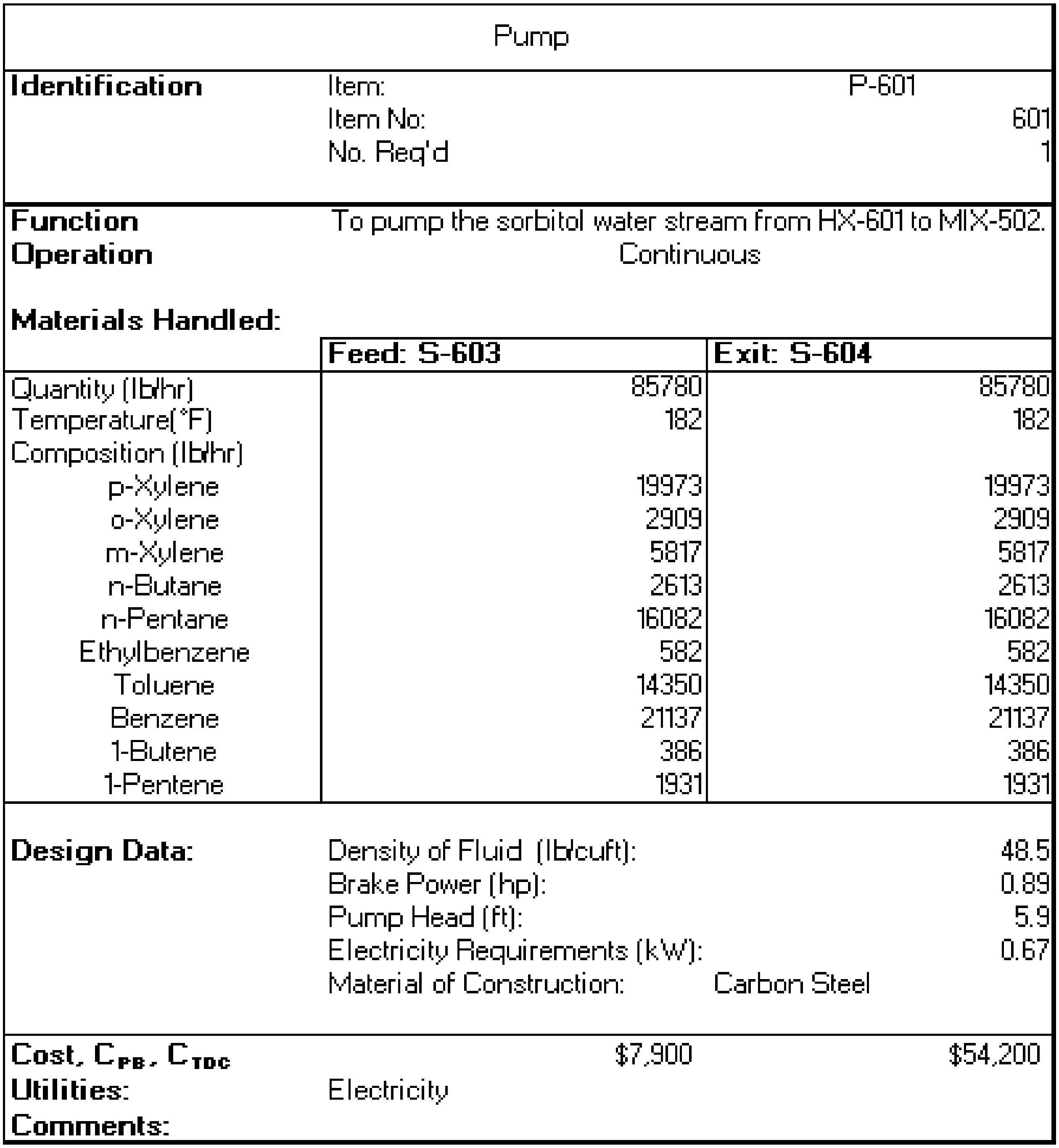
Heat Exchanger				
Identification	Item:		HX-500	
	Item No:			500
	No. Req'd			1
Function	Cools the xylene other aromatic mix before the crystallizer.			
Operation	Continuous			
Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In: S-521	Stream Out: S-508	Stream In:	Stream Out:
Quantity (lb/hr)	74508	74508		
Temperature(˚F)	60	-22		
Composition (lb/hr)				
p-Xylene	53936	53936		
o-Xylene	2490	2490		
m-Xylene	5216	5216		
Ethylbenzene	877	877		
Toluene	6745	6745		
1,2,4-Trimethylbenzene	60	60		
Isopropylbenzene	5184	5184		
Design Data:	Heat Duty (BTU):			-2,163,272
	Overal Heat Coefficient (BTU/hr-ft'			50
	Heat Transfer Area (ft^{2}):			2858
	Type:		Floating Head	
	Material of Construction			
		Shell:	Carbon Steel	
		Tube:	Carbon Steel	
Cost, C_{PB}, C_{TDC}:		\$54,200		\$150,200
Utilities:				
Comments:	Heat from furnace			



	Heat Exchanger			
Identification	Item:		HX-501	
	Item No:			501
	No. Req'd			1
Function	Cools the xylene other aromatic mix before the crystallizer.			
Operation	Continuous			
Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In: S-520	Stream Out: S-521	Stream In: CW-502	Stream Out: CW-503
Quantity (lb/hr)	74508	74508	507520	507520
Temperature(°F)	226	60	40	49
Composition (lb/hr)				
p-Xylene	53936	53936	0	0
o-Xylene	2490	2490	0	0
m-Xylene	5216	5216	0	0
Water	0	0	507520	507520
Ethylbenzene	877	877	0	0
Toluene	6745	6745	0	0
1,2,4-Trimethylbenzene	60	60	0	0
Isopropylbenzene	5184	5184	0	0
Design Data:	Heat Duty (BTU):			5,221,359
	Overal Heat Coefficient (BTU/hr-ft			80
	Heat Transfer Area (ft^2):			907
	Type:		Floating Head	
	Material of Construction			
		Shell:	Carbon Steel	
		Tube:	Carbon Steel	
Cost, C_{PB}, C_{TDC}:		$24,200		$96,300
Utilities:				
Comments:	Heat from furnace			

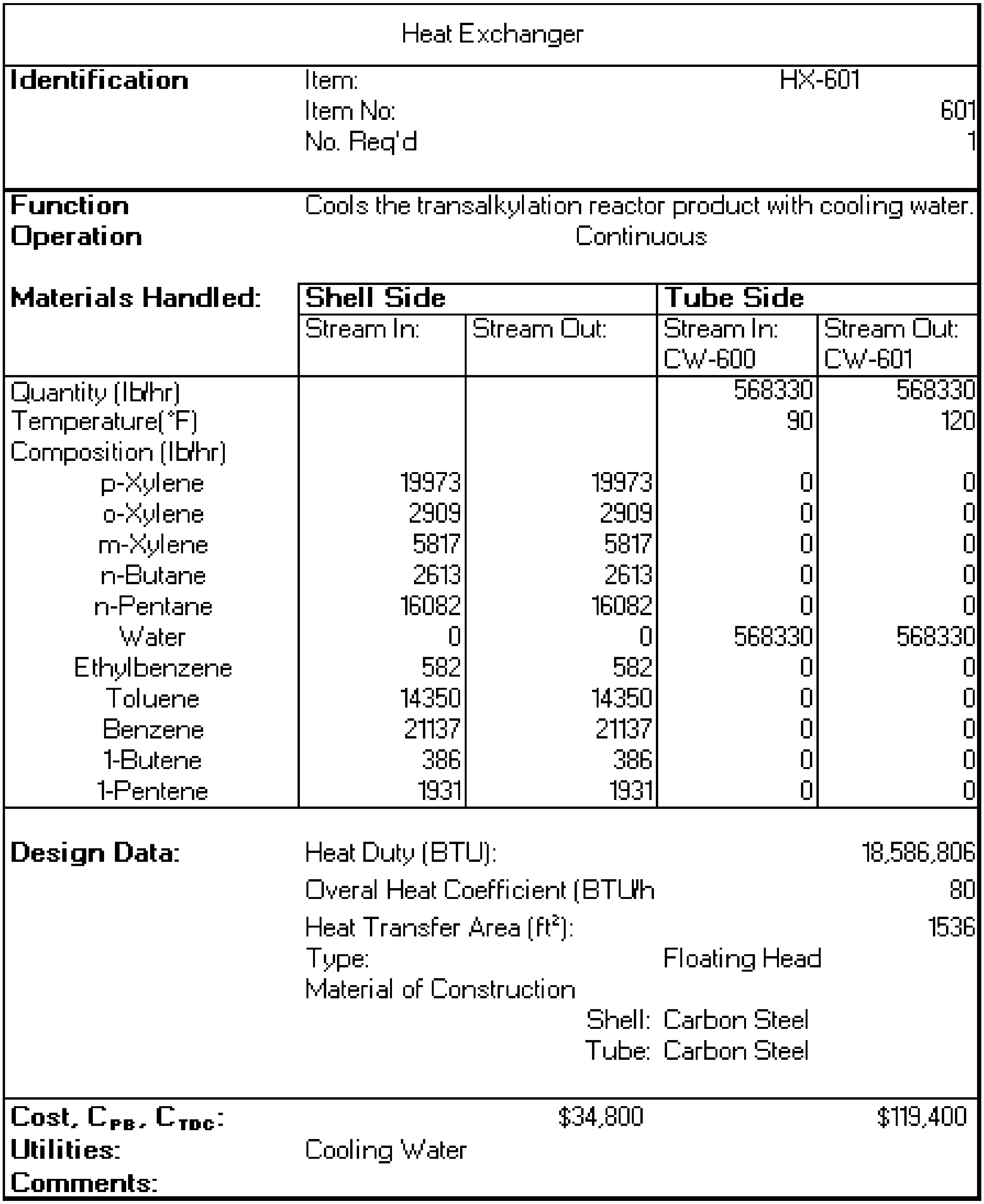


Separator				
Identification	Item:			SEP-500
	Item No:			500
	No. Req'd			1
Function			3 phase separator	
Operation			Continuous	
Materials Handled:				
	Streams In:		Streams Out:	
	S-508		S-510	S-509
Quantity (lb/hr)	67763		50431	17332
Temperature(°F)	-22		-22	-22
Composition (lb/hr)				
p-Xylene	53936		50431	3505
o-Xylene	2490		0	2490
m-Xylene	5216		0	5216
Ethylbenzene	877		0	877
1,2,4-Trimethylbenzene	60		0	60
Isopropylbenzene	5184		0	5184
Design Data:				
	Heat Duty (BTU/hr)			-85
	Height (ft):			16.5
	Diameter (ft):			7.5
	Material of Construction:		304 Stainless Steel	
Cost, C_{PB}, C_{TDC}:		$15,000,000		$15,000,000
Utilities:				
Comments:	See utilites section			



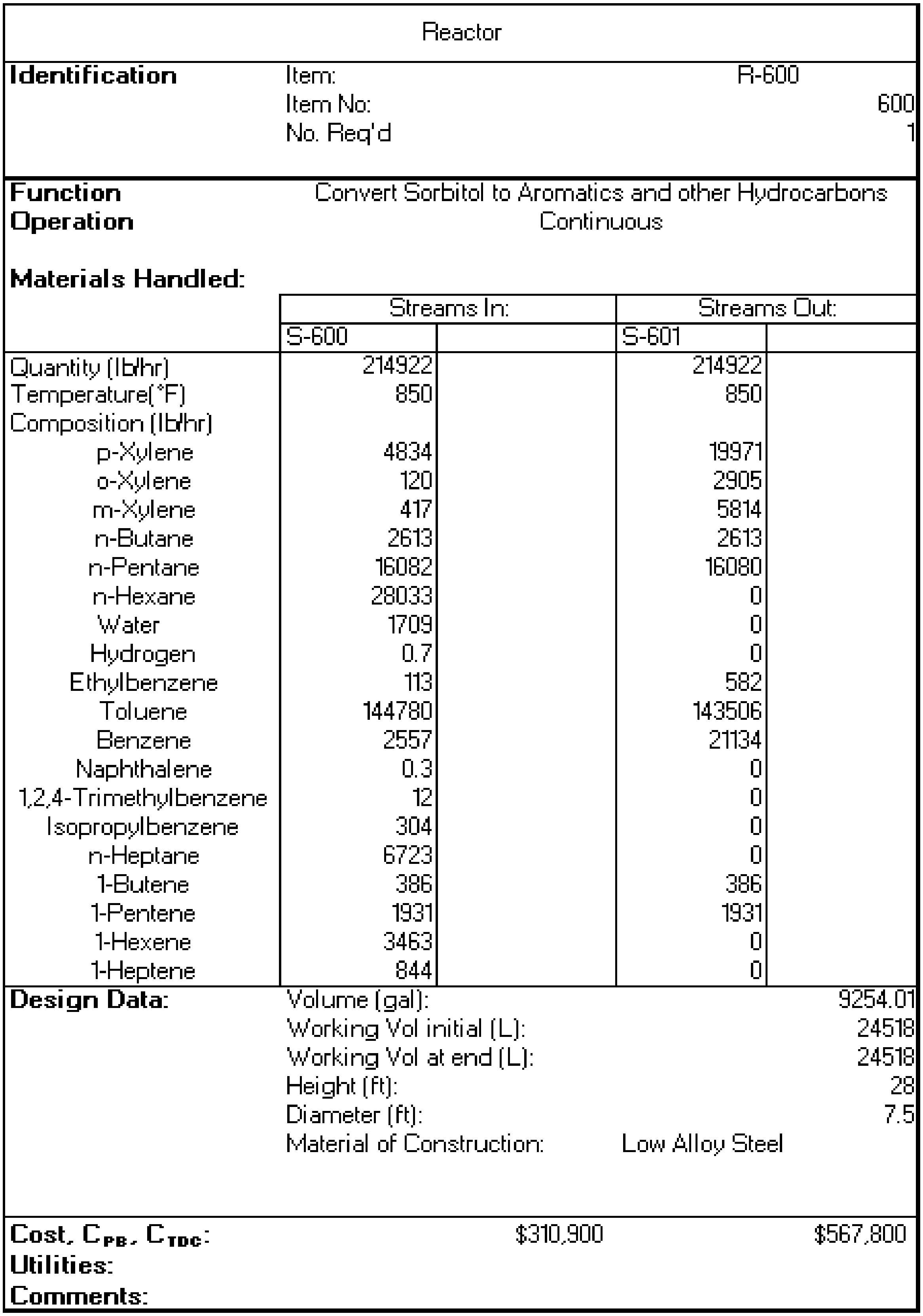
	Pump	
Identification	Item:	P-601
	Item No:	601
	No. Req'd	1
Function	To pump the sorbitol water stream from HX-601 to MIX-502.	
Operation	Continuous	
Materials Handled:		
	Feed: S-603	**Exit: S-604**
Quantity (lb/hr)	85780	85780
Temperature(°F)	182	182
Composition (lb/hr)		
p-Xylene	19973	19973
o-Xylene	2909	2909
m-Xylene	5817	5817
n-Butane	2613	2613
n-Pentane	16082	16082
Ethylbenzene	582	582
Toluene	14350	14350
Benzene	21137	21137
1-Butene	386	386
1-Pentene	1931	1931
Design Data:	Density of Fluid (lb/cuft):	48.5
	Brake Power (hp):	0.89
	Pump Head (ft):	5.9
	Electricity Requirements (kW):	0.67
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$7,900	$54,200
Utilities:	Electricity	
Comments:		

Heat Exchanger				
Identification	Item:			HX-600
	Item No:			600
	No. Req'd			1
Function	ats the distillate of DC-500 to transalkylation reactor temperat			
Operation			Continuous	
Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In:	Stream Out:	Stream In: S-512	Stream Out: S-600
Quantity (lb/hr)			214922	214922
Temperature(°F)			209	850
Composition (lb/hr)				
p-Xylene			4834	4834
o-Xylene			120	120
m-Xylene			417	417
n-Butane			2613	2613
n-Pentane			16082	16082
n-Hexane			28033	28033
Water			1709	1709
Hydrogen			0.7	0.7
Ethylbenzene			113	113
Toluene			144780	144780
Benzene			2557	2557
Naphthalene			0.3	0.3
1,2,4-Trimethylbenzene			12	12
Isopropylbenzene			304	304
n-Heptene			6723	6723
1-Butene			386	386
1-Pentene			1931	1931
1-Hexene			3463	3463
1-Heptene			844	844
Design Data:	Heat Duty (BTU):			527,756,123
	Overal Heat Coefficient (BTU/h			50
	Heat Transfer Area (ft^2):		??	
	Type:		Floating Head	
	Material of Construction			
		Shell:	Carbon Steel	
		Tube:	Carbon Steel	
Cost, C_{PB}, C_{TDC}:		$96,700		$541,900
Utilities:				
Comments:	Heat from furnace			



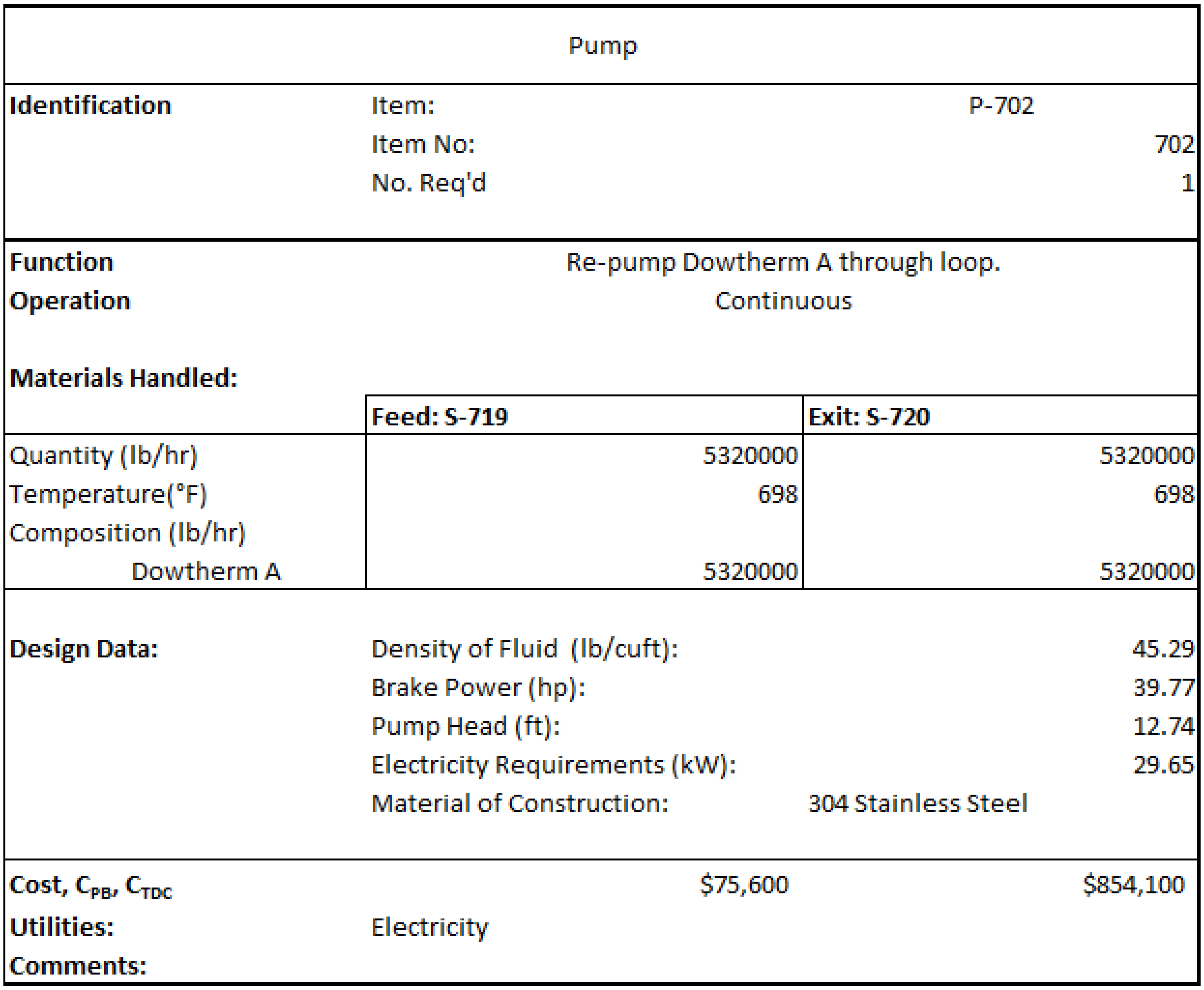
Heat Exchanger

Identification	Item:		HX-601	
	Item No:			601
	No. Req'd			1
Function	Cools the transalkylation reactor product with cooling water.			
Operation	Continuous			
Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In:	Stream Out:	Stream In: CW-600	Stream Out: CW-601
Quantity (lb/hr)			568330	568330
Temperature(°F)			90	120
Composition (lb/hr)				
p-Xylene	19973	19973	0	0
o-Xylene	2909	2909	0	0
m-Xylene	5817	5817	0	0
n-Butane	2613	2613	0	0
n-Pentane	16082	16082	0	0
Water	0	0	568330	568330
Ethylbenzene	582	582	0	0
Toluene	14350	14350	0	0
Benzene	21137	21137	0	0
1-Butene	386	386	0	0
1-Pentene	1931	1931	0	0
Design Data:	Heat Duty (BTU):			18,586,806
	Overal Heat Coefficient (BTU/h			80
	Heat Transfer Area (ft^2):			1536
	Type:		Floating Head	
	Material of Construction			
		Shell:	Carbon Steel	
		Tube:	Carbon Steel	
Cost, C_{PB}, C_{TDC}:		$34,800		$119,400
Utilities:	Cooling Water			
Comments:				

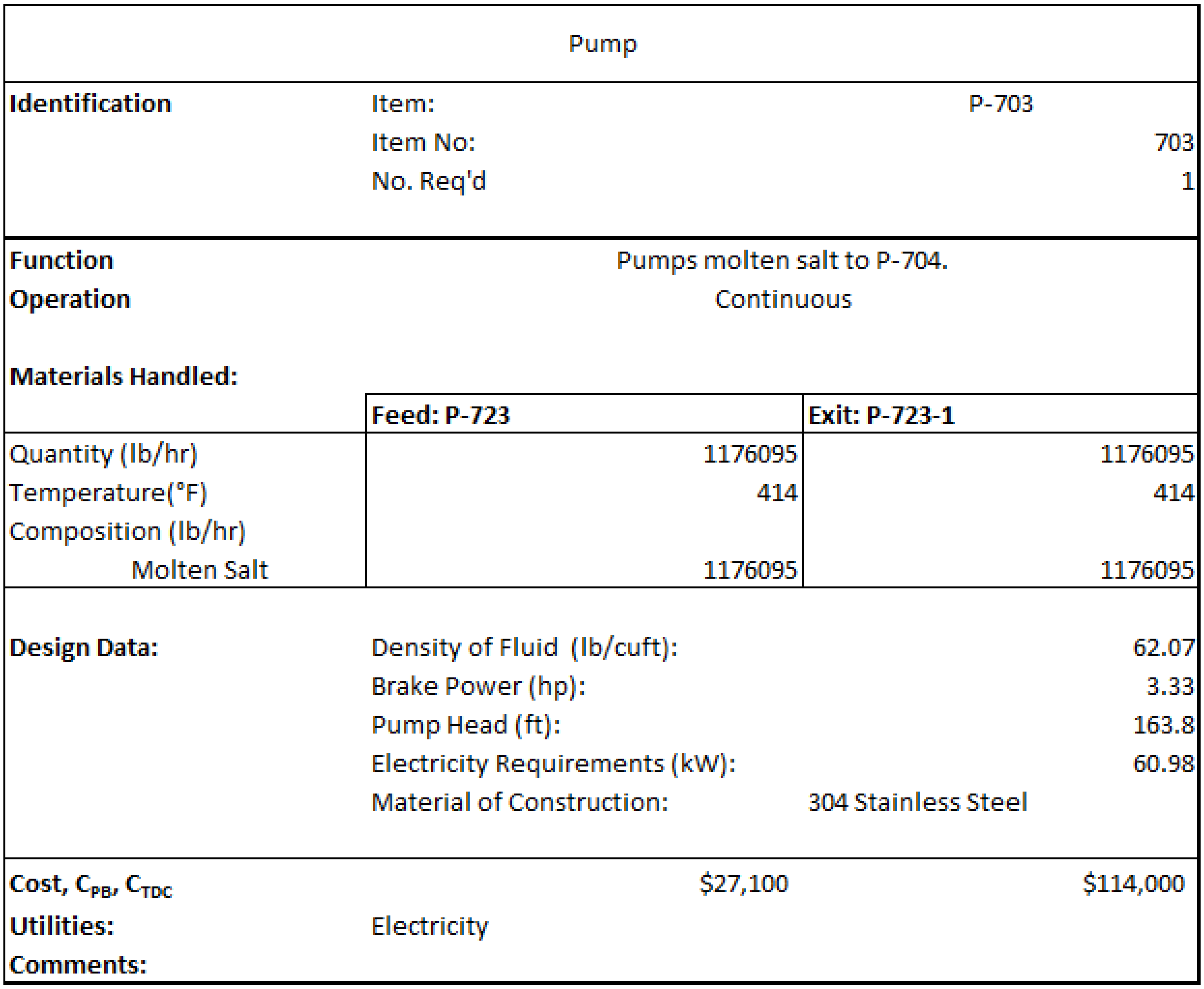


Reactor				
Identification	Item:		R-600	
	Item No:			600
	No. Req'd			1
Function	Convert Sorbitol to Aromatics and other Hydrocarbons			
Operation	Continuous			
Materials Handled:				
	Streams In:		Streams Out:	
	S-600		S-601	
Quantity (lb/hr)	214922		214922	
Temperature(°F)	850		850	
Composition (lb/hr)				
p-Xylene	4834		19971	
o-Xylene	120		2905	
m-Xylene	417		5814	
n-Butane	2613		2613	
n-Pentane	16082		16080	
n-Hexane	28033		0	
Water	1709		0	
Hydrogen	0.7		0	
Ethylbenzene	113		582	
Toluene	144780		143506	
Benzene	2557		21134	
Naphthalene	0.3		0	
1,2,4-Trimethylbenzene	12		0	
Isopropylbenzene	304		0	
n-Heptane	6723		0	
1-Butene	386		386	
1-Pentene	1931		1931	
1-Hexene	3463		0	
1-Heptene	844		0	
Design Data:	Volume (gal):			9254.01
	Working Vol initial (L):			24518
	Working Vol at end (L):			24518
	Height (ft):			28
	Diameter (ft):			7.5
	Material of Construction:		Low Alloy Steel	
Cost, C_{PB}, C_{TDC}:		$310,900		$567,800
Utilities:				
Comments:				

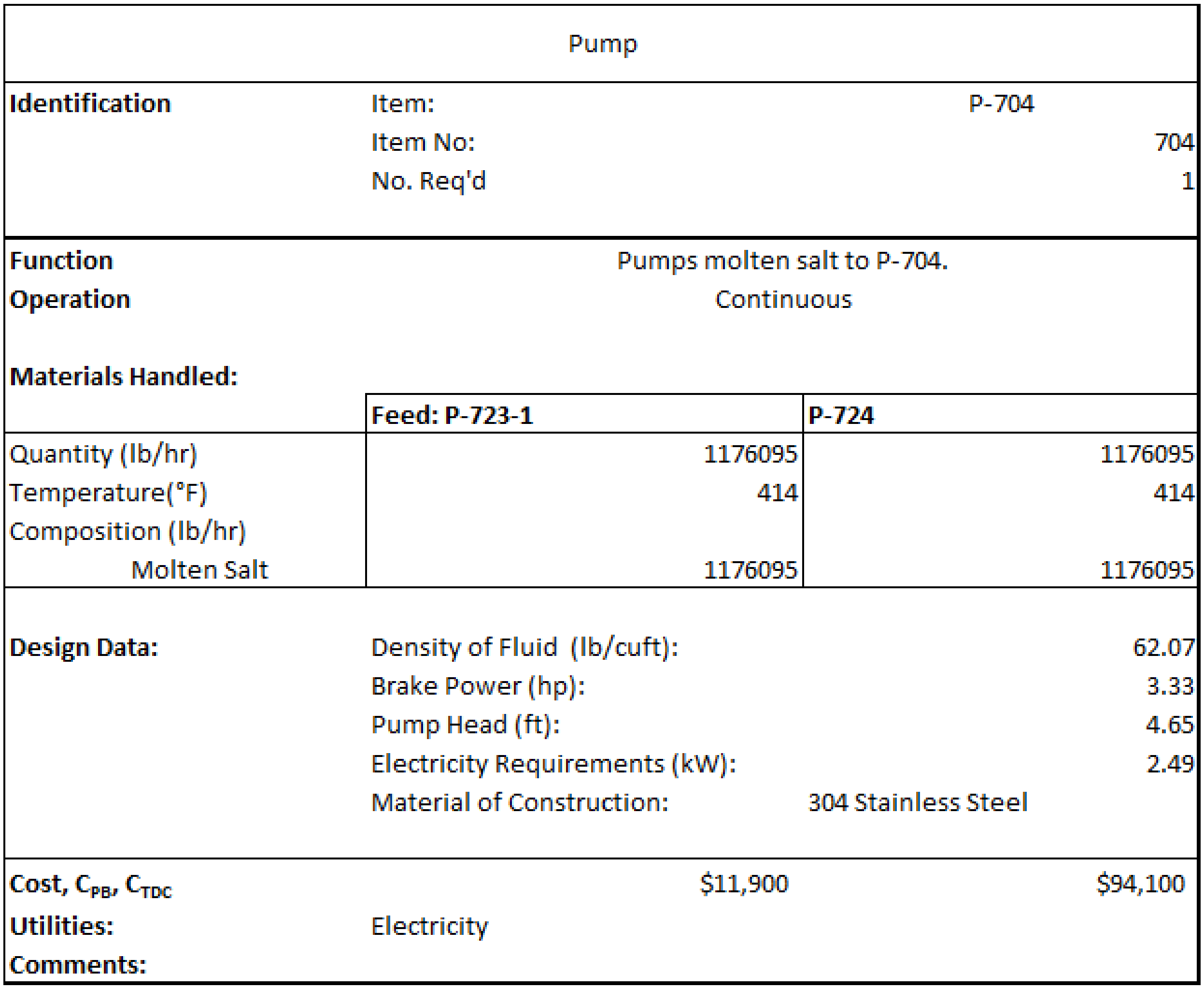
Pump			
Identification	Item:		P-700
	Item No:		700
	No. Req'd		2
Function		Pump Dowtherm A to HX-701	
Operation		Continuous	
Materials Handled:			
	Feed: S-713	**Exit: S-721**	
Quantity (lb/hr)	2660000	2660000	
Temperature(°F)	698	698	
Composition (lb/hr)			
Dowtherm A	2660000	2660000	
Design Data:	Density of Fluid (lb/cuft):		45.29
	Brake Power (hp):		9.94
	Pump Head (ft):		79.13
	Electricity Requirements (kW):		7.84
	Material of Construction:	304 Stainless Steel	
Cost, C_{PB}, C_{TDC}	$51,300	$481,700	
Utilities:	Electricity		
Comments:			



	Pump	
Identification	Item:	P-702
	Item No:	702
	No. Req'd	1
Function	Re-pump Dowtherm A through loop.	
Operation	Continuous	
Materials Handled:		
	Feed: S-719	**Exit: S-720**
Quantity (lb/hr)	5320000	5320000
Temperature(°F)	698	698
Composition (lb/hr)		
Dowtherm A	5320000	5320000
Design Data:	Density of Fluid (lb/cuft):	45.29
	Brake Power (hp):	39.77
	Pump Head (ft):	12.74
	Electricity Requirements (kW):	29.65
	Material of Construction:	304 Stainless Steel
Cost, C_{PB}, C_{TDC}	$75,600	$854,100
Utilities:	Electricity	
Comments:		

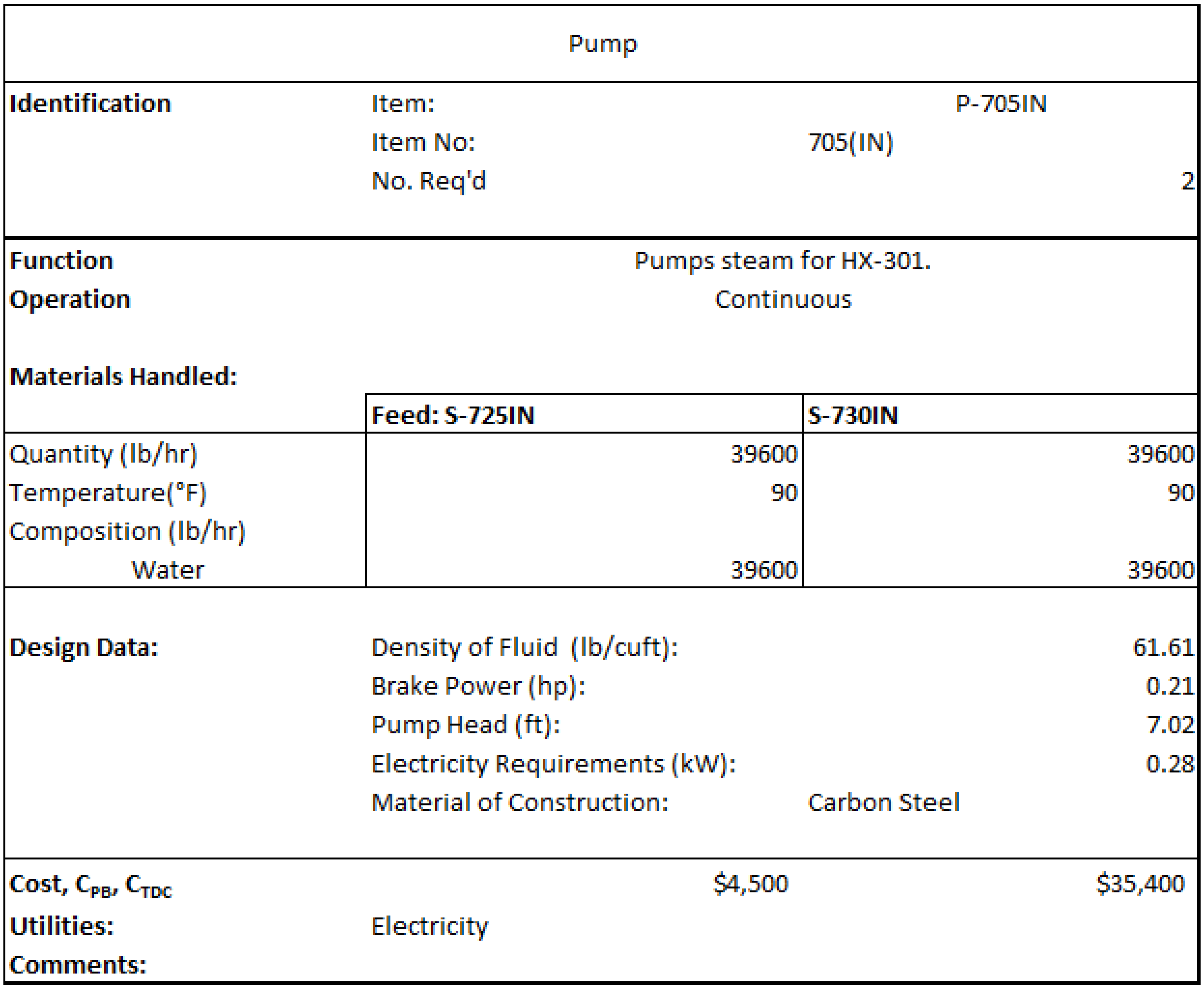


Pump		
Identification	Item:	P-703
	Item No:	703
	No. Req'd	1
Function	Pumps molten salt to P-704.	
Operation	Continuous	
Materials Handled:		
	Feed: P-723	**Exit: P-723-1**
Quantity (lb/hr)	1176095	1176095
Temperature(°F)	414	414
Composition (lb/hr)		
Molten Salt	1176095	1176095
Design Data:	Density of Fluid (lb/cuft):	62.07
	Brake Power (hp):	3.33
	Pump Head (ft):	163.8
	Electricity Requirements (kW):	60.98
	Material of Construction:	304 Stainless Steel
Cost, C_{PB}, C_{TDC}	$27,100	$114,000
Utilities:	Electricity	
Comments:		



	Pump		
Identification	Item:	P-704	
	Item No:		704
	No. Req'd		1
Function	Pumps molten salt to P-704.		
Operation	Continuous		
Materials Handled:			
	Feed: P-723-1	**P-724**	
Quantity (lb/hr)	1176095	1176095	
Temperature(°F)	414	414	
Composition (lb/hr)			
Molten Salt	1176095	1176095	
Design Data:	Density of Fluid (lb/cuft):		62.07
	Brake Power (hp):		3.33
	Pump Head (ft):		4.65
	Electricity Requirements (kW):		2.49
	Material of Construction:	304 Stainless Steel	
Cost, C_{PB}, C_{TDC}	$11,900	$94,100	
Utilities:	Electricity		
Comments:			

	Pump	
Identification	Item:	P-705
	Item No:	705
	No. Req'd	2
Function	Pumps steam for HX-301.	
Operation	Continuous	
Materials Handled:		
	Feed: S-725	**S-730**
Quantity (lb/hr)	39600	39600
Temperature(°F)	90	90
Composition (lb/hr)		
Water	39600	39600
Design Data:	Density of Fluid (lb/cuft):	61.61
	Brake Power (hp):	0.14
	Pump Head (ft):	4.68
	Electricity Requirements (kW):	0.18
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$4,500	$35,400
Utilities:	Electricity	
Comments:		

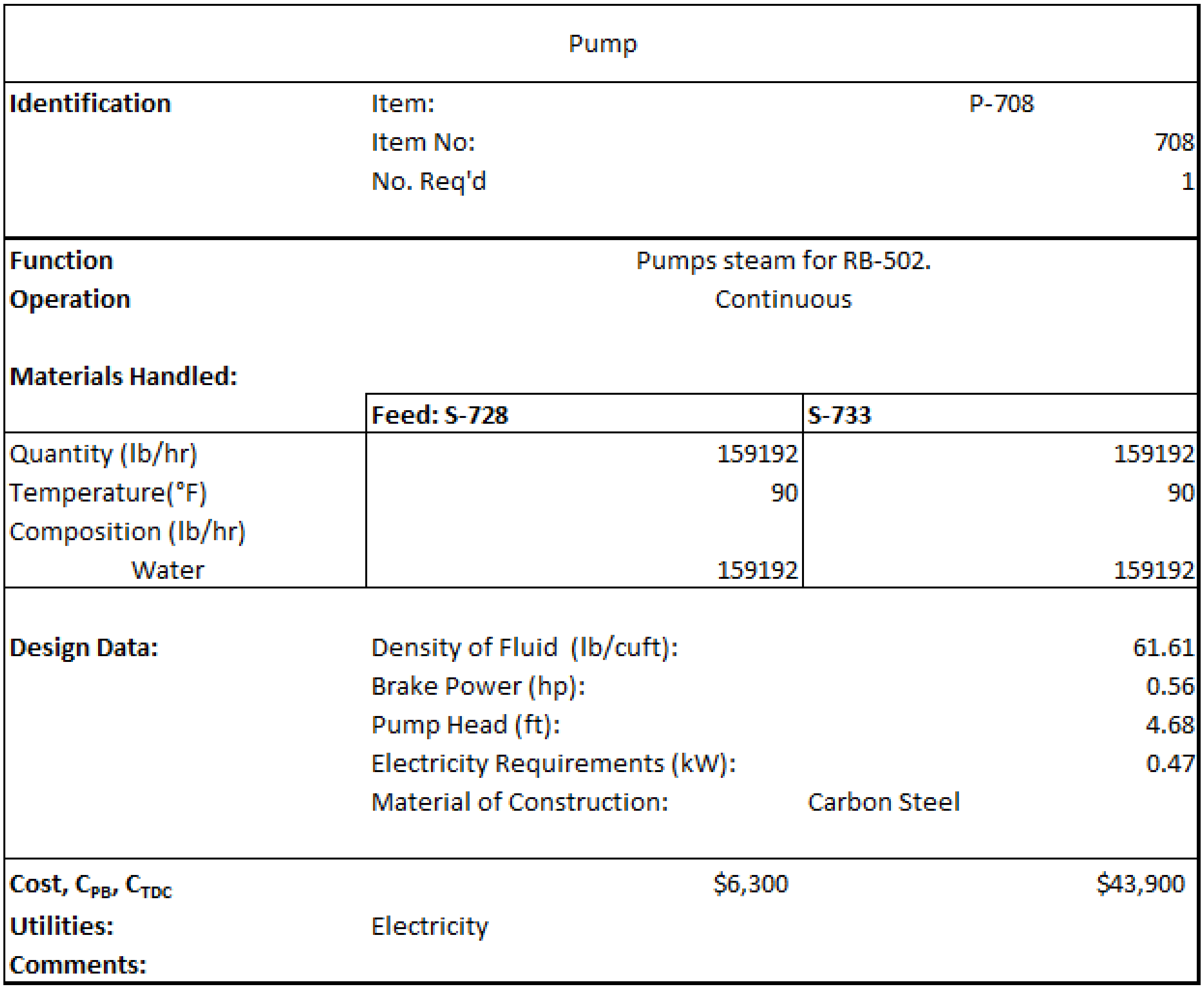


Pump		
Identification	Item:	P-705IN
	Item No:	705(IN)
	No. Req'd	2
Function	Pumps steam for HX-301.	
Operation	Continuous	
Materials Handled:		
	Feed: S-725IN	**S-730IN**
Quantity (lb/hr)	39600	39600
Temperature(°F)	90	90
Composition (lb/hr)		
Water	39600	39600
Design Data:	Density of Fluid (lb/cuft):	61.61
	Brake Power (hp):	0.21
	Pump Head (ft):	7.02
	Electricity Requirements (kW):	0.28
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$4,500	$35,400
Utilities:	Electricity	
Comments:		

Pump		
Identification	Item:	P-706
	Item No:	706
	No. Req'd	1
Function	Pumps steam for RB-500.	
Operation	Continuous	
Materials Handled:		
	Feed: S-726	**S-731**
Quantity (lb/hr)	86174	86174
Temperature(°F)	90	90
Composition (lb/hr)		
Water	86174	86174
Design Data:	Density of Fluid (lb/cuft):	61.61
	Brake Power (hp):	0.34
	Pump Head (ft):	4.68
	Electricity Requirements (kW):	0.25
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$5,200	$40,500
Utilities:	Electricity	
Comments:		

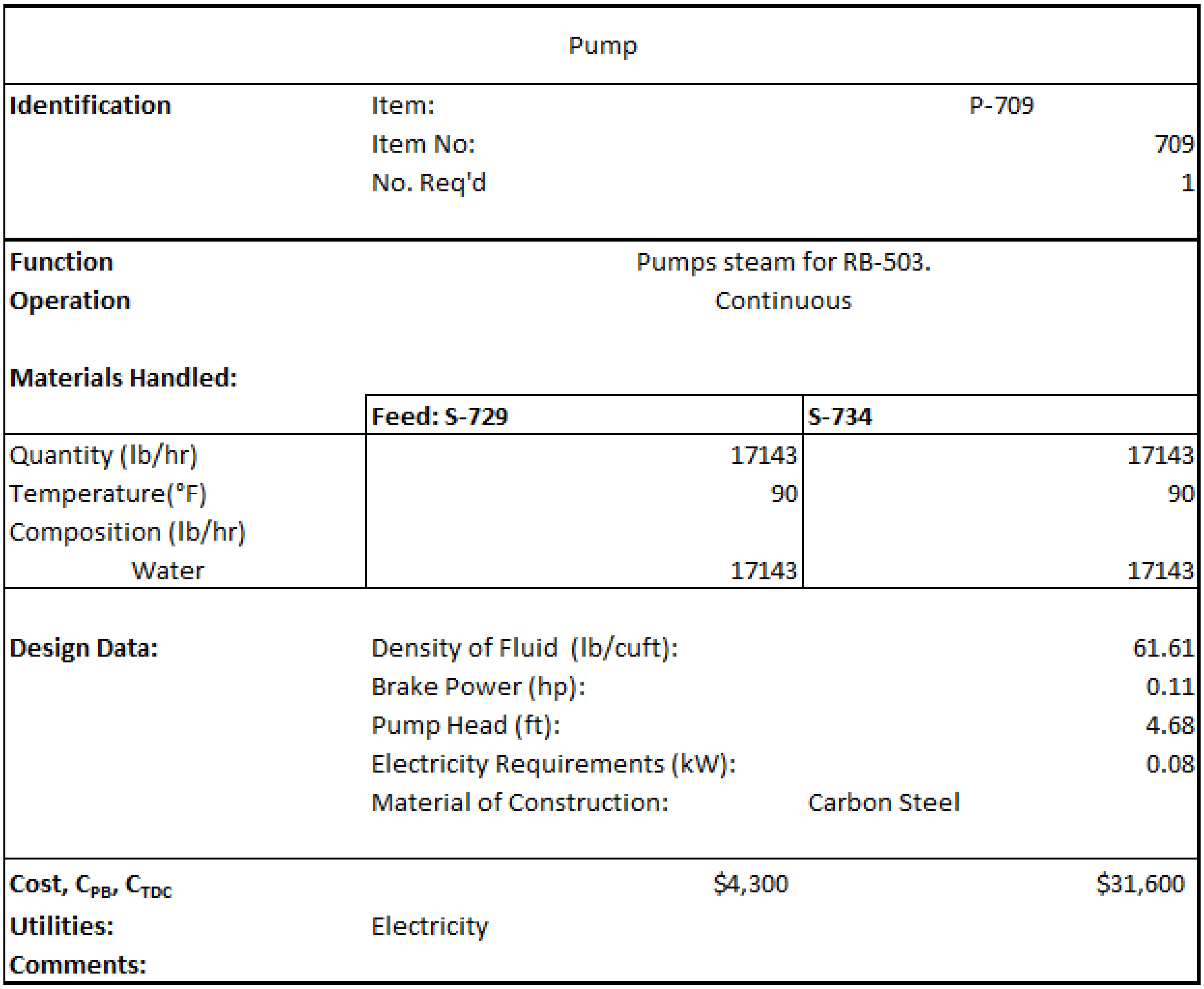
	Pump	
Identification	Item:	P-706IN
	Item No:	706(IN)
	No. Req'd	1
Function	Pumps steam for HX-301.	
Operation	Continuous	
Materials Handled:		
	Feed: S-726IN	**S-731IN**
Quantity (lb/hr)	86174	86174
Temperature(°F)	90	90
Composition (lb/hr)		
Water	86174	86174
Design Data:	Density of Fluid (lb/cuft):	61.61
	Brake Power (hp):	0.51
	Pump Head (ft):	7.02
	Electricity Requirements (kW):	0.38
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$4,500	$36,600
Utilities:	Electricity	
Comments:		

	Pump		
Identification	Item:	P-707	
	Item No:		707
	No. Req'd		1
Function		Pumps steam for RB-501.	
Operation		Continuous	
Materials Handled:			
	Feed: S-727	**S-732**	
Quantity (lb/hr)	53087	53087	
Temperature(°F)	90	90	
Composition (lb/hr)			
Water	53087	53087	
Design Data:	Density of Fluid (lb/cuft):		61.61
	Brake Power (hp):		0.23
	Pump Head (ft):		4.68
	Electricity Requirements (kW):		0.17
	Material of Construction:	Carbon Steel	
Cost, C_{PB}, C_{TDC}	$4,700	$36,600	
Utilities:	Electricity		
Comments:			



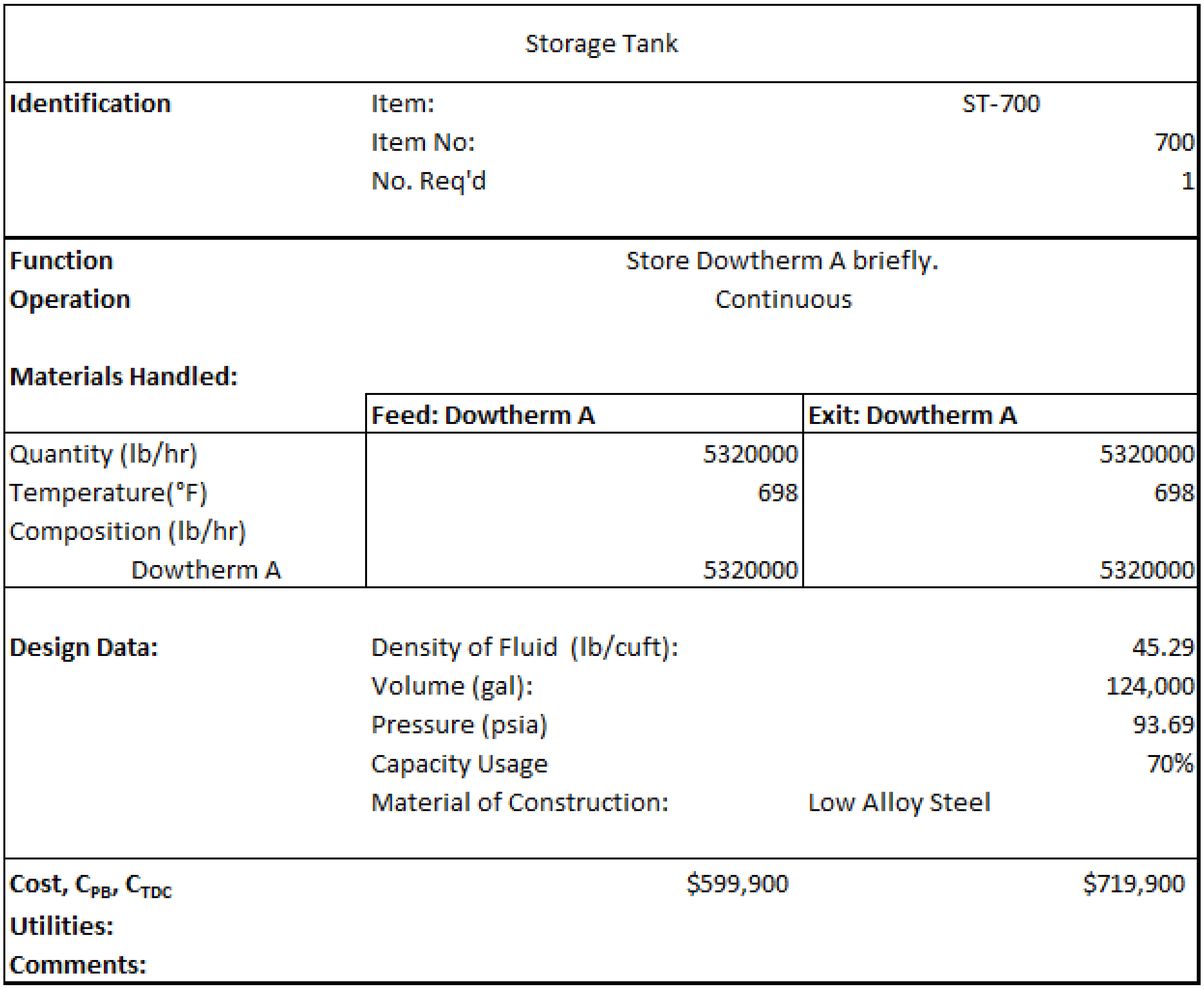
Pump		
Identification	Item:	P-708
	Item No:	708
	No. Req'd	1
Function	Pumps steam for RB-502.	
Operation	Continuous	
Materials Handled:		
	Feed: S-728	**S-733**
Quantity (lb/hr)	159192	159192
Temperature(°F)	90	90
Composition (lb/hr)		
Water	159192	159192
Design Data:	Density of Fluid (lb/cuft):	61.61
	Brake Power (hp):	0.56
	Pump Head (ft):	4.68
	Electricity Requirements (kW):	0.47
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$6,300	$43,900
Utilities:	Electricity	
Comments:		

Pump		
Identification	Item:	P-708IN
	Item No:	708IN
	No. Req'd	1
Function	Pumps steam for RB-502.	
Operation	Continuous	
Materials Handled:		
	Feed: S-728IN	**S-733IN**
Quantity (lb/hr)	159192	159192
Temperature(°F)	90	90
Composition (lb/hr)		
Water	159192	159192
Design Data:	Density of Fluid (lb/cuft):	61.61
	Brake Power (hp):	0.84
	Pump Head (ft):	7.02
	Electricity Requirements (kW):	0.63
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$6,300	$43,900
Utilities:	Electricity	
Comments:		



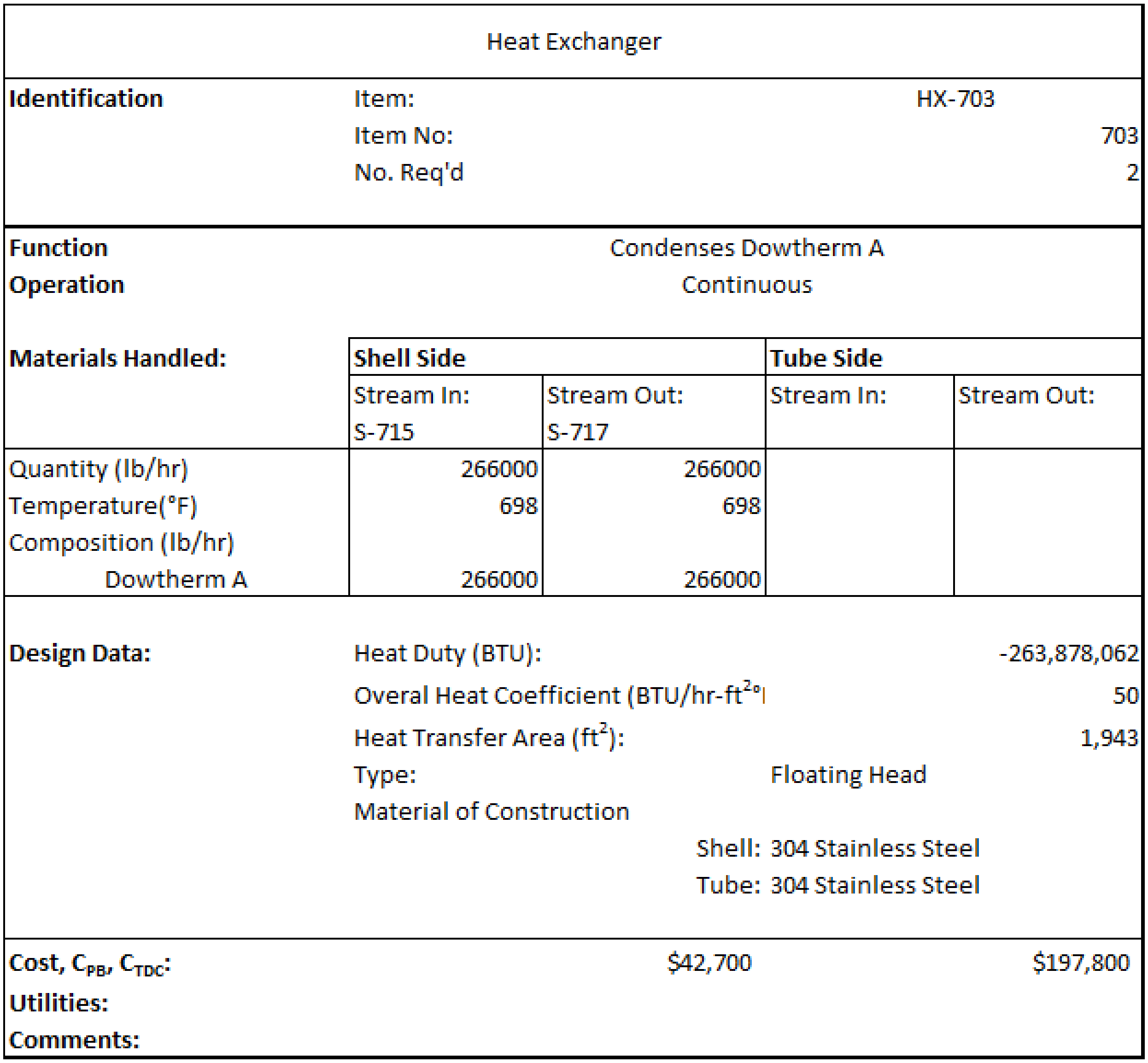
Pump		
Identification	Item:	P-709
	Item No:	709
	No. Req'd	1
Function	Pumps steam for RB-503.	
Operation	Continuous	
Materials Handled:		
	Feed: S-729	**S-734**
Quantity (lb/hr)	17143	17143
Temperature(°F)	90	90
Composition (lb/hr)		
Water	17143	17143
Design Data:	Density of Fluid (lb/cuft):	61.61
	Brake Power (hp):	0.11
	Pump Head (ft):	4.68
	Electricity Requirements (kW):	0.08
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$4,300	$31,600
Utilities:	Electricity	
Comments:		

Pump		
Identification	Item:	P-709IN
	Item No:	709IN
	No. Req'd	1
Function	Pumps steam for RB-503.	
Operation	Continuous	
Materials Handled:		
	Feed: S-729IN	**S-734IN**
Quantity (lb/hr)	17143	17143
Temperature(°F)	90	90
Composition (lb/hr)		
Water	17143	17143
Design Data:	Density of Fluid (lb/cuft):	61.61
	Brake Power (hp):	0.16
	Pump Head (ft):	7.02
	Electricity Requirements (kW):	0.12
	Material of Construction:	Carbon Steel
Cost, C_{PB}, C_{TDC}	$4,300	$31,600
Utilities:	Electricity	
Comments:		



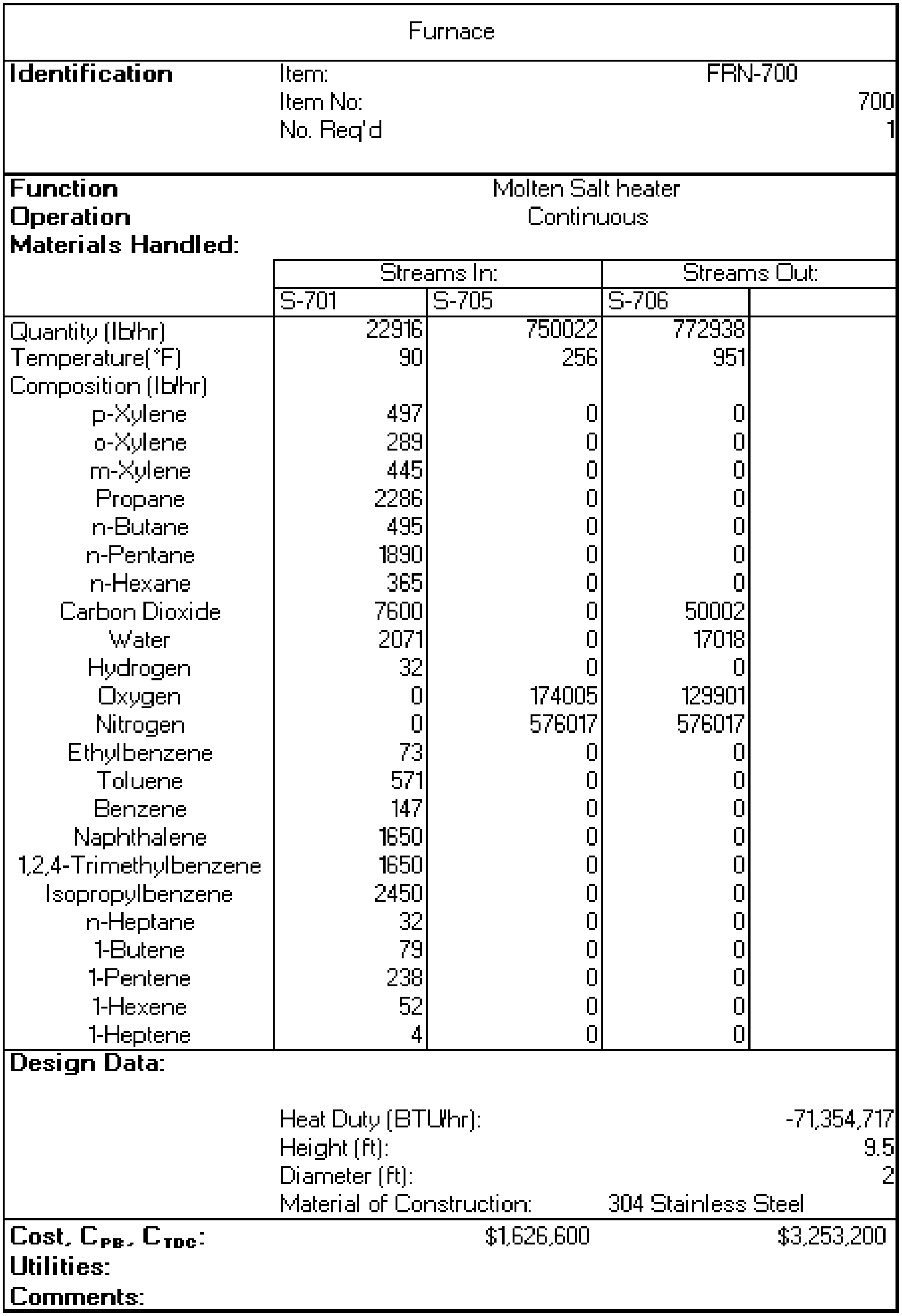
	Storage Tank		
Identification	Item:		ST-700
	Item No:		700
	No. Req'd		1
Function		Store Dowtherm A briefly.	
Operation		Continuous	
Materials Handled:			
	Feed: Dowtherm A	**Exit: Dowtherm A**	
Quantity (lb/hr)	5320000	5320000	
Temperature(°F)	698	698	
Composition (lb/hr)			
Dowtherm A	5320000	5320000	
Design Data:	Density of Fluid (lb/cuft):		45.29
	Volume (gal):		124,000
	Pressure (psia)		93.69
	Capacity Usage		70%
	Material of Construction:	Low Alloy Steel	
Cost, C_{PB}, C_{TDC}	$599,900	$719,900	
Utilities:			
Comments:			

Storage Tank		
Identification	Item:	ST-701
	Item No:	701
	No. Req'd	1
Function	Store Dowtherm A briefly.	
Operation	Continuous	
Materials Handled:		
	Feed: Solar Salt	**Exit: Solar Salt**
Quantity (lb/hr)	1176095	1176095
Temperature(°F)	900	900
Composition (lb/hr)		
Dowtherm A	1176095	1176095
Design Data:	Density of Fluid (lb/cuft):	62.07
	Volume (gal):	639,300
	Pressure (psia)	17.7
	Capacity Usage	70%
	Material of Construction:	304 Stainless Steel
Cost, C_{PB}, C_{TDC}	$329,400	$658,800
Utilities:		
Comments:		



		Heat Exchanger		
Identification	Item:			HX-703
	Item No:			703
	No. Req'd			2
Function		Condenses Dowtherm A		
Operation		Continuous		
Materials Handled:	**Shell Side**		**Tube Side**	
	Stream In: S-715	Stream Out: S-717	Stream In:	Stream Out:
Quantity (lb/hr)	266000	266000		
Temperature(°F)	698	698		
Composition (lb/hr)				
Dowtherm A	266000	266000		
Design Data:	Heat Duty (BTU):			-263,878,062
	Overal Heat Coefficient (BTU/hr-ft^{2}°			50
	Heat Transfer Area (ft^{2}):			1,943
	Type:		Floating Head	
	Material of Construction			
		Shell:	304 Stainless Steel	
		Tube:	304 Stainless Steel	
Cost, C_{PB}, C_{TDC}:		$42,700		$197,800
Utilities:				
Comments:				

Furnace				
Identification	Item:		FRN-701	
	Item No:			701
	No. Req'd			2
Function		Dowtherm A heater		
Operation		Continuous		
Materials Handled:				
	Streams In:		Streams Out:	
	S-703	S-707	S-708	
Quantity (lb/hr)	89889	3750111	3840000	
Temperature(°F)	90	256	1103	
Composition (lb/hr)				
p-Xylene	1951	0	0	
o-Xylene	1132	0	0	
m-Xylene	1754	0	0	
Propane	8966	0	0	
n-Butane	1941	0	0	
n-Pentane	7410	0	0	
n-Hexane	1433	0	0	
Carbon Dioxide	29809	0	196120	
Water	8122	0	66750	
Hydrogen	124	0	0	
Oxygen	0	870026	697045	
Nitrogen	0	2880085	2880085	
Ethylbenzene	285	0	0	
Toluene	2241	0	0	
Benzene	577	0	0	
Naphthalene	6471	0	0	
1,2,4-Trimethylbenzene	6467	0	0	
Isopropylbenzene	9610	0	0	
n-Heptane	125	0	0	
1-Butene	312	0	0	
1-Pentene	935	0	0	
1-Hexene	206	0	0	
1-Heptene	18	0	0	
Design Data:				
	Heat Duty (BTU/hr):			-263,915,627
	Height (ft):			13
	Diameter (ft):			3
	Material of Construction:		Carbon Steel	
Cost, C_{PB}, C_{TDC}:		$5,186,600		$5,186,000
Utilities:				
Comments:				



Furnace

Identification Item: FRN-700

Item No: 700

No. Req'd 1

Function Molten Salt heater

Operation Continuous

Materials Handled:

	Streams In:		Streams Out:	
	S-701	S-705	S-706	
Quantity (lb/hr)	22916	750022	772938	
Temperature(°F)	90	256	951	
Composition (lb/hr)				
p-Xylene	497	0	0	
o-Xylene	289	0	0	
m-Xylene	445	0	0	
Propane	2286	0	0	
n-Butane	495	0	0	
n-Pentane	1890	0	0	
n-Hexane	365	0	0	
Carbon Dioxide	7600	0	50002	
Water	2071	0	17018	
Hydrogen	32	0	0	
Oxygen	0	174005	129901	
Nitrogen	0	576017	576017	
Ethylbenzene	73	0	0	
Toluene	571	0	0	
Benzene	147	0	0	
Naphthalene	1650	0	0	
1,2,4-Trimethylbenzene	1650	0	0	
Isopropylbenzene	2450	0	0	
n-Heptane	32	0	0	
1-Butene	79	0	0	
1-Pentene	238	0	0	
1-Hexene	52	0	0	
1-Heptene	4	0	0	

Design Data:

Heat Duty (BTU/hr): -71,354,717

Height (ft): 9.5

Diameter (ft): 2

Material of Construction: 304 Stainless Steel

Cost, C_{PB}, C_{TDC}: $1,626,600 $3,253,200

Utilities:

Comments:

Furnace

Identification	Item:	FRN-703
	Item No:	703
	No. Req'd	1

Function	Provides steam for reboilers, WC-500 and HX-301
Operation	Continuous
Materials Handled:	

	Streams In:		Streams Out:	
	S-704	S-711	S-712	
Quantity (lb/hr)	79783	8365631	8445414	
Temperature(°F)	90	256	508	
Composition (lb/hr)				
p-Xylene	1732	0	0	
o-Xylene	1005	0	0	
m-Xylene	1550	0	0	
Propane	7959	0	0	
n-Butane	1723	0	0	
n-Pentane	6577	0	0	
n-Hexane	1272	0	0	
Carbon Dioxide	26460	0	174086	
Water	7210	0	59248	
Hydrogen	110	0	0	
Oxygen	0	1940826	1787275	
Nitrogen	0	6424805	6424805	
Ethylbenzene	253	0	0	
Toluene	1989	0	0	
Benzene	512	0	0	
Naphthalene	5744	0	0	
1,2,4-Trimethylbenzene	5740	0	0	
Isopropylbenzene	8530	0	0	
n-Heptane	111	0	0	
1-Butene	277	0	0	
1-Pentene	830	0	0	
1-Hexene	183	0	0	
1-Heptene	16	0	0	

Design Data:

Heat Duty (BTU/hr):		-315,781,138
Height (ft):		12.5
Diameter (ft):		3
Material of Construction:	Carbon Steel	

Cost, C_{PB}, C_{TDC}:	$1,495,600	$1,495,600
Utilities:		
Comments:		

Section VII

Other Considerations

VII. OTHER CONSIDERATIONS

Alternate Design Considerations

Removal of Aqueous Phase Reforming Section

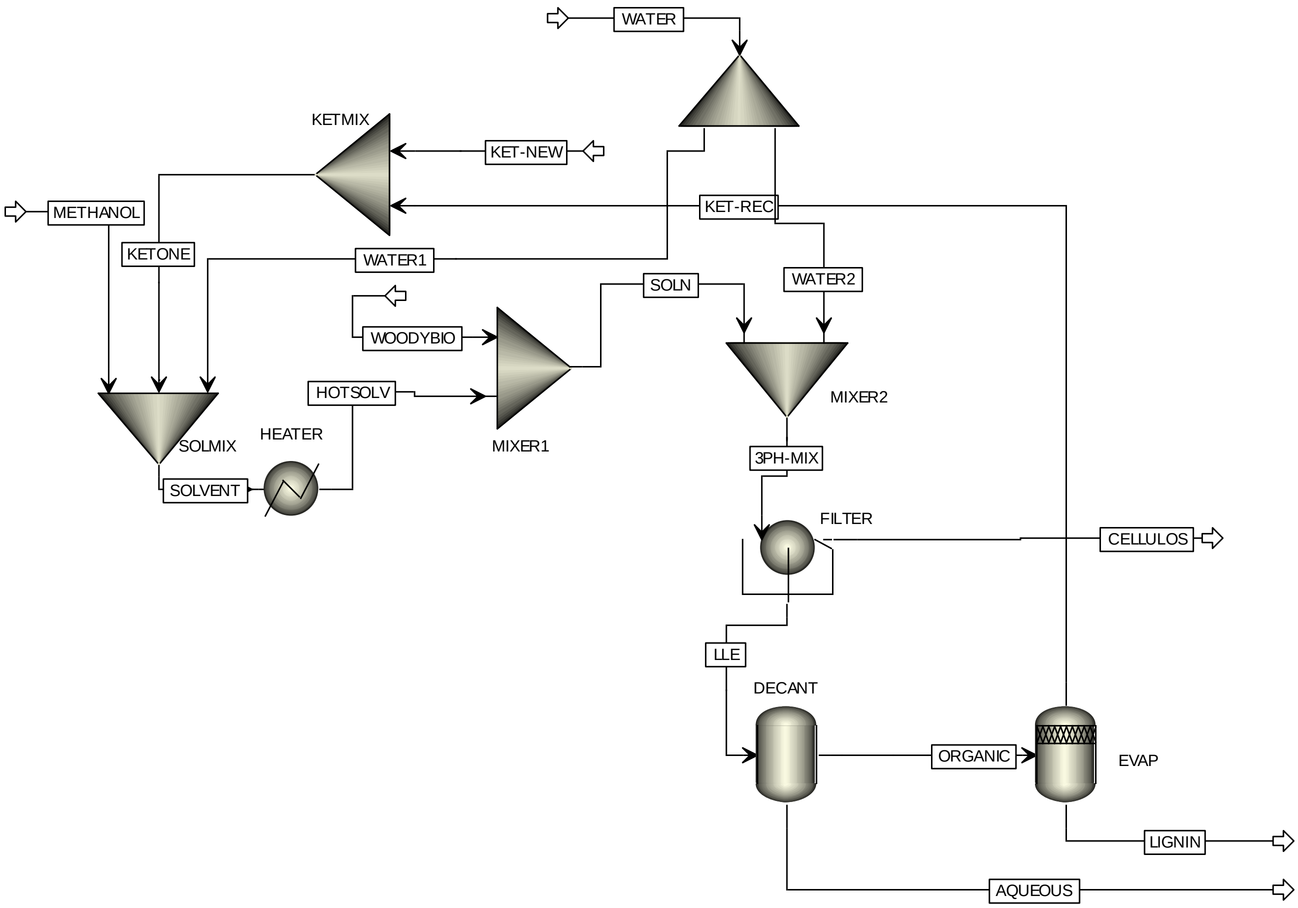
A major section of this process is based upon Virent Corporation's aqueous phase reforming technology, which is detailed in WO2007/075476-A2 and several other patents. The appeal of the aqueous phase reforming technology is that it generates hydrogen *in situ* for use in hydrogenation, a necessary step in getting from oxygenated hydrocarbon to p-xylene. Unfortunately, however, the analysis presented herein reveals that APR is quite costly due to the compression needs and exotic catalysts. This resulted in consideration of removing the APR section. Doing so would eliminate about six process units, $2M in electricity, and over $78M of catalyst technology. The substitute cost would be the external purchase of hydrogen. However, purchasing hydrogen from an economical source goes hand-in-hand with purchasing it from a non-green source, which goes against the purpose of this design. This would not be justified unless savings and impact on NPV were dramatic. As it turns out, even removing the entire 300 section of the flowsheet has limited impact on bottom line profitability. Although the large capital outlay, much of which is directly traceable to section 300, contributes to a large negative NPV, the major cost driver is input materials. Therefore, even a change as substantial as this is not enough to turn NPV positive (although it should be noted that IRR becomes positive, without accounting for the cost of hydrogen).Thus, this design is discarded because its benefit is not nearly enough to justify its lack of sustainability.

Woody Biomass with Three-Phase Hot Water Extraction

Due to its high per pound cost, corn dry grind was never an attractive feedstock. Of the two remaining options, woody biomass was the cheaper raw material. However, two unique processing steps were necessary to convert it into usable simple sugars: extraction of the cellulose, and enzymatic cleaving of the ether bonds in the cellulose chains. In contrast, molasses was slightly more expensive upfront, but required only the additional clarification step prior to hydrolysis.

Initially, separating the biomass into its different components, each of which served a different purpose, posed a challenge. However, US Patent 5730837 described a unique, one-step sequence that generated three phases, each of which contained one of the necessary components. In short, the biomass would be heated in a mixture of ketone and water insoluble at room temperature until a single-phase solution was obtained. Then, by cooling and/or adding additional water, the three phases would separate into three separate phases. The cellulose would remain as solid precipitate to filter out and convert enzymatically into simple sugars.. The hemicelluloses and simple sugars would remain aqueous, and could be sent for completed breakdown into simple sugars. Finally, the lignin would remain in the organic solvent, most of which could be recovered before sending the lignin to the furnace to burn. An example of this process is shown in Figure 14 below.

Figure 14

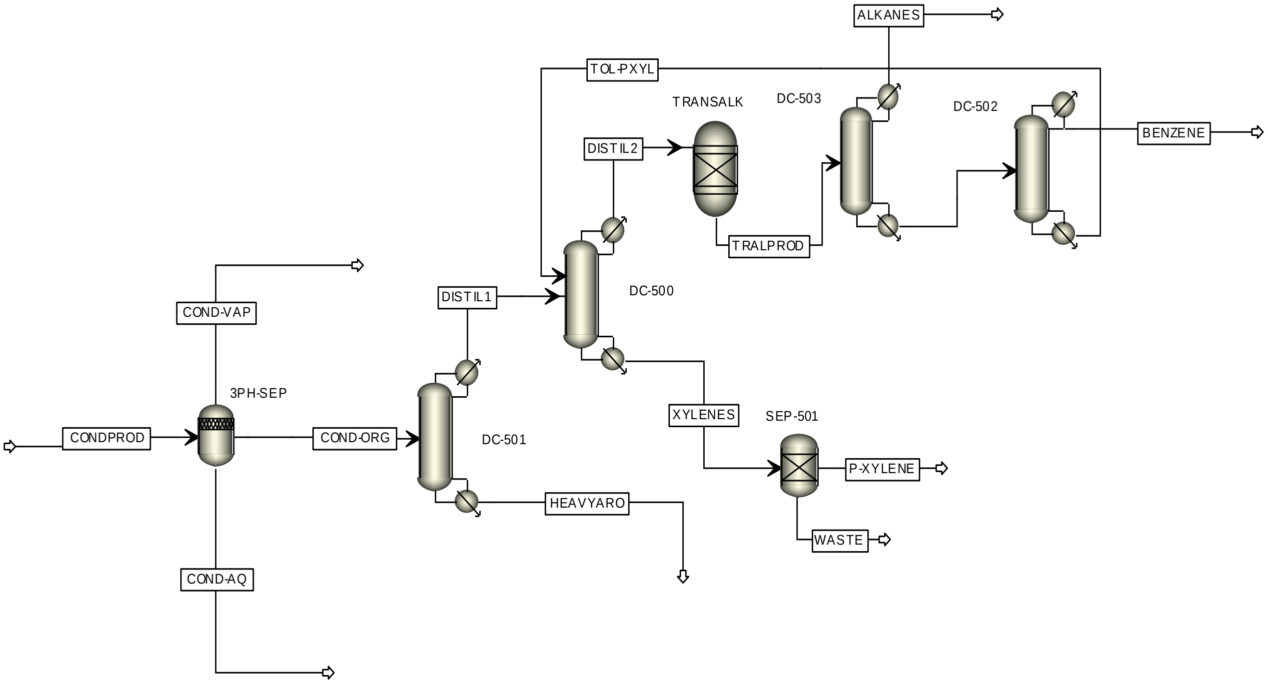


Even with this streamlined separation process, the high cost of enzymes required to process the cellulose, from which the majority of the sugar for para-xylene production would be derived, rendered woody biomass economically inferior to molasses.

Alternative Separation Scheme

The separation scheme used for the renewable production of para-xylene can be varied drastically. An alternative design is presented in Figure 15 below. Note that the blocks are labeled such that the columns in the actual process have the same light and heavy key’s as blocks with the same name below (e.g. DC-500 always separates between xylenes and toluene).

Figure 15



In this scheme, DC-500 and DC-501 have been switched, meaning the heavy aromatics are taken off before the light in the isolation of para-xylene. While certainly possible, this option was not pursued because the separation between para-xylene and the next heaviest species, isopropylbenzene, in DC-501 is far more difficult and requires a larger column and more stages than the xylene/toluene separation in DC-500. It is cheaper to deal with the larger quantity of material in the shorter column, DC-500. In addition, because the three phase separator operates at cooler temperatures than the distillation columns, it is also cheaper to do the lower-temperature distillation (DC-500) first, rather than heating to the higher temperature and then cooling again.

In this scheme, DC-502 and DC-503 have also been switched. This decision can be made independently of the order of DC-500 and DC-501. In this case, the pentane separation is easier, and, all other things being equal, it would be cheaper to drive off the alkanes first, as depicted above. However, the transalkylation occurs at temperatures higher than the distillation columns. As such, it is actually cheaper to take off the heavy constituents, xylene and toluene, as they condense, rather than to condense everything other than the alkanes and reheat afterwards, as depicted above.

Invertase-Catalyzed Sucrose Hydrolysis

In the food industry, the enzyme invertase is commonly used to catalyze the sucrose hydrolysis reaction. It is a proven technology which operates under easily attainable conditions. Invertase is added to a 60% sucrose solution and then heated to 60 °C. Citric acid is then added to make the solution have a pH of 4.5. The invertase takes 12 hours to fully convert the sucrose into fructose and glucose.

However, the prohibiting factor is that invertase costs around $40 per kilogram and a kilogram of invertase is required to invert one metric ton of sucrose. Invertase is also difficult to recover from the product. Because of the high cost, the choice was made to use a zeolite catalyst in a fixed bed reactor instead.

Plant Startup

Because the hydrogenation section requires a large amount of hydrogen (3655 lbmol per hour), a supply of hydrogen will have to be available until the plant can produce enough hydrogen to sustain itself through the aqueous phase reforming reaction. The pressure swing adsorption contains a large pressure vessel used to store up to a 21 hour supply of hydrogen. This storage vessel will be able to supply hydrogen for any future plant startups after the first time.

The furnaces are fired from byproduct gases such as alkanes and aromatics so a supply of natural gas will have to be available to fire the furnaces in order to produce process steam and heat the Dowtherm A and molten salt. Additionally, the salt will have to be melted if allowed to solidify.

On startup, auxiliary heat might have to be provided to several streams since streams farther down the process would not be heated to their expected values, causing heat exchangers to operate at non-ideal conditions. Because the plant utilizes many heat exchangers to preheat and cool streams, this could pose a major challenge.

The aqueous phase separated from the flash vessel in the separation section (SEP-500) is used as cooling water for a high temperature stream, so a secondary source of cooling water must be provided to operate HX-601.

Sodium hydroxide is used as a catalyst in the APR reaction, and is recovered through the flash vessel after the reaction (F-300), so no additional sodium hydroxide needs to be added after startup. The sodium hydroxide will have to be added into the recycle loop as the plant starts up.

Environmental Considerations

The primary impact on the environment is the release of waste carbon dioxide. The plant releases approximately 1.5 million tons per year of carbon dioxide. In addition, 20,000 tons per year of carbon monoxide are released into the atmosphere. Approximately 10,000 tons per year of propane and other alkanes are released as well.

A 2005 report by the Center for Climate and Energy Solutions reported that the cost to sequester carbon dioxide ranged from $30 to $90 per ton of carbon dioxide. At $30 per ton it would cost $45 million per year to sequester all of the carbon released from the plant. This is clearly an expensive option, but it is not unfeasible given the expected $325M/yr revenue. That said, the operating margin is currently nowhere near able to support a variable cost of this magnitude.

The process also requires 40.3 bgal/y of water, or 11.8 bgal/y excluding HX-401. As noted earlier, HX-401 is a serious cause for concern, but it will likely be straightforward to discover improvements. Ignoring HX-401 for now, the process uses about 4.1 gal water/gal of p-xylene, which is higher than the industry benchmark of 3 gal/gal. However, it is close enough to be encouraging. In fact, excluding chilled water, the ratio is 3.7 gal/gal. Clearly there is room for improvement in term of cooling water recycle. With a bit of careful consideration – specifically with regard to water cooling rates in open air – a zero-discharge plant is well within reach.

In addition, some organic compounds, mostly naphthalene, 1,2,4-trimethylbenzene, and isopropylbenzene, are encountered as waste products from DC-501. These compounds are currently burned in the furnace; however, they could be separated further and sold, although the economics of this have not been explored.

The plant succeeds at producing para-xylene from renewable sources. The only input to the process is molasses. Cooling water is used extensively, but the plant could easily switch to a closed loop cooling water system.

Process Control

The process operates at temperatures and pressures provided in specific examples found in patents and other relevant literature. Consequently, a narrow acceptable range of operating conditions are assumed for all sections of the process and all reactors in particular. Further research may reveal a wider range of acceptable operating conditions for some or all process units. However, the strategies for control explained within this section should still apply.

A full analysis of process control requirements, as well as the design of a corresponding system, falls beyond the scope of this report. However, the critical elements of the process variables to be controlled, as well as potential strategies for controlling these variables, are disclosed. Following the additional research recommended by this report, the following concerns should be addressed in the next iteration of this process's design.

Section 100: Hydrolysis

The streams and blocks associated with hydrolysis must be controlled such that (a) the sucrose feed (S-100) to each hydrolysis reactor (R-100, R-101, and R-102) enters at 212.0 degrees

Fahrenheit and 41.1 psia, and (b) the glucose/fructose stream (S-119) is feed to hydrogenation at the proper pressure.

To set pressure, power to the pre-hydrolysis pumps (P-100, P-101, and P-102) and post-hydrolysis pumps (P-103, P-104, and P-105) will adjusted as necessary in response to readings from a pressure sensors, most likely variable capacitance differential pressure transducers.

The temperature poses a greater challenge, as it results only from the exchange of heat between the sucrose feeds (S-104, S-105, and S-106) and the condensation product streams (S-417, S-418, S-419). For mild temperature disturbances, increasing or decreasing the flow rate of the condensation product (S-416) would raise or lower (respectively) the temperature of the sucrose streams (S-106, S-107, and S-108) exiting the heat exchangers and entering the hydrolysis reactors. This control system would require holdup tanks both preceding and following the heat exchangers (HX-100, HX-101, and HX-102) in order to ensure no disturbances elsewhere in the process. Because cooling water is ultimately used to bring the condensation product to an appropriate temperature for separation, the flow rate of the cooling water can be varied to compensate for the discrepancies in cooling achieved in the heat exchangers (HX-100, HX-101, and HX-102) as a result of these techniques. If severe disturbances are expected, the process will require investment in an additional heater and/or cooler to which a fraction of the disturbed stream (S-100) can be diverted.

Section 200: Hydrogenation

Successful hydrogenation will rely on proper control of the temperature and pressure of both the hydrogen (S-316) and sugar (S-226) feeds to the reactors. Discussion of the hydrogen stream (S-316) can be found in this section under Aqueous Phase Reforming, below. Pressure of the sugar stream (S-119) was set using automated pumps (P-103, P-104, and P-105) discussed under Hydrolysis, above. Cooling water (CW-100) in heat exchanger (HX-200) sets the temperature. As such, the flow rate of the cooling water (CW-100) can be varied to achieve the desired temperature.

Section 300: Aqueous Phase Reforming

Although more complex than previous sections, the Aqueous Phase Reforming has only one block that requires precise control: the reforming reactor itself (R-300). The feed stream (S-305) must enter the reactor at the desired conditions, 360 degrees Fahrenheit and 725 psia. The pressure is achieved through a pair of pumps (P-302 and P-300), and power to the latter can be varied based on information from a sensor, most likely a variable capacitance differential pressure transducer on the second pump's feed stream (S-303) in order to achieve the desired pressure. Although heat is recovered from the hydrogen product stream (S-311) in a heat exchanger located between the pumps (HX-300), the temperature of the sorbitol feed (S-305) is ultimately set by a second heat exchanger (HX-301) that uses steam (S-727) heated by the furnace as a heat source. As such, the temperature or the flow rate of the steam (S-727) can be varied based on a temperature sensor, most likely a thermocouple on the pressurized sorbitol stream (S-304), to achieve the desired temperature.

Other streams of direct consequence include the exiting hydrogen (S-316) for hydrogenation and exiting sorbitol (S-402) for condensation; the alkanes leaving the separator are simply sent to the furnace. After recovering some heat in a first pair of exchangers (HX-300 and HX-400) as well as cooling prior to entering the compressor (HX-303 prior to flash drum F-301 and compressor SEP-300), the outlet temperature of the hydrogen is ultimately set by a final heat exchanger (HX-302) which uses cooling water; as such, the flow rate of the cooling water can be varied to control the temperature based on information obtained from a temperature sensor, most likely a thermocouple on the post-heat-recovery stream (S-315). The sorbitol outlet (S-402) undergoes recovers some heat from the hydrogen (S-314 in heat exchanger HX-400) but will undergo much more processing in the condensation region of the process before it must be fed to the condensation reactors (R-400, R-401, R-402, and R-403).

Section 400: Condensation

For condensation, feed sorbitol stream (S-407) must enter at the proper conditions, 204 degrees Fahrenheit and 640 psia. Both the transalkylation product (S-601) and pre-crystallization xylenes (S-507), from which heat is recovered via heat exchangers (HX-402 and HX-403), are cooled later using either cooling water or chilled water, and can more easily be controlled in those later exchangers. The sorbitol feed (S-407) ultimately enters the condensation reactors (R-400, R-401, R-402, and R-403) at the exit temperature of the final heat exchanger (HX-404), which uses Dowtherm A as a hot stream. Since the Dowtherm's only function is to transfer heat from the furnace to the condensation feed, the temperature or flow rate of the Dowtherm can be varied based on temperature data from the pre-exchanger (HX-404) sorbitol stream (S-405) collected via sensor, most likely a thermocouple. Heat recovery and cooling of the condensation product stream (S-416) is discussed in other sections.

Section 500: Separation

The separations section of the process requires little control. All separators operate at atmospheric pressure, and the transalkylation product (S-604) is cooled in Section 600.The only streams requiring control are the crystallization feed (S-520) and initial condensation product (S-423). The crystallization feed temperature is controlled by changing the flow rate of chilled water (CW-502) and ethylene refrigerant through the two pre-crystallization heat-exchangers (HX-501 and REF-500) based on temperature data obtained from a sensor, most likely a thermocouple on the pre-cooling stream (S-520). Similarly, after expansion to near atmospheric pressure, the proper temperature for the condensation product (S-423) is achieved by exchanging heat with cooling water (CW-400) in a pre-separation heat exchanger (HX-401). If the temperature of the post-heat-recovery stream (S-423) varies, either randomly or as a result of the control system described for Section 100, the flow rate of the cooling water can be varied to compensate based on information from a temperature sensor, most likely a thermocouple, on the pre-cooling stream (S-424). If the flow rate were to vary as a result of the same control scheme, the holdup tank previously discussed in Section 100 would be used to prevent disturbance in Section 500.

Following the first three-phase separator (SEP-500), each distillation column (DC-500, DC-501, DC-502, and DC-503) is designed to operate with feed at the outlet temperature from the previous column. The designs are also robust enough that mild variation in the outlet temperatures does not dramatically affect the quality of separation. Properties of all streams exiting Section 500 are controlled elsewhere in the process: the vapor (S-500) from the three-phase separator (SEP-500), the heavy aromatics (S-509) from the crystallizer (SEP-501) and the alkanes (S-518) from the second post-transalkylation column (DC-503) are burned in the furnace; the distillate (S-512) from the first column (DC-500) is heated elsewhere prior to transalkylation; the xylenes-rich distillate (S-507) from the second column (DC-501) is cooled using heat recovery and chilled water prior to crystallization; finally, the benzene in the bottoms (S-519) from the second post-transalkylation column (DC-503) and para-xylene (S-510) leaving the crystallizer (SEP-501) are final products requiring no further treatment. Look at SC-500 for three-phase separation calculation.

Section 600: Transalkylation

The temperature and pressure of the transalkylation feed (S-600) must be controlled to the specified temperature and pressure, 850 degrees Fahrenheit and 150 psia. To achieve these conditions, the distillate (S-512) from the first distillation column (DC-500) is heated in a heat exchanger (HX-600) using molten-salt (S-723). Since the salt’s only function is to heat the transalkylation feed, the temperature or flow rate of the salt can be varied based on information from a temperature sensor, most likely a thermocouple on the pre-heating stream (S-512), to achieve the desired cold stream (S-600) outlet temperature.

The reactor outlet (S-601) must be cooled to an appropriate temperature to reenter the distillation columns. This control can be fairly loose, as the column design is robust enough to handle a moderate range of entry conditions. However, if necessary the flow rate of cooling water (CW-600) through the final post-transalkylation heat exchanger (HW-601) can be varied to ensure an appropriate temperature based on information obtained from a temperature sensor, most likely a thermocouple on the post-heat-recovery transalkylation product stream (S-602).

Section 700: Furnace

In Section 700, the outlet temperatures and flow rates of the Dowtherm A (S-719), process steam (S-727), and molten salt (S-723) streams must be controlled such that they provide the necessary heat duties in other sections of the process. This will rely on data from a variety of temperature sensors, most likely thermocouples, placed on the cold stream feeds entering each heat exchanger that uses these heating streams. The system will also require thermocouples on each exiting stream (S-719, S-723, and S-727) in order to ensure proper exit temperatures. Alternatively and more likely, given the high temperatures these streams reach, the flow rates, rather than the temperatures, will be controlled in by valves in response to temperature data from the thermocouples.

In order to control the outlet temperatures, data from the thermocouples will also be sent to valves located in the combined waste stream (S-700). These valves will divert the flow of flammable waste in order to achieve the required heating duties. A holdup tank within the combined stream (S-700) will likely be necessary in order to enable the desired level of control over burn rates. In addition, this tank may need to have supplemental fuel feeds available to counter unexpected energy losses. Overall, this section represents the most complex system of interrelated controls and responses in the process; designers should build in as much flexibility as possible in order to enable successful operation of control systems implemented elsewhere in the process.

Safety Considerations

Many of the materials used in this process are highly flammable such as hydrocarbons and hydrogen. Extreme care must be exercised, despite the lack of oxygen in the feed streams, because of the possibility of an explosion caused by a leak. For this reason open flames and sparks should not be permitted anywhere near the hydrogenation, condensation, aqueous phase reforming, transalkylation and separation processes in particular. Emergency shut-off valves should be installed into the process to prevent large scale accidents. Nitrogen should be used to flush pipes of any combustible residue when performing catalyst recharge or cleaning.

In addition to the risks of explosions and fires due to the large amounts of hydrocarbons flowing through the system, hydrocarbon gases often present health risks via inhalation. For this reason, prolonged exposure to gases should be avoided at all costs. Additionally, risks of incomplete combustion within the furnaces could produce carbon monoxide. Carbon monoxide is very hazardous as it is both highly flammable and quite deadly if inhaled. Carbon dioxide also poses health risks if inhaled in large quantities. For these reasons, contact with the furnace should be avoided.

Many of the reactors are require high temperatures and pressures to react so reactors that can withstand intense conditions must be used. For this reason, contact with any of the reactors or heated streams should be avoided to prevent burns.

São Paolo, Brazil is known for its highly unreliable weather as it can vary drastically from day to day. It is also the location of tremendous amounts of rainfall. For this reason much of the pipes and equipment should be made of stainless steel to avoid corrosion and rusting particularly if it is to be kept outdoors.

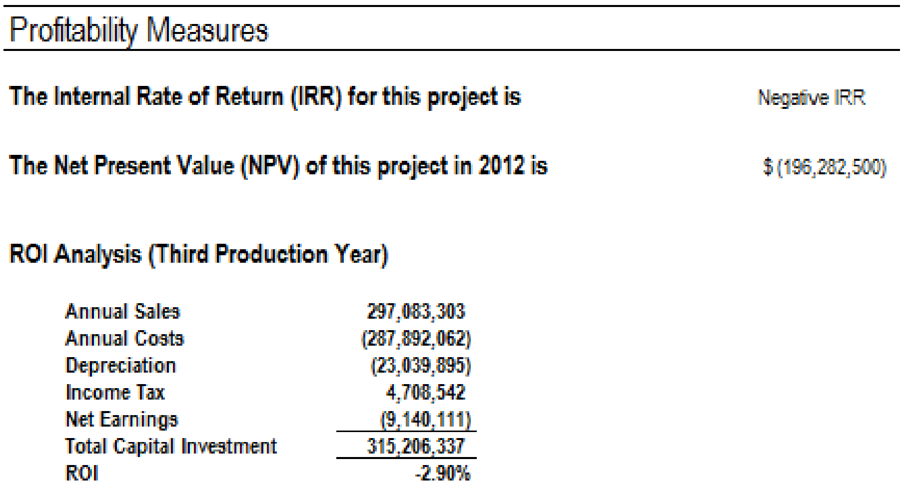
Section VIII

Process Economics

VIII. PROCESS ECONOMICS

At a p-xylene price of $0.83/lb, a benzene price of $0.45/lb, and a sugar cane molasses price of $0.03/lb, this process is unprofitable, with an ROI of -2.90%. Profitability measures are summarized in Figure 16. The inputs leading up to these findings are described in the following sections: overview and materials, equipment cost estimates, utility requirements, cost summaries, and cash flows. This section concludes with a series of sensitivity analyses. Although profitability is feasible under certain conditions, the primary hurdle is that of overall conversion. Given the already optimistic assumptions throughout the process, making this investment is not recommended without technological advances. Namely, unless overall conversion can increase from 4.3% to 5.6%, the outlay is undesirable.

Figure 16



Profitability Measures

The Internal Rate of Return (IRR) for this project is Negative IRR

The Net Present Value (NPV) of this project in 2012 is $ (196,282,500)

ROI Analysis (Third Production Year)

Annual Sales	297,083,303
Annual Costs	(287,892,062)
Depreciation	(23,039,895)
Income Tax	4,708,542
Net Earnings	(9,140,111)
Total Capital Investment	315,206,337
ROI	-2.90%

Overview & Materials

Due to the choice of sugar cane molasses as a primary input, the process would be located in Brazil. A site factor of 0.85 is chosen as representative of the BRIC countries (Table 22.13, PPDP). Allowing for 35 days per year of down time, an operating factor of 0.9041 is selected. Therefore, 50,505 lb/h of p-xylene is required to achieve the requisite 400,000,000 lb/y. One year is permitted for design and for construction. Under the assumption that standard bulk contract pricing applies, prices of $1,818/MT, $1,001/MT, and $60/MT are used for p-xylene, benzene (ICIS), and sugar cane molasses. These prices have a large impact on bottom-line profit and tend to fluctuate widely. Their impact is examined in the sensitivity analyses.

General Information

Process Title:	**P-Xylene from Sugar Cane Molasses**
Product:	**Para-Xylene**
Plant Site Location:	**Brazil**
Site Factor:	**0.85**
Operating Hours per Year:	**7920**
Operating Days Per Year:	**330**
Operating Factor:	**0.9041**

Product Information

This Process will Yield

50,505	lb of Para-Xylene per hour
1,212,121	lb of Para-Xylene per day
400,000,000	lb of Para-Xylene per year

Price **$0.83** **/lb**

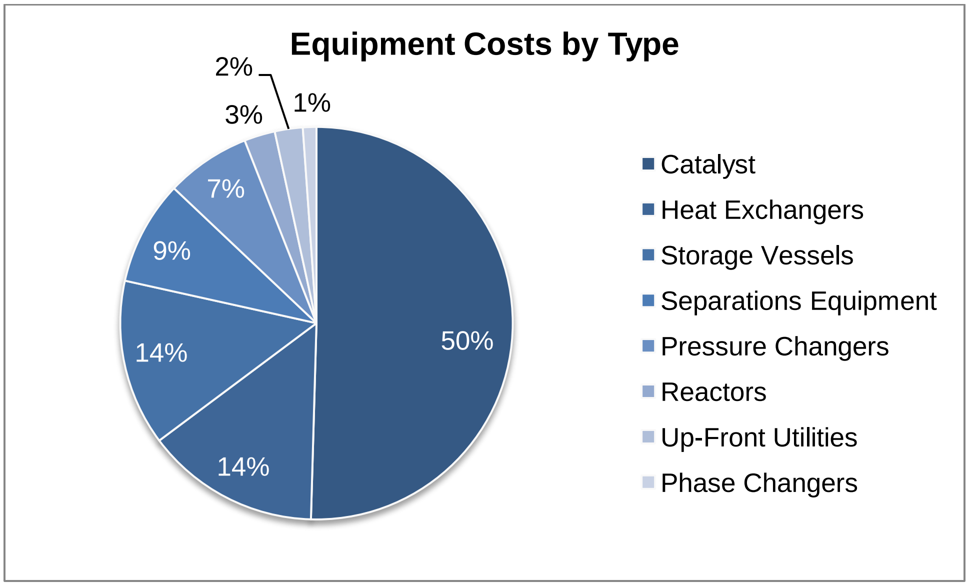
Chronology

Year	Action	Distribution of Permanent Investment	Production Capacity	Depreciation 5 year MACRS	Product Price
2012	Design		0.0%		
2013	Construction	100%	0.0%		
2014	Production	0%	45.0%	20.00%	$0.83
2015	Production	0%	67.5%	32.00%	$0.83
2016	Production	0%	90.0%	19.20%	$0.83
2017	Production		90.0%	11.52%	$0.83
2018	Production		90.0%	11.52%	$0.83
2019	Production		90.0%	5.76%	$0.83
2020	Production		90.0%		$0.83
2021	Production		90.0%		$0.83
2022	Production		90.0%		$0.83
2023	Production		90.0%		$0.83
2043	Production		90.0%		$0.83

Equipment Cost Estimates

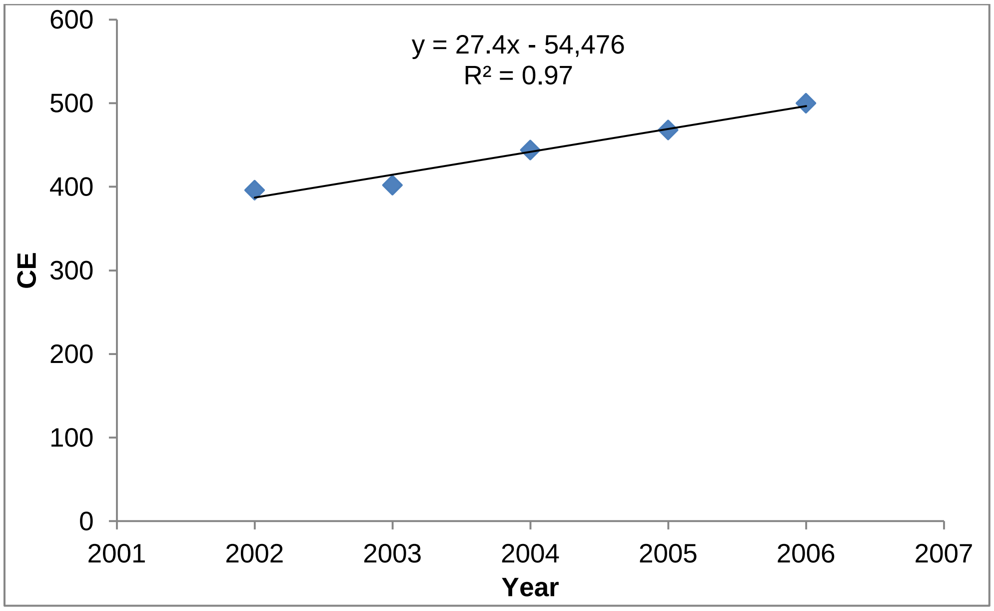
Equipment costs represent a large portion of the overall initial capital investment, totaling over $230 million. The largest expenditure categories are catalysts, heat exchange equipment, and storage vessels. Most equipment prices are reported according to ASPEN IPE estimates. Catalysts are discussed throughout the unit descriptions. Storage vessels, one heat exchanger, and furnaces are priced using the equations of Table 22.32 in PPDP – details are reported in the respective sections. Figure 17 summarizes equipment expenditure by type. Storage and catalyst are two significant costs that should be first priorities for cost reduction. Storage is especially significant because it also represents a large opportunity cost (two-thirds of storage vessels are unused for three-quarters of the year, for example – see Section 700.

Figure 17

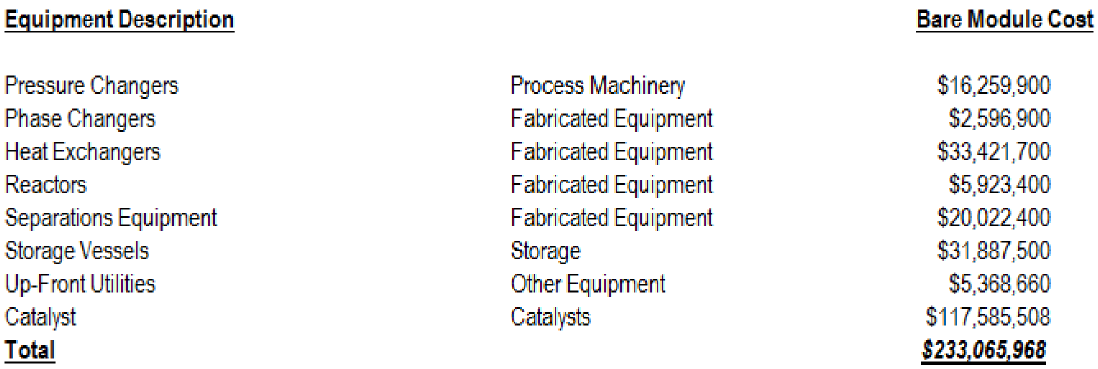


Note that “hand-priced” equipment was adjusted for the change in the Chemical Engineering Cost Index (data from Table 22.6, PPDP), extrapolation shown in Figure 18. Statistically speaking, predictive extrapolation is extremely dangerous; however, there was little other choice available. The period from 2002-2006 appears to be a “new normal,” and, if this assumption holds, the extrapolation will not be far off the true value. That said, it is likely that the financial events since 2008 have had a negative impact on the CE growth. Fortunately, this affects a small number of units.

Figure 18



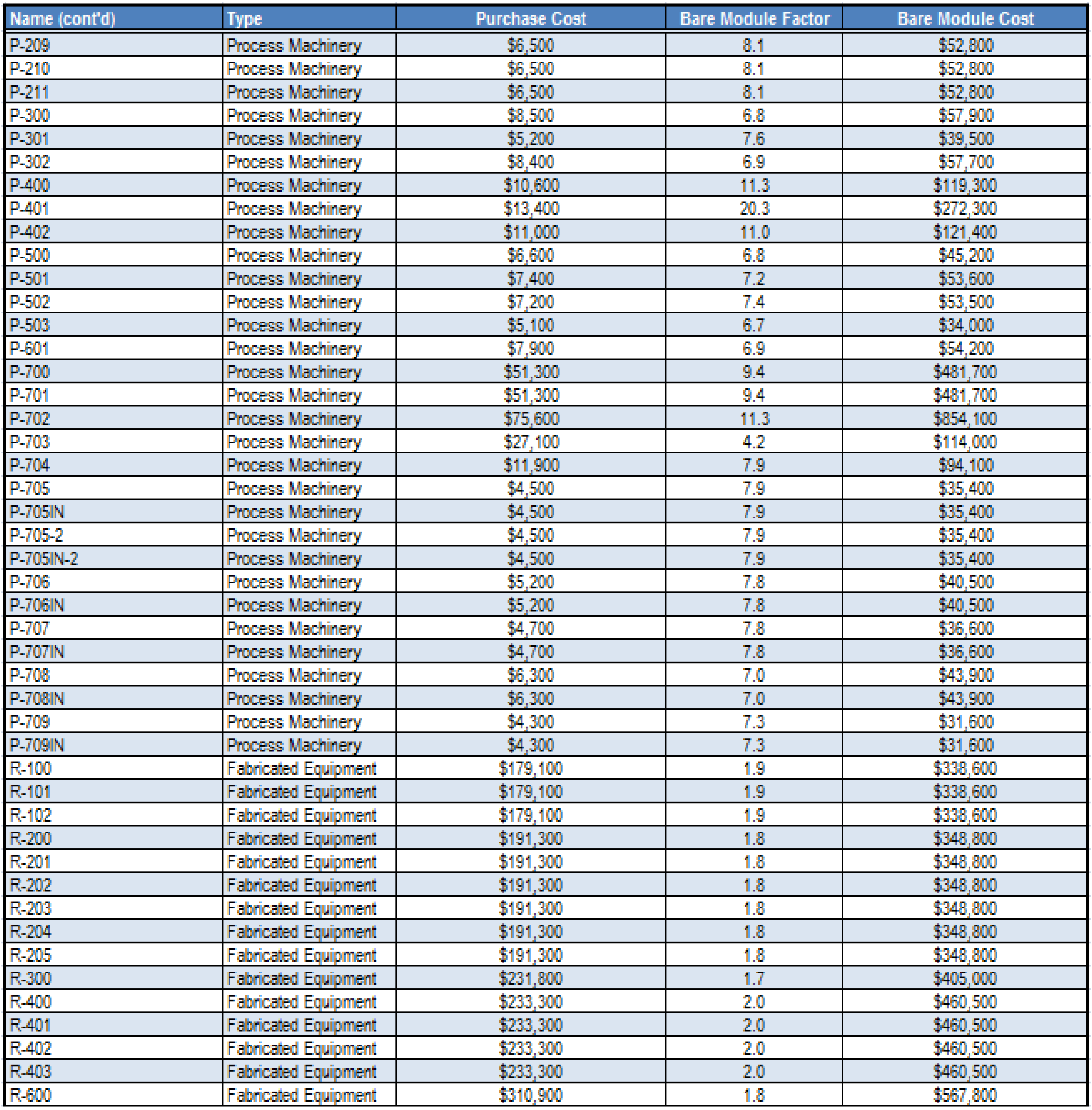
Equipment Cost Summary



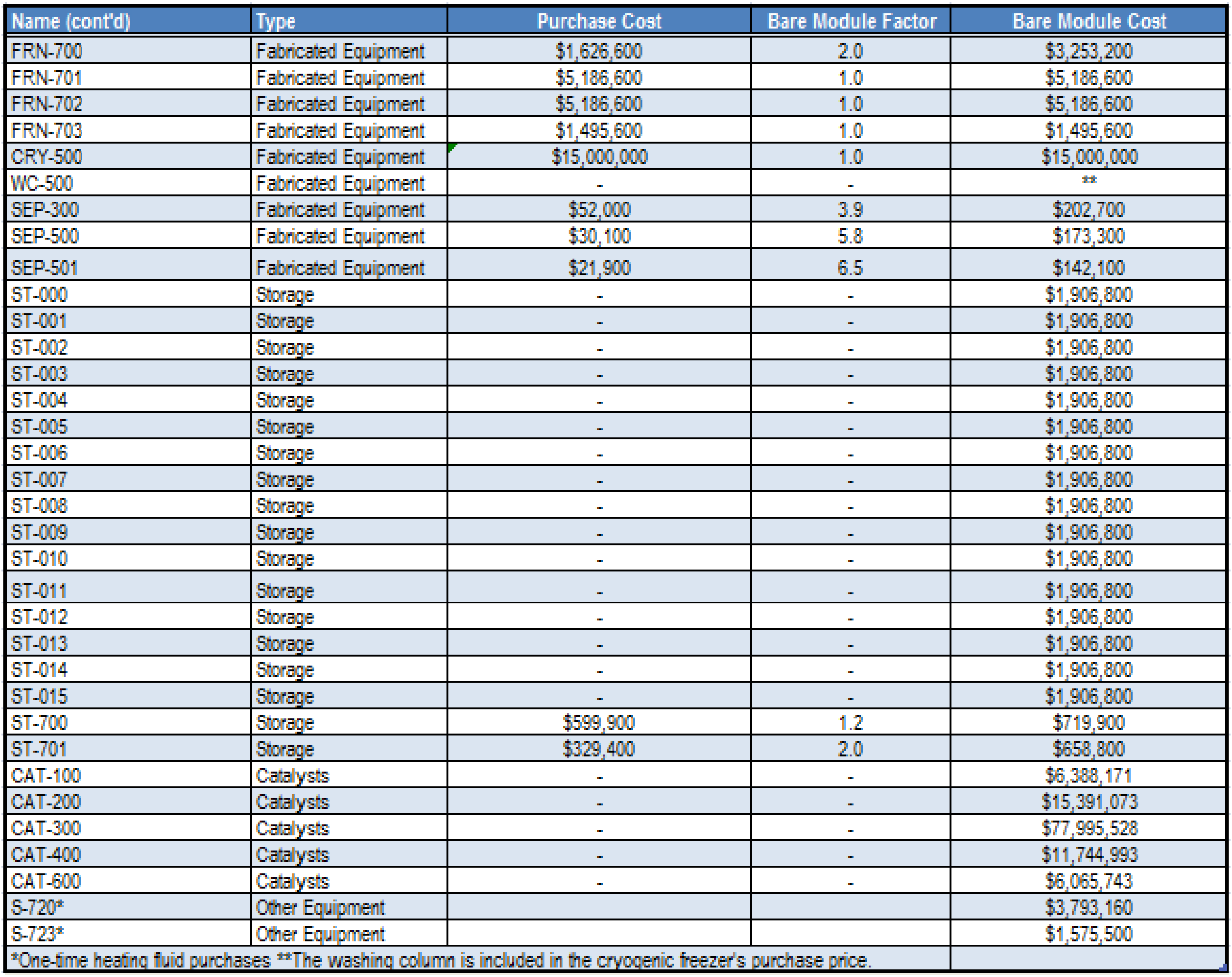
Equipment Description		Bare Module Cost
Pressure Changers	Process Machinery	$16,259,900
Phase Changers	Fabricated Equipment	$2,596,900
Heat Exchangers	Fabricated Equipment	$33,421,700
Reactors	Fabricated Equipment	$5,923,400
Separations Equipment	Fabricated Equipment	$20,022,400
Storage Vessels	Storage	$31,887,500
Up-Front Utilities	Other Equipment	$5,368,660
Catalyst	Catalysts	$117,585,508
Total		***$233,065,968***

Equipment Cost Details

Name	Type	Purchase Cost	Bare Module Factor	Bare Module Cost
CMP-300	Process Machinery	$10,132,800	1.1	$10,868,300
CND-500	Fabricated Equipment	$33,800	3.4	$115,600
AD-500	Fabricated Equipment	$27,700	5.7	$158,500
RB-500	Fabricated Equipment	$381,200	1.5	$558,700
DP-500	Process Machinery	$9,900	5.8	$57,800
DC-500	Fabricated Equipment	$528,900	2.0	$1,050,200
CND-501	Fabricated Equipment	$31,000	3.7	$113,300
AD-501	Fabricated Equipment	$35,100	5.1	$180,600
RB-501	Fabricated Equipment	$238,100	1.6	$371,900
DP-501	Process Machinery	$13,600	4.9	$67,200
DC-501	Fabricated Equipment	$458,000	2.0	$898,800
CND-502	Fabricated Equipment	$215,100	1.8	$380,300
AD-502	Fabricated Equipment	$51,600	3.9	$199,500
RB-502	Fabricated Equipment	$313,700	1.7	$522,000
DP-502	Process Machinery	$26,600	3.9	$104,200
DC-502	Fabricated Equipment	$580,000	2.2	$1,279,600
CND-503	Fabricated Equipment	$266,100	1.6	$421,600
AD-503	Fabricated Equipment	$18,700	5.7	$106,000
RB-503	Fabricated Equipment	$29,600	3.8	$113,500
DP-503	Process Machinery	$6,200	6.3	$39,000
DC-503	Fabricated Equipment	$117,600	2.8	$330,800
F-300	Fabricated Equipment	$35,100	4.1	$142,900
F-301	Fabricated Equipment	$34,600	4.5	$157,400
HX-100	Fabricated Equipment	$51,200	4.4	$226,000
HX-101	Fabricated Equipment	$51,200	4.4	$226,000
HX-102	Fabricated Equipment	$51,200	4.4	$226,000
HX-200	Fabricated Equipment	$286,600	1.7	$485,300
HX-300	Fabricated Equipment	$56,000	3.1	$174,400
HX-301	Fabricated Equipment	$174,200	1.9	$335,000
HX-302	Fabricated Equipment	$16,000	5.2	$83,100
HX-303	Fabricated Equipment	$185,100	1.9	$347,600
HX-400	Fabricated Equipment	$156,900	4.9	$764,100
HX-401	Fabricated Equipment	$834,400	1.6	$1,375,300
HX-402	Fabricated Equipment	$39,400	3.5	$136,400
HX-403	Fabricated Equipment	$383,200	2.0	$762,600
HX-404	Fabricated Equipment	$3,568,600	3.3	$11,854,500
HX-500	Fabricated Equipment	$54,200	2.8	$150,200
HX-501	Fabricated Equipment	$24,200	4.0	$96,300
HX-600	Fabricated Equipment	$96,700	5.6	$541,900
HX-601	Fabricated Equipment	$34,800	3.4	$119,400
HX-703	Fabricated Equipment	$42,700	4.6	$197,800
HX-704	Fabricated Equipment	$42,700	4.6	$197,800
P-000	Process Machinery	$11,400	7.4	$84,300
P-100	Process Machinery	$10,200	5.6	$57,500
P-101	Process Machinery	$10,200	5.6	$57,500
P-102	Process Machinery	$10,200	5.6	$57,500
P-103	Process Machinery	$179,700	1.6	$284,000
P-104	Process Machinery	$179,700	1.6	$284,000
P-105	Process Machinery	$179,700	1.6	$284,000
P-200	Process Machinery	$6,500	8.1	$52,800
P-201	Process Machinery	$6,500	8.1	$52,800
P-202	Process Machinery	$6,500	8.1	$52,800
P-203	Process Machinery	$6,500	8.1	$52,800
P-204	Process Machinery	$6,500	8.1	$52,800
P-205	Process Machinery	$6,500	8.1	$52,800
P-206	Process Machinery	$6,500	8.1	$52,800
P-207	Process Machinery	$6,500	8.1	$52,800
P-208	Process Machinery	$6,500	8.1	$52,800
P-209	Process Machinery	$6,500	8.1	$52,800



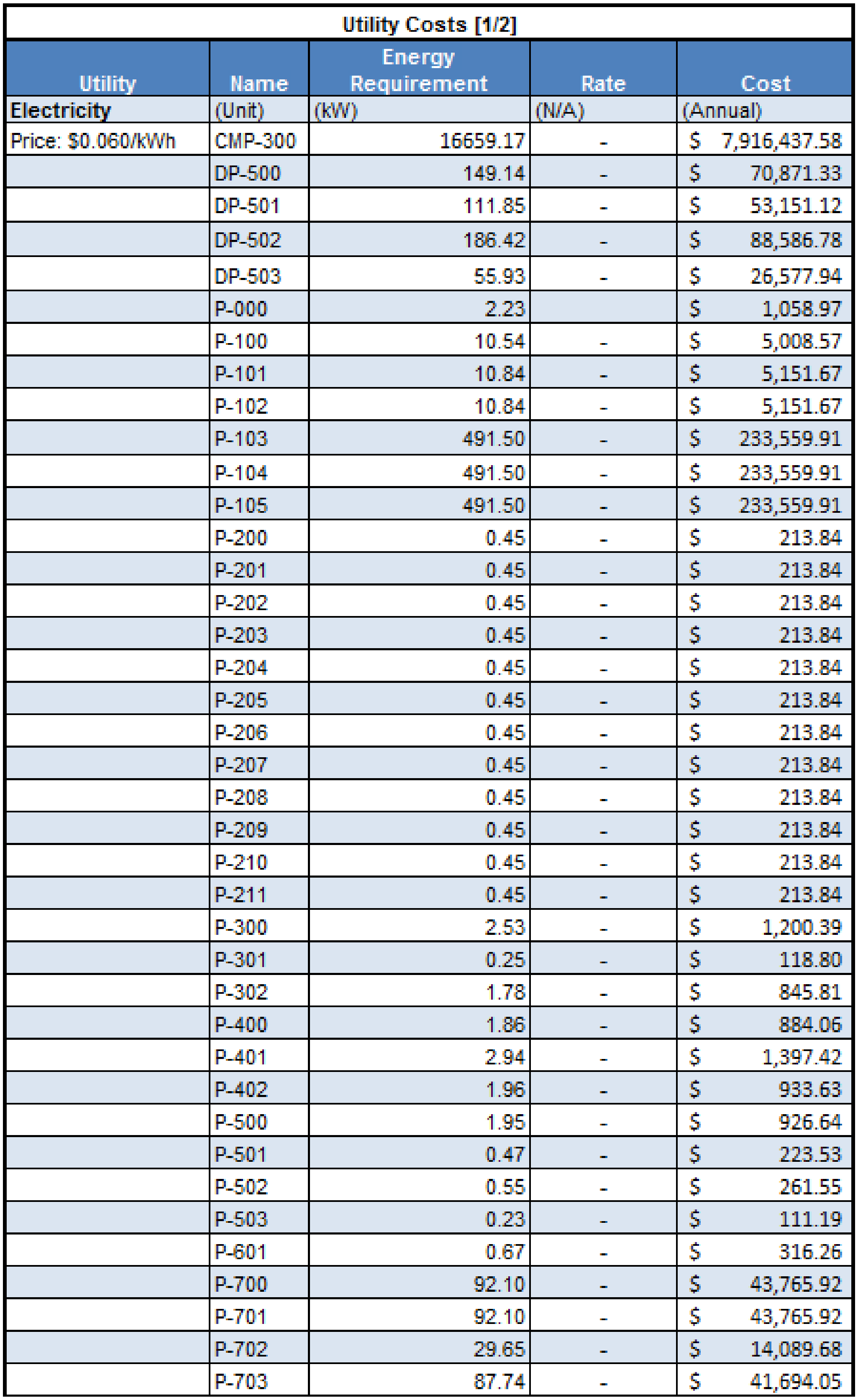
Name (cont'd)	Type	Purchase Cost	Bare Module Factor	Bare Module Cost
P-209	Process Machinery	$6,500	8.1	$52,800
P-210	Process Machinery	$6,500	8.1	$52,800
P-211	Process Machinery	$6,500	8.1	$52,800
P-300	Process Machinery	$8,500	6.8	$57,900
P-301	Process Machinery	$5,200	7.6	$39,500
P-302	Process Machinery	$8,400	6.9	$57,700
P-400	Process Machinery	$10,600	11.3	$119,300
P-401	Process Machinery	$13,400	20.3	$272,300
P-402	Process Machinery	$11,000	11.0	$121,400
P-500	Process Machinery	$6,600	6.8	$45,200
P-501	Process Machinery	$7,400	7.2	$53,600
P-502	Process Machinery	$7,200	7.4	$53,500
P-503	Process Machinery	$5,100	6.7	$34,000
P-601	Process Machinery	$7,900	6.9	$54,200
P-700	Process Machinery	$51,300	9.4	$481,700
P-701	Process Machinery	$51,300	9.4	$481,700
P-702	Process Machinery	$75,600	11.3	$854,100
P-703	Process Machinery	$27,100	4.2	$114,000
P-704	Process Machinery	$11,900	7.9	$94,100
P-705	Process Machinery	$4,500	7.9	$35,400
P-705IN	Process Machinery	$4,500	7.9	$35,400
P-705-2	Process Machinery	$4,500	7.9	$35,400
P-705IN-2	Process Machinery	$4,500	7.9	$35,400
P-706	Process Machinery	$5,200	7.8	$40,500
P-706IN	Process Machinery	$5,200	7.8	$40,500
P-707	Process Machinery	$4,700	7.8	$36,600
P-707IN	Process Machinery	$4,700	7.8	$36,600
P-708	Process Machinery	$6,300	7.0	$43,900
P-708IN	Process Machinery	$6,300	7.0	$43,900
P-709	Process Machinery	$4,300	7.3	$31,600
P-709IN	Process Machinery	$4,300	7.3	$31,600
R-100	Fabricated Equipment	$179,100	1.9	$338,600
R-101	Fabricated Equipment	$179,100	1.9	$338,600
R-102	Fabricated Equipment	$179,100	1.9	$338,600
R-200	Fabricated Equipment	$191,300	1.8	$348,800
R-201	Fabricated Equipment	$191,300	1.8	$348,800
R-202	Fabricated Equipment	$191,300	1.8	$348,800
R-203	Fabricated Equipment	$191,300	1.8	$348,800
R-204	Fabricated Equipment	$191,300	1.8	$348,800
R-205	Fabricated Equipment	$191,300	1.8	$348,800
R-300	Fabricated Equipment	$231,800	1.7	$405,000
R-400	Fabricated Equipment	$233,300	2.0	$460,500
R-401	Fabricated Equipment	$233,300	2.0	$460,500
R-402	Fabricated Equipment	$233,300	2.0	$460,500
R-403	Fabricated Equipment	$233,300	2.0	$460,500
R-600	Fabricated Equipment	$310,900	1.8	$567,800



Name (cont'd)	Type	Purchase Cost	Bare Module Factor	Bare Module Cost
FRN-700	Fabricated Equipment	$1,626,600	2.0	$3,253,200
FRN-701	Fabricated Equipment	$5,186,600	1.0	$5,186,600
FRN-702	Fabricated Equipment	$5,186,600	1.0	$5,186,600
FRN-703	Fabricated Equipment	$1,495,600	1.0	$1,495,600
CRY-500	Fabricated Equipment	$15,000,000	1.0	$15,000,000
WC-500	Fabricated Equipment	-	-	**
SEP-300	Fabricated Equipment	$52,000	3.9	$202,700
SEP-500	Fabricated Equipment	$30,100	5.8	$173,300
SEP-501	Fabricated Equipment	$21,900	6.5	$142,100
ST-000	Storage	-	-	$1,906,800
ST-001	Storage	-	-	$1,906,800
ST-002	Storage	-	-	$1,906,800
ST-003	Storage	-	-	$1,906,800
ST-004	Storage	-	-	$1,906,800
ST-005	Storage	-	-	$1,906,800
ST-006	Storage	-	-	$1,906,800
ST-007	Storage	-	-	$1,906,800
ST-008	Storage	-	-	$1,906,800
ST-009	Storage	-	-	$1,906,800
ST-010	Storage	-	-	$1,906,800
ST-011	Storage	-	-	$1,906,800
ST-012	Storage	-	-	$1,906,800
ST-013	Storage	-	-	$1,906,800
ST-014	Storage	-	-	$1,906,800
ST-015	Storage	-	-	$1,906,800
ST-700	Storage	$599,900	1.2	$719,900
ST-701	Storage	$329,400	2.0	$658,800
CAT-100	Catalysts	-	-	$6,388,171
CAT-200	Catalysts	-	-	$15,391,073
CAT-300	Catalysts	-	-	$77,995,528
CAT-400	Catalysts	-	-	$11,744,993
CAT-600	Catalysts	-	-	$6,065,743
S-720*	Other Equipment			$3,793,160
S-723*	Other Equipment			$1,575,500
*One-time heating fluid purchases **The washing column is included in the cryogenic freezer's purchase price.				

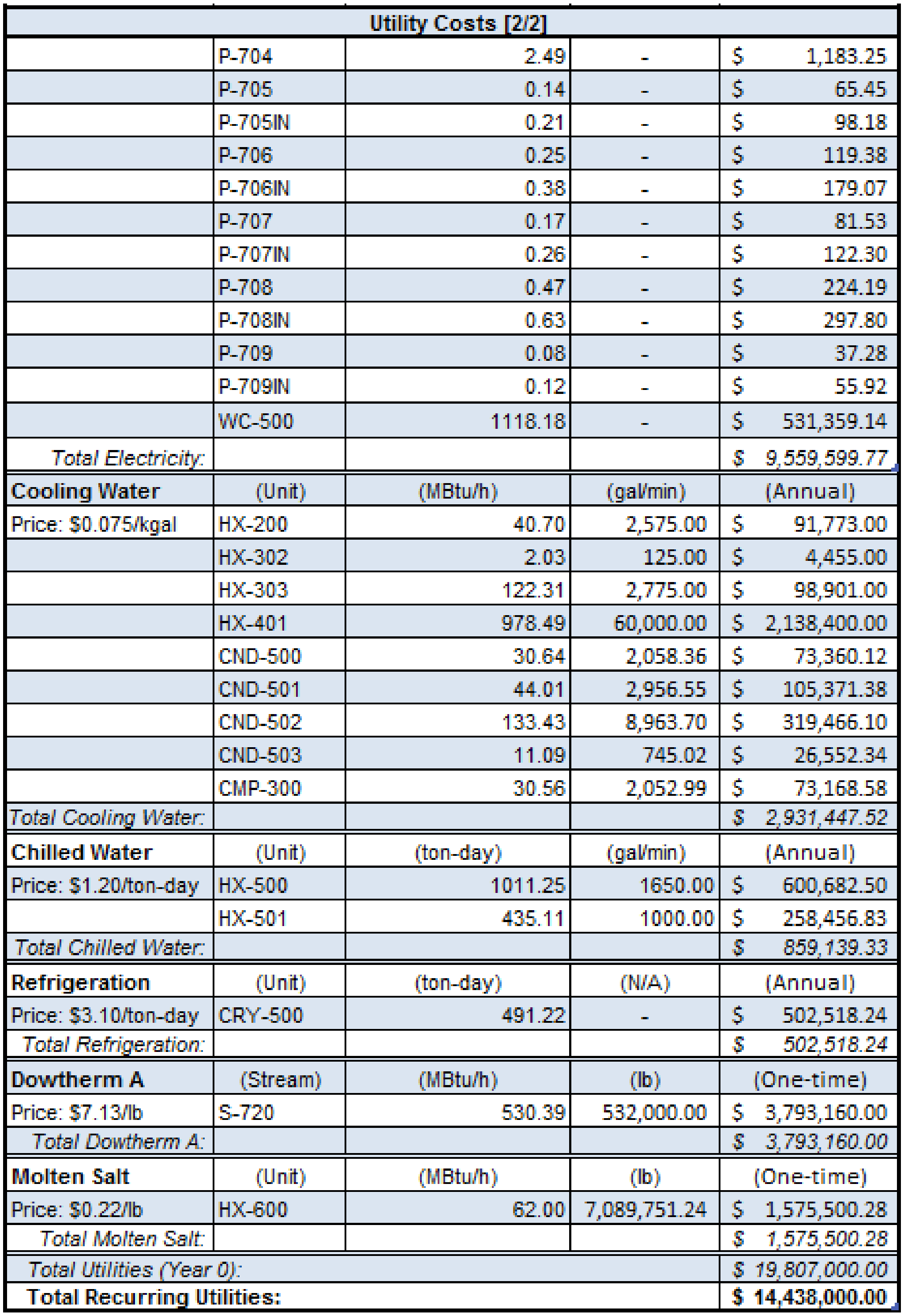
Utility Requirements

The utility cost for the plant is calculated using prices from Table 23.1 of PPDP, and the utility requirements as derived from ASPEN or as calculated according to various heating requirements. More information on utilities can be found in Section IV: Energy Balance.



Utility Costs [1/2]

Utility	Name	Energy Requirement	Rate	Cost
Electricity	(Unit)	(kW)	(N/A)	(Annual)
Price: $0.060/kWh	CMP-300	16659.17	-	$ 7,916,437.58
	DP-500	149.14	-	$ 70,871.33
	DP-501	111.85	-	$ 53,151.12
	DP-502	186.42	-	$ 88,586.78
	DP-503	55.93	-	$ 26,577.94
	P-000	2.23		$ 1,058.97
	P-100	10.54	-	$ 5,008.57
	P-101	10.84	-	$ 5,151.67
	P-102	10.84	-	$ 5,151.67
	P-103	491.50	-	$ 233,559.91
	P-104	491.50	-	$ 233,559.91
	P-105	491.50	-	$ 233,559.91
	P-200	0.45	-	$ 213.84
	P-201	0.45	-	$ 213.84
	P-202	0.45	-	$ 213.84
	P-203	0.45	-	$ 213.84
	P-204	0.45	-	$ 213.84
	P-205	0.45	-	$ 213.84
	P-206	0.45	-	$ 213.84
	P-207	0.45	-	$ 213.84
	P-208	0.45	-	$ 213.84
	P-209	0.45	-	$ 213.84
	P-210	0.45	-	$ 213.84
	P-211	0.45	-	$ 213.84
	P-300	2.53	-	$ 1,200.39
	P-301	0.25	-	$ 118.80
	P-302	1.78	-	$ 845.81
	P-400	1.86	-	$ 884.06
	P-401	2.94	-	$ 1,397.42
	P-402	1.96	-	$ 933.63
	P-500	1.95	-	$ 926.64
	P-501	0.47	-	$ 223.53
	P-502	0.55	-	$ 261.55
	P-503	0.23	-	$ 111.19
	P-601	0.67	-	$ 316.26
	P-700	92.10	-	$ 43,765.92
	P-701	92.10	-	$ 43,765.92
	P-702	29.65	-	$ 14,089.68
	P-703	87.74	-	$ 41,694.05



Utility Costs [2/2]				
	P-704	2.49	-	$ 1,183.25
	P-705	0.14	-	$ 65.45
	P-705IN	0.21	-	$ 98.18
	P-706	0.25	-	$ 119.38
	P-706IN	0.38	-	$ 179.07
	P-707	0.17	-	$ 81.53
	P-707IN	0.26	-	$ 122.30
	P-708	0.47	-	$ 224.19
	P-708IN	0.63	-	$ 297.80
	P-709	0.08	-	$ 37.28
	P-709IN	0.12	-	$ 55.92
	WC-500	1118.18	-	$ 531,359.14
Total Electricity:				*$ 9,559,599.77*
Cooling Water	(Unit)	(MBtu/h)	(gal/min)	(Annual)
Price: $0.075/kgal	HX-200	40.70	2,575.00	$ 91,773.00
	HX-302	2.03	125.00	$ 4,455.00
	HX-303	122.31	2,775.00	$ 98,901.00
	HX-401	978.49	60,000.00	$ 2,138,400.00
	CND-500	30.64	2,058.36	$ 73,360.12
	CND-501	44.01	2,956.55	$ 105,371.38
	CND-502	133.43	8,963.70	$ 319,466.10
	CND-503	11.09	745.02	$ 26,552.34
	CMP-300	30.56	2,052.99	$ 73,168.58
Total Cooling Water:				*$ 2,931,447.52*
Chilled Water	(Unit)	(ton-day)	(gal/min)	(Annual)
Price: $1.20/ton-day	HX-500	1011.25	1650.00	$ 600,682.50
	HX-501	435.11	1000.00	$ 258,456.83
Total Chilled Water:				*$ 859,139.33*
Refrigeration	(Unit)	(ton-day)	(N/A)	(Annual)
Price: $3.10/ton-day	CRY-500	491.22	-	$ 502,518.24
Total Refrigeration:				*$ 502,518.24*
Dowtherm A	(Stream)	(MBtu/h)	(lb)	(One-time)
Price: $7.13/lb	S-720	530.39	532,000.00	$ 3,793,160.00
Total Dowtherm A:				*$ 3,793,160.00*
Molten Salt	(Unit)	(MBtu/h)	(lb)	(One-time)
Price: $0.22/lb	HX-600	62.00	7,089,751.24	$ 1,575,500.28
Total Molten Salt:				*$ 1,575,500.28*
Total Utilities (Year 0):				*$ 19,807,000.00*
Total Recurring Utilities:				**$ 14,438,000.00**

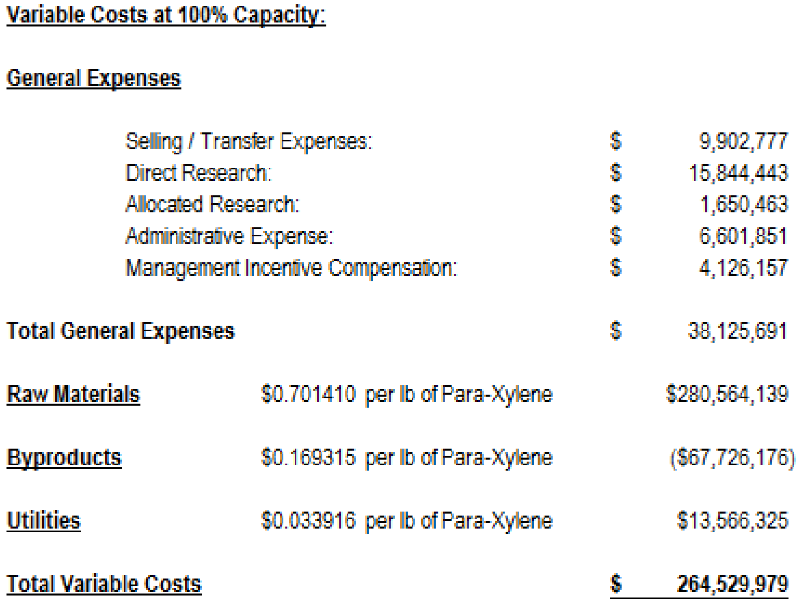
Cost Summaries

Variable costs, working capital, fixed costs, and investment requirements are taken according to specifications in PPDP Table 23.1.

Working capital is taken to include four days of p-xylene inventory and 24 days of raw materials (four tanks of residence time six days not in use at any given time during peak production season).

Direct operating expenses total just over $7,000,000 per year, over 83% of which stems from wages and benefits. These wages and benefits are based on the operator wage of $35/h, which was fair in the United States in 2006, and still applies today in Brazil. The number of operators is determined from recommendations in Table 23.3 PPDP. The process has seven main sections, six of which are continuous fluids and one of which involves some solids handling. Therefore, at a scale of 610 tons per operating day, the recommended number of operators on-hand is 16: two for each fluids portion and four for the separations section that involves solids. This amounts to $6.7M per annum in wages, salary, and benefits.

Variable Cost Summary



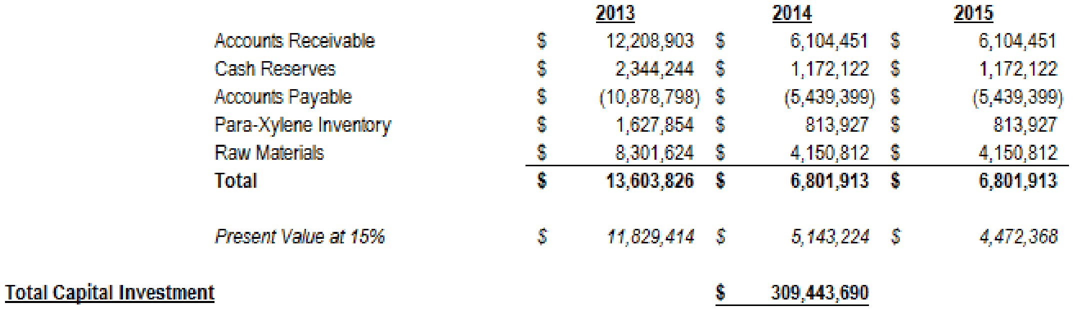
Variable Costs at 100% Capacity:

General Expenses

Selling / Transfer Expenses:	$	9,902,777
Direct Research:	$	15,844,443
Allocated Research:	$	1,650,463
Administrative Expense:	$	6,601,851
Management Incentive Compensation:	$	4,126,157
Total General Expenses	$	38,125,691

Raw Materials	$0.701410 per lb of Para-Xylene	$280,564,139
Byproducts	$0.169315 per lb of Para-Xylene	($67,726,176)
Utilities	$0.033916 per lb of Para-Xylene	$13,566,325
Total Variable Costs		**$ 264,529,979**

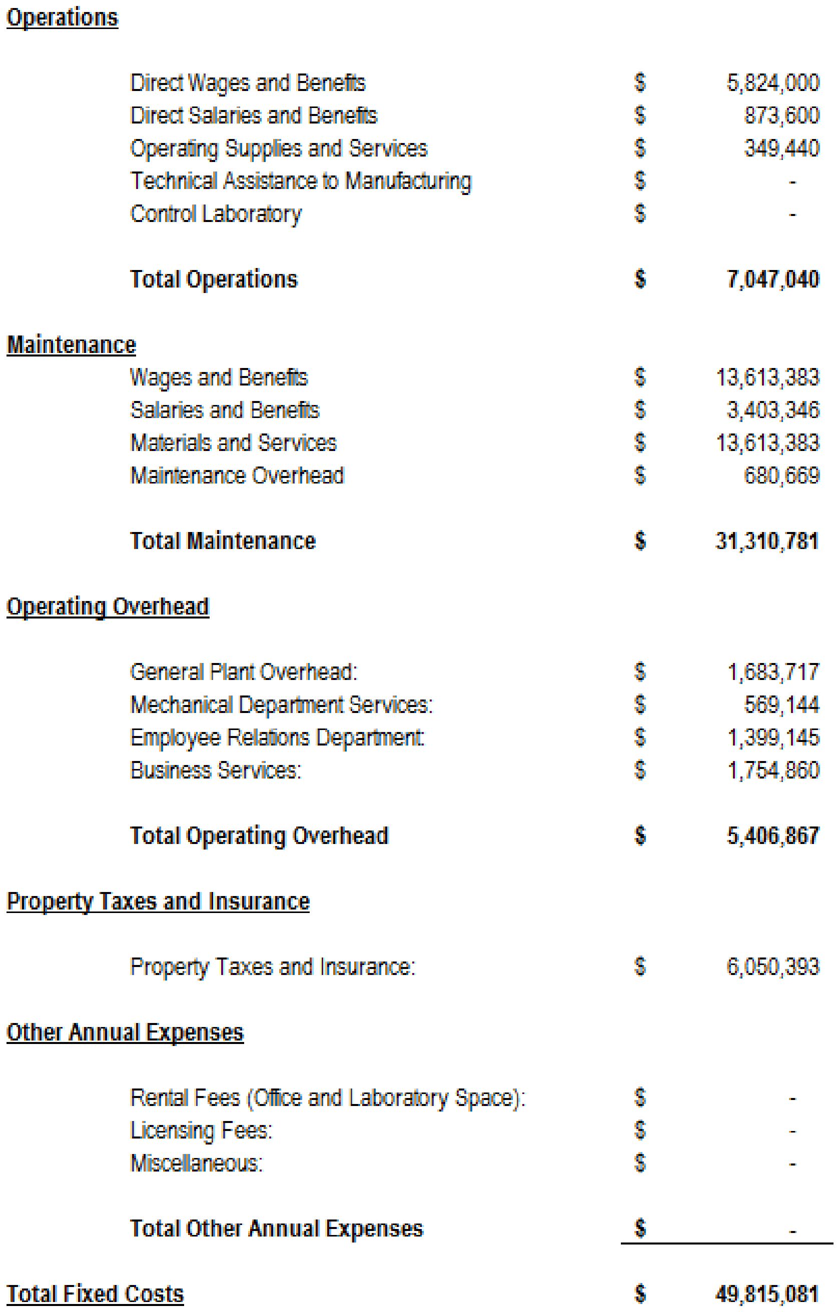
Working Capital



		2013		2014		2015
Accounts Receivable	$	12,208,903	$	6,104,451	$	6,104,451
Cash Reserves	$	2,344,244	$	1,172,122	$	1,172,122
Accounts Payable	$	(10,878,798)	$	(5,439,399)	$	(5,439,399)
Para-Xylene Inventory	$	1,627,854	$	813,927	$	813,927
Raw Materials	$	8,301,624	$	4,150,812	$	4,150,812
Total	**$**	**13,603,826**	**$**	**6,801,913**	**$**	**6,801,913**
Present Value at 15%	*$*	*11,829,414*	*$*	*5,143,224*	*$*	*4,472,368*

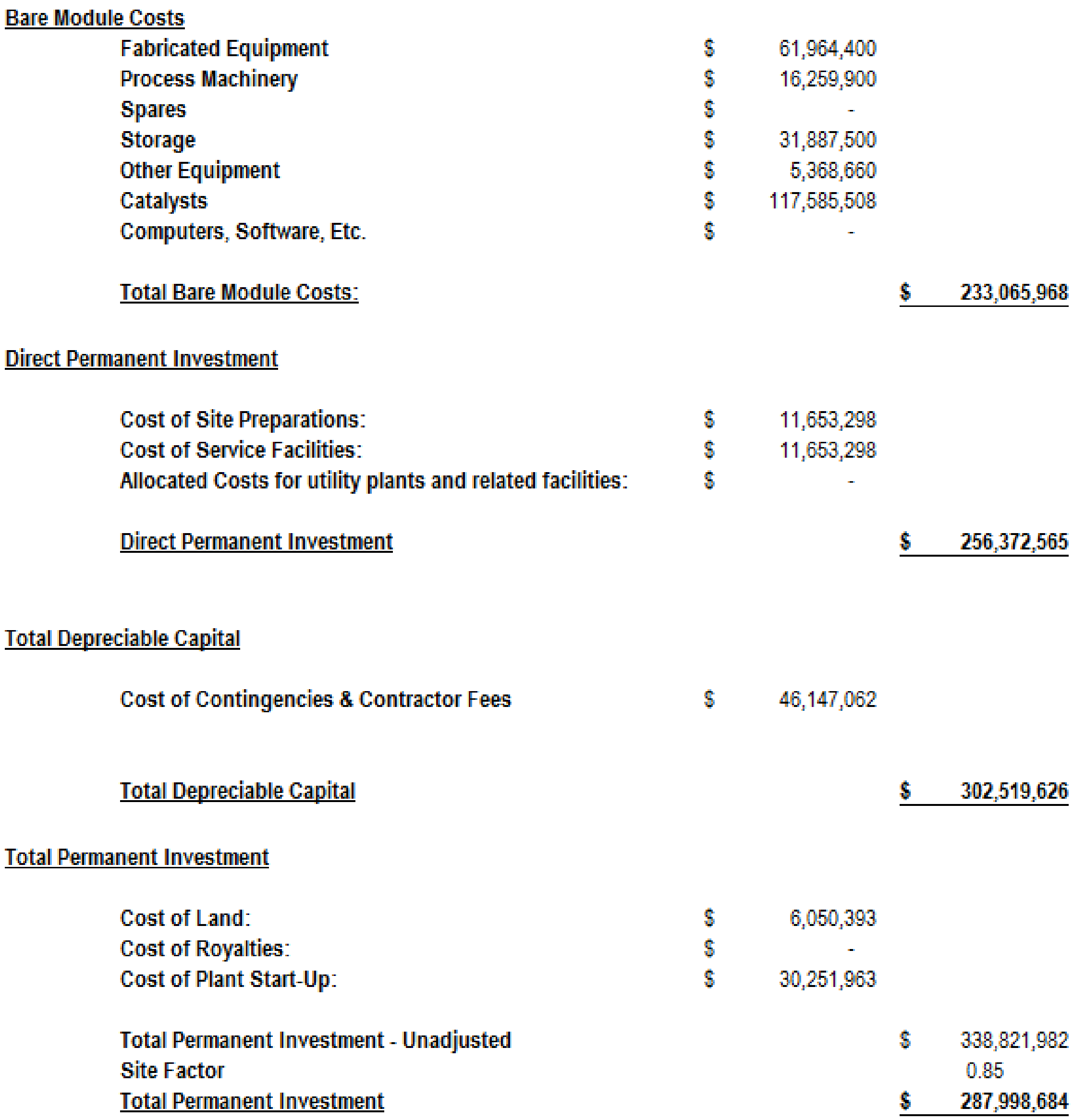
Total Capital Investment **$ 309,443,690**

Fixed Cost Summary



Operations			
	Direct Wages and Benefits	$	5,824,000
	Direct Salaries and Benefits	$	873,600
	Operating Supplies and Services	$	349,440
	Technical Assistance to Manufacturing	$	-
	Control Laboratory	$	-
	Total Operations	**$**	**7,047,040**
Maintenance			
	Wages and Benefits	$	13,613,383
	Salaries and Benefits	$	3,403,346
	Materials and Services	$	13,613,383
	Maintenance Overhead	$	680,669
	Total Maintenance	**$**	**31,310,781**
Operating Overhead			
	General Plant Overhead:	$	1,683,717
	Mechanical Department Services:	$	569,144
	Employee Relations Department:	$	1,399,145
	Business Services:	$	1,754,860
	Total Operating Overhead	**$**	**5,406,867**
Property Taxes and Insurance			
	Property Taxes and Insurance:	$	6,050,393
Other Annual Expenses			
	Rental Fees (Office and Laboratory Space):	$	-
	Licensing Fees:	$	-
	Miscellaneous:	$	-
	Total Other Annual Expenses	**$**	**-**
Total Fixed Costs		**$**	**49,815,081**

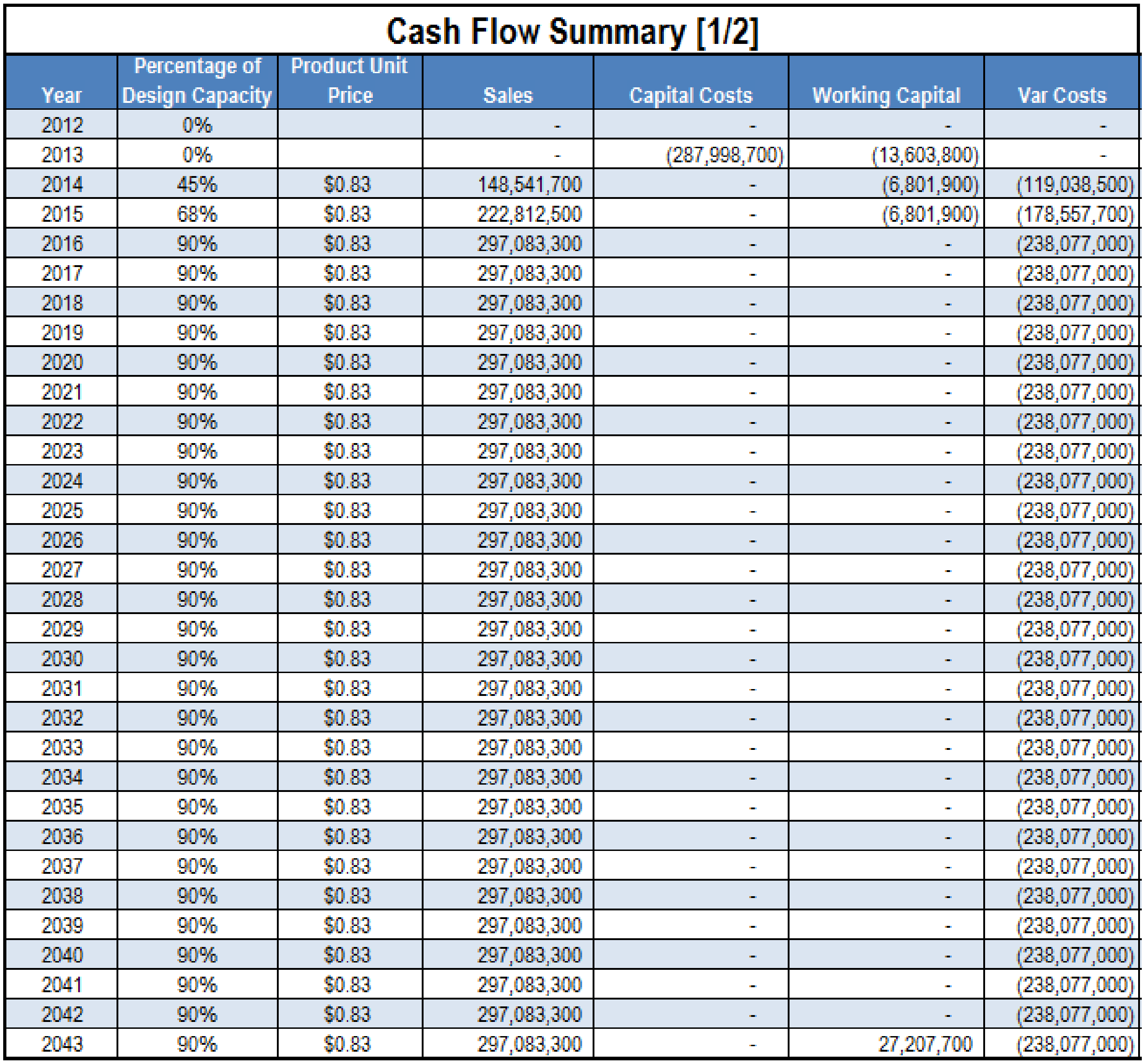
Investment Summary



Bare Module Costs				
Fabricated Equipment	$	61,964,400		
Process Machinery	$	16,259,900		
Spares	$	-		
Storage	$	31,887,500		
Other Equipment	$	5,368,660		
Catalysts	$	117,585,508		
Computers, Software, Etc.	$	-		
Total Bare Module Costs:			**$**	**233,065,968**
Direct Permanent Investment				
Cost of Site Preparations:	$	11,653,298		
Cost of Service Facilities:	$	11,653,298		
Allocated Costs for utility plants and related facilities:	$	-		
Direct Permanent Investment			**$**	**256,372,565**
Total Depreciable Capital				
Cost of Contingencies & Contractor Fees	$	46,147,062		
Total Depreciable Capital			**$**	**302,519,626**
Total Permanent Investment				
Cost of Land:	$	6,050,393		
Cost of Royalties:	$	-		
Cost of Plant Start-Up:	$	30,251,963		
Total Permanent Investment - Unadjusted			$	338,821,982
Site Factor				0.85
Total Permanent Investment			**$**	**287,998,684**

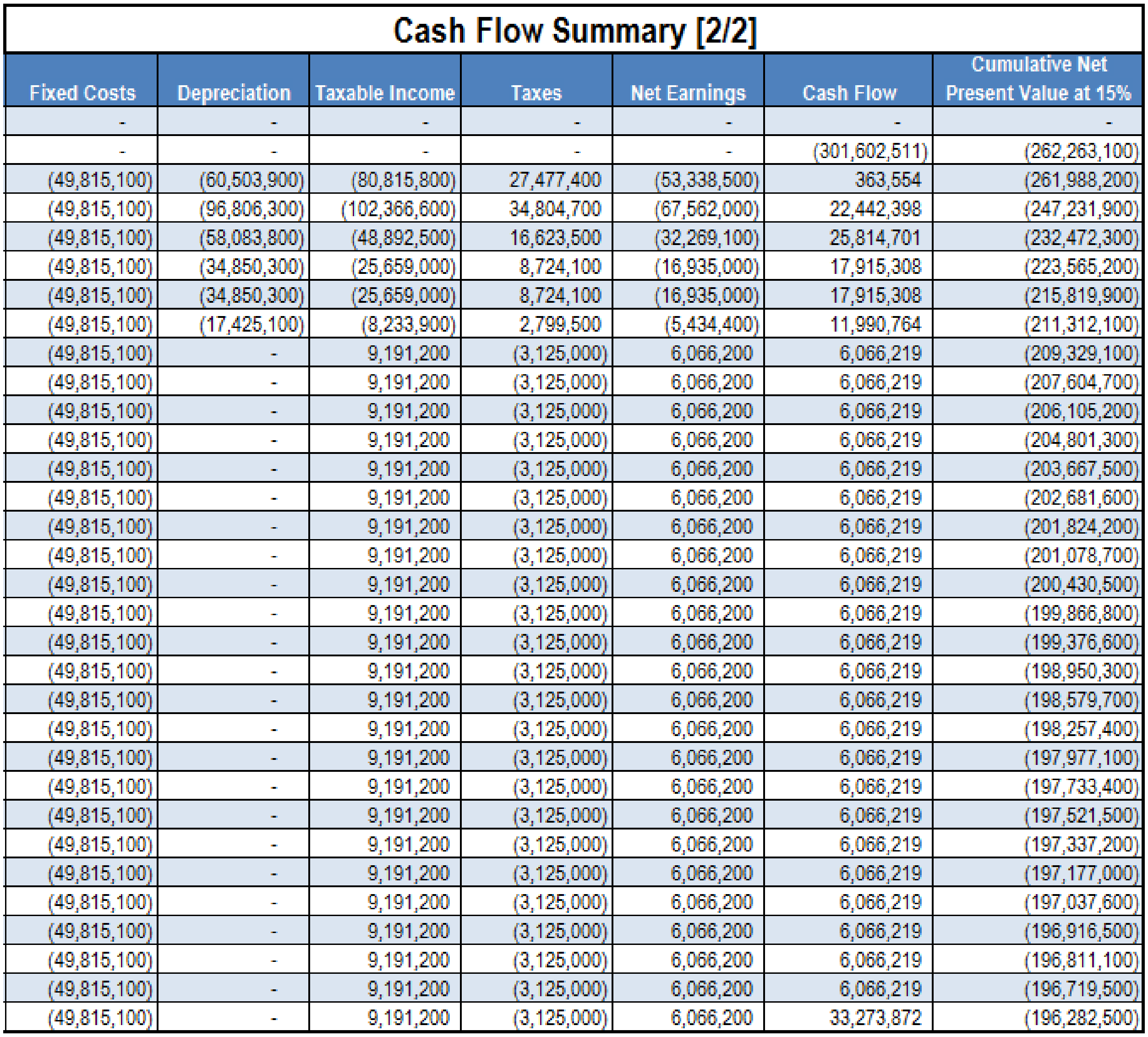
Cash Flows

The most important features of the cash flow summary in this instance are the initial capital costs, the year of positive cash flow, and the ultimate NPV. The summary shows that, although the process becomes profitable in year seven of operation, the small cash flows (~$6M) never fully compensate for the large initial capital outlay, $288M. Ultimately, at a discount rate of 15%, which is conservative, the net present value of the process is $(196,282,500). This investment is not recommended under the given assumptions.



Cash Flow Summary [1/2]

Year	Percentage of Design Capacity	Product Unit Price	Sales	Capital Costs	Working Capital	Var Costs
2012	0%		-	-	-	-
2013	0%		-	(287,998,700)	(13,603,800)	-
2014	45%	$0.83	148,541,700	-	(6,801,900)	(119,038,500)
2015	68%	$0.83	222,812,500	-	(6,801,900)	(178,557,700)
2016	90%	$0.83	297,083,300	-	-	(238,077,000)
2017	90%	$0.83	297,083,300	-	-	(238,077,000)
2018	90%	$0.83	297,083,300	-	-	(238,077,000)
2019	90%	$0.83	297,083,300	-	-	(238,077,000)
2020	90%	$0.83	297,083,300	-	-	(238,077,000)
2021	90%	$0.83	297,083,300	-	-	(238,077,000)
2022	90%	$0.83	297,083,300	-	-	(238,077,000)
2023	90%	$0.83	297,083,300	-	-	(238,077,000)
2024	90%	$0.83	297,083,300	-	-	(238,077,000)
2025	90%	$0.83	297,083,300	-	-	(238,077,000)
2026	90%	$0.83	297,083,300	-	-	(238,077,000)
2027	90%	$0.83	297,083,300	-	-	(238,077,000)
2028	90%	$0.83	297,083,300	-	-	(238,077,000)
2029	90%	$0.83	297,083,300	-	-	(238,077,000)
2030	90%	$0.83	297,083,300	-	-	(238,077,000)
2031	90%	$0.83	297,083,300	-	-	(238,077,000)
2032	90%	$0.83	297,083,300	-	-	(238,077,000)
2033	90%	$0.83	297,083,300	-	-	(238,077,000)
2034	90%	$0.83	297,083,300	-	-	(238,077,000)
2035	90%	$0.83	297,083,300	-	-	(238,077,000)
2036	90%	$0.83	297,083,300	-	-	(238,077,000)
2037	90%	$0.83	297,083,300	-	-	(238,077,000)
2038	90%	$0.83	297,083,300	-	-	(238,077,000)
2039	90%	$0.83	297,083,300	-	-	(238,077,000)
2040	90%	$0.83	297,083,300	-	-	(238,077,000)
2041	90%	$0.83	297,083,300	-	-	(238,077,000)
2042	90%	$0.83	297,083,300	-	-	(238,077,000)
2043	90%	$0.83	297,083,300	-	27,207,700	(238,077,000)



Cash Flow Summary [2/2]

Fixed Costs	Depreciation	Taxable Income	Taxes	Net Earnings	Cash Flow	Cumulative Net Present Value at 15%
-	-	-	-	-	-	-
-	-	-	-	-	(301,602,511)	(262,263,100)
(49,815,100)	(60,503,900)	(80,815,800)	27,477,400	(53,338,500)	363,554	(261,988,200)
(49,815,100)	(96,806,300)	(102,366,600)	34,804,700	(67,562,000)	22,442,398	(247,231,900)
(49,815,100)	(58,083,800)	(48,892,500)	16,623,500	(32,269,100)	25,814,701	(232,472,300)
(49,815,100)	(34,850,300)	(25,659,000)	8,724,100	(16,935,000)	17,915,308	(223,565,200)
(49,815,100)	(34,850,300)	(25,659,000)	8,724,100	(16,935,000)	17,915,308	(215,819,900)
(49,815,100)	(17,425,100)	(8,233,900)	2,799,500	(5,434,400)	11,990,764	(211,312,100)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(209,329,100)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(207,604,700)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(206,105,200)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(204,801,300)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(203,667,500)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(202,681,600)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(201,824,200)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(201,078,700)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(200,430,500)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(199,866,800)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(199,376,600)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(198,950,300)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(198,579,700)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(198,257,400)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(197,977,100)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(197,733,400)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(197,521,500)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(197,337,200)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(197,177,000)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(197,037,600)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(196,916,500)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(196,811,100)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	6,066,219	(196,719,500)
(49,815,100)	-	9,191,200	(3,125,000)	6,066,200	33,273,872	(196,282,500)

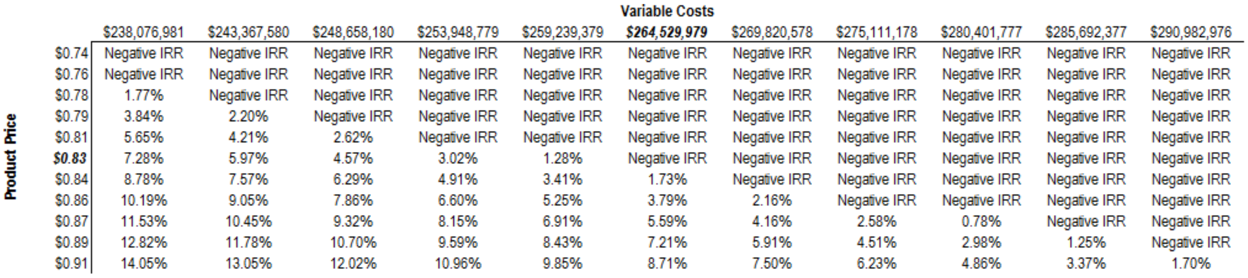
Sensitivity Analyses

The most significant and the most variable cost and revenue drivers should always be examined for bottom-line impact, in order to be prepared for different operating scenarios. Key cost drivers of this process include the cost of sugar cane molasses, the price of electricity, the price of catalyst, and the overall conversion rate of molasses to p-xylene. Key revenue drivers include the price of p-xylene and the price of benzene.

IRR sensitivity tables are shown for product price against variable costs (Figure 19), fixed costs (Figure 20), and total permanent investment (Figure 21). These are rather generic measures intended to demonstrate the robustness of the assumptions detailed heretofore. Price fluctuations are taken at ±10%, which is reasonable given para-xylene's recent performance and which is well within the norm of commodities markets.

More incisive sensitivity analyses are summarized in a Strauss plot, Figure 22 (Fig. 9-14, Perry's).

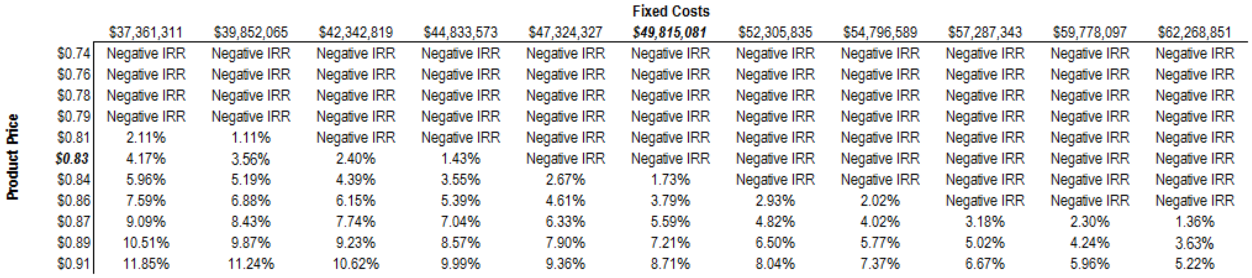
Figure 19



						Variable Costs					
		$238,076,981	$243,367,580	$248,658,180	$253,948,779	$259,239,379	***$264,529,979***	$269,820,578	$275,111,178	$280,401,777	$285,692,377	$290,982,976
Product Price	$0.74	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	$0.76	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	$0.78	1.77%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	$0.79	3.84%	2.20%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	$0.81	5.65%	4.21%	2.62%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	$0.83	7.28%	5.97%	4.57%	3.02%	1.28%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	$0.84	8.78%	7.57%	6.29%	4.91%	3.41%	1.73%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	$0.86	10.19%	9.05%	7.86%	6.60%	5.25%	3.79%	2.16%	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	$0.87	11.53%	10.45%	9.32%	8.15%	6.91%	5.59%	4.16%	2.58%	0.78%	Negative IRR	Negative IRR
	$0.89	12.82%	11.78%	10.70%	9.59%	8.43%	7.21%	5.91%	4.51%	2.98%	1.25%	Negative IRR
	$0.91	14.05%	13.05%	12.02%	10.96%	9.85%	8.71%	7.50%	6.23%	4.86%	3.37%	1.70%

This figure demonstrates relationship between product price (±10%) and variable cost (±10%). If product price were to increase any amount while variable cost either decreased or stayed constant, positive IRR would be achievable.

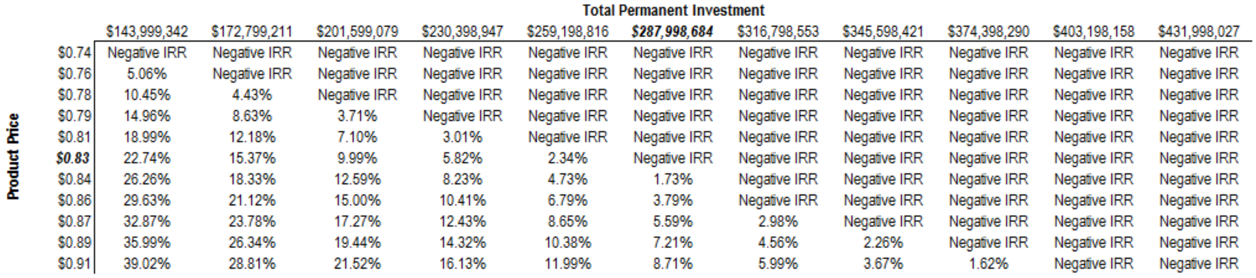
Figure 20



Product Price	Fixed Costs										
	$37,361,311	$39,852,065	$42,342,819	$44,833,573	$47,324,327	***$49,815,081***	$52,305,835	$54,796,589	$57,287,343	$59,778,097	$62,268,851
$0.74	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.76	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.78	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.79	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.81	2.11%	1.11%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.83	4.17%	3.56%	2.40%	1.43%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.84	5.96%	5.19%	4.39%	3.55%	2.67%	1.73%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.86	7.59%	6.88%	6.15%	5.39%	4.61%	3.79%	2.93%	2.02%	Negative IRR	Negative IRR	Negative IRR
$0.87	9.09%	8.43%	7.74%	7.04%	6.33%	5.59%	4.82%	4.02%	3.18%	2.30%	1.36%
$0.89	10.51%	9.87%	9.23%	8.57%	7.90%	7.21%	6.50%	5.77%	5.02%	4.24%	3.63%
$0.91	11.85%	11.24%	10.62%	9.99%	9.36%	8.71%	8.04%	7.37%	6.67%	5.96%	5.22%

This figure demonstrates relationship between product price (±10%) and fixed cost (±25%). If product price were to increase any amount while fixed cost either decreased or stayed constant, positive IRR would be achievable.

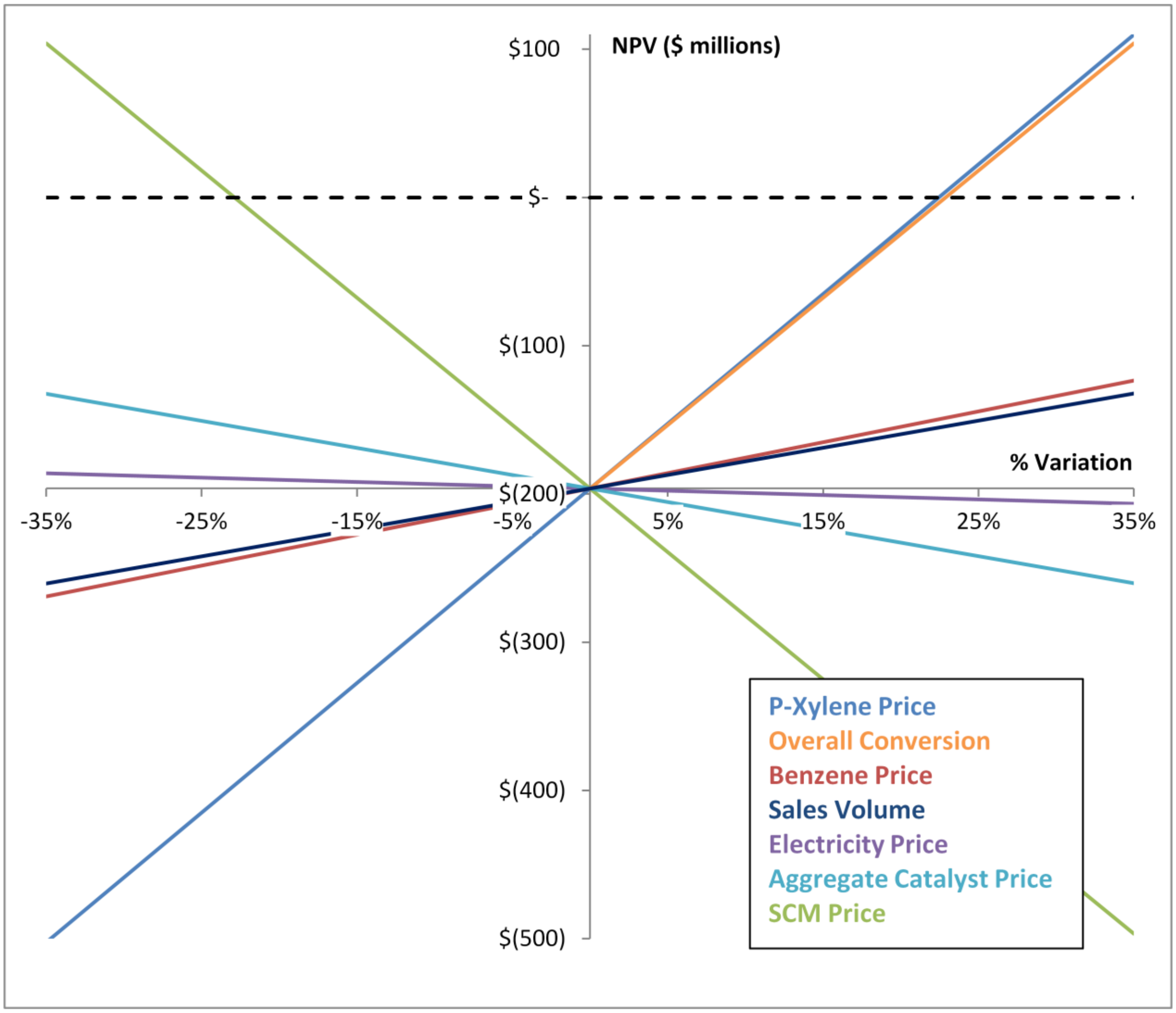
Figure 21



Product Price	Total Permanent Investment										
	$143,999,342	$172,799,211	$201,599,079	$230,398,947	$259,198,816	***$287,998,684***	$316,798,553	$345,598,421	$374,398,290	$403,198,158	$431,998,027
$0.74	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.76	5.06%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.78	10.45%	4.43%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.79	14.96%	8.63%	3.71%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.81	18.99%	12.18%	7.10%	3.01%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.83	22.74%	15.37%	9.99%	5.82%	2.34%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.84	26.26%	18.33%	12.59%	8.23%	4.73%	1.73%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.86	29.63%	21.12%	15.00%	10.41%	6.79%	3.79%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.87	32.87%	23.78%	17.27%	12.43%	8.65%	5.59%	2.98%	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.89	35.99%	26.34%	19.44%	14.32%	10.38%	7.21%	4.56%	2.26%	Negative IRR	Negative IRR	Negative IRR
$0.91	39.02%	28.81%	21.52%	16.13%	11.99%	8.71%	5.99%	3.67%	1.62%	Negative IRR	Negative IRR

This figure demonstrates relationship between product price (±10%) and total permanent investment (±50%). If product price were to increase any amount while TPI either decreased or stayed constant, positive IRR would be achievable.

Figure 22



This Strauss plot shows what percent change of which inputs would result in positive NPV. Notice, for example, that the effect of catalyst price is shown to be minimal at small price changes; however, if it increases to its full potential (see **Catalyst**), a 300% change, the effect could be devastating on profitability. It is clear that focus areas for improvement – those where positive NPV seems even feasible – should be the price of sugar cane molasses, the price of para-xylene, and the overall process conversion. Since the former two cannot be controlled, the best one can do is hedge against price fluctuations with futures contracts. Since the later is directly related to technological improvements, it makes sense to invest heavily in improving the overall process conversion. A 23%

increase in conversion – from the current 4.28% to a hopeful 5.55% - would achieve breakeven. Incremental improvements above 5.55% overall conversion result in strongly positive NPV. This conversion is a clear and attainable goal, which would serve as a “green light” for the investment, if demonstrable.

Section IX

Conclusion & Recommendations

IX. CONCLUSION & RECOMMENDATIONS

Conclusion

At a para-xylene price of $0.83 per pound, a benzene price of $0.45 per pound, and a price for sugar cane molasses of $0.03 per pound, the renewable production of para-xylene is unprofitable, and earns a **negative** 2.90% return on investment (ROI). Furthermore, the net present value (NPV) of this project at a discount rate of 15% is a **negative** $196 million. This results from two facts. First, the process requires an initial investment of $309 million; this is difficult to recover given the time value of money. Second, while the process ultimately becomes cash flow positive, this only occurs after six years of operation, and expected yearly profits are only $6 million. These conclusions were reached using conservative assumptions; as such, construction of the process should not proceed.

However, the three key factors merit further research. The market for para-xylene still represents a great opportunity due to steadily growing demand, both renewable and in general (see Market Analysis). New findings in any of the three areas below would mitigate the low annual profits and possibly the high initial investment. The project could then proceed to a more rigorous design.

Recommendations

Recommendation 1: Reactor Yields

Overall, 23.38 pounds or molasses are consumed for every pound of para-xylene produced. This is a direct consequence of yields in the Aqueous Phase Reforming (APR) and Condensation sections (300 and 400, respectively) of the process. Even after recycling unconverted sorbitol, only 1.25% of sorbitol mass consumed by the APR is produced as hydrogen; the remainder consists of light hydrocarbons, which can be burned, and a major fraction of carbon-dioxide, which must simply be vented. In addition, only 8.27% of sorbitol consumed by the condensation reactions is produced as para-xylene. Even increasing this yield by 27% via transalkylation results in only a 10.5% overall yield through the condensation and transalkylation combined.

However, these figures were conservatively restricted to specific examples found in patents and other relevant literature. Conditions in the aqueous phase reforming can likely be tailored to ensure full conversion of the leftover hydrocarbons to carbon dioxide and hydrogen; this would decrease the amount of additional feed required to supply hydrogen to the process. It is even more likely that the condensation reaction can be modified to generate a higher yield of para-xylene (currently only obtained in 46% of its theoretical yield). If both sections were to produce 100% of their theoretical hydrogen and para-xylene yields, the process would require 59.5% less molasses and save $167 million in raw materials costs every year. Decreasing the molasses costs by 23.2% of this 59.5%, which corresponds to increasing yields by 30% out of a potential 247%, causes the process to break even; any further advancement and the process returns a positive ROI and NPV.

Recommendation 2: Catalysts

The hydrolysis, hydrogenation, aqueous phase reforming, condensation, and transalkylation each require a substantial amount of zeolite catalyst. For most of these sections, no suitable catalysts were available for purchase. Instead, the process accounts for raw materials and manufacturing costs to provide the necessary catalysts. Following the advice of Professor Fabiano, we evaluated the process for three scenarios: raw material prices are not substantially lower in bulk than small quantities; raw material prices drop by 50% when purchased in bulk, and raw material prices drop by 25% when purchased in bulk. Due to the high cost of the raw materials, the process was modeled using the 25% price. Even so, the purchase and maintenance of the necessary amount of catalyst in perpetuity has a negative NPV of $117.6 million.

Further market and laboratory research is required to validate these pricing assumptions. It is possible that in large quantities the raw materials cost less than assumed, but the catalyst could also cost significantly more. In the event that reactor yields can be improved, the catalyst costs must be accurately estimated in order to ensure economic viability of the project.

If catalyst costs prove to be the deciding prohibitive factor, research into alternative catalyst systems based on cheaper raw materials may be merited. Such research, if fruitful, would be beneficial regardless of whether the renewable production of para-xylene was ultimately deemed economically viable. If the process is to be constructed, the cheaper catalyst system would provide a source of sustained competitive advantage. If not, the catalyst technology could be licensed to incumbent producers of para-xylene, who no doubt also suffer from the high cost of their catalysts.

Recommendation 3: Plant Acquisition and Reconstruction

Even at low yields and high catalyst costs, the process ultimately generates $6 million in profit per annum. However, this still represents a negative ROI and NPV due to the high amount of initial investment necessary for this process. However, offsetting this cost would make the process profitable as modeled in this report. One way to offset this cost would be the purchase and repurposing of a similar plant. Condensation and transalkylation are fairly common practices in the field, and it may be possible to acquire a facility with these capabilities already constructed. Alternatively, the manufacture of sugar alcohols from biofuel materials as well as the production of hydrogen via aqueous phase reforming are also reasonably common practices, either in separate or combined plants. If available at a low price, purchasing an unwanted plant with one of these subset of capabilities, then constructing the remaining sections of the plant necessary, could represent a cheaper initial investment than construction from scratch.

Section X

Acknowledgments

X. ACKNOWLEDGMENTS

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Section XI

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Section XII

Appendices

XII. APPENDICES

Appendix A: Problem Statement

Renewable Para-Xylene

The international demand for xylene isomers continues to increase steadily, with p-xylene in high demand as a key raw material in the bottling, packaging, materials, and fiber industries. Climate change, dwindling petroleum resources, a desire for energy independence, and consumer behavior are driving significant research and investment into the development of technologies that reduce energy consumption, improve efficiency, and produce chemicals and fuels from renewable resources. The disposition of agricultural resources and production to support both this transition from fossil to renewable fuels, while providing food to meet the demands of the increasing global population, is a source of controversy and significant discussion. Additionally, several beverage makers are actively seeking a plant-based route to plastics for their product packaging, to actively demonstrate their commitment to sustainability and the global environment.

Through its research efforts, your company has developed new and innovative technology to convert biomass-derived material into para-xylene, as an alternative to traditional production routes. Because the material from this innovative catalytic technology has the same composition as traditional petroleum-based para-xylene, it can be used directly in current manufacturing processes, or blended with conventional petroleum-based material, and distributed through existing supply chains without equipment modifications or separate shipping containers. In its current state, this technology is flexible to be optimized and modified to convert multiple renewable feedstocks to para-xylene, using a patented catalytic process to convert the plant-based sugars into monomer. In laboratory and pilot- scale testing, the technology has proven to be equally flexible with respect to potential raw materials, and able to accommodate a varying range of feed materials from glucose and sucrose (derived from sugar crops), starches, glycerol, polymers of glucose contained in cellulose (plant-cell walls), and longer chain C_5 and C_6 sugars (such as those contained in hemi-cellulose). Your company's product trials show that the *p*-xylene produced using this technology is suitable for conversion into the polyethylene terephthalate (PET) raw material, purified terephthalic acid.

Your team has been assembled to design the first commercial facility, and to identify the optimal raw material to demonstrate the commercial viability of this new technology, using assumptions identified by your research and business directors. Your directors agree that the biomass options for this first facility should be limited to woody biomass, sugar cane, and corn grain. It's expected that woody biomass can be converted to sugars using standard enzymatic technology developed for the corn and cellulosic ethanol industry and available from industrial enzyme suppliers. However, they have concerns that the additional investment necessary for pre-treatment and enzymatic conversion of the biomass to sugars may restrict the economic viability of the innovation.

Your company recently acquired both corn dry-grind and sugar-cane ethanol facilities, in an effort to proactively provide access to the necessary raw material supplies (corn grain and sugar cane) at market pricing. These facilities are in Nebraska (U.S.) and in the Sao Paolo region of

Brazil, respectively. Partnership discussions for woody biomass supply, in the Pacific Northwestern region of the United States, are currently in progress. This material is expected to be available in Washington State, and in the form of mill residue (but also land clearing debris and forest thinnings). Sugar supply from the dry mill is expected to be typical of that currently used to supply fuel-ethanol fermentations, while the Brazilian facility will supply molasses and cane juice at standard cane industry concentrations. In addition to raw material economics, your team will need to consider carefully the advantages, disadvantages, potential obstacles, and restrictions for each sugar supply option when making its selection; e.g., the sugar-cane crushing season in Brazil is 8-9 months long. Current market pricing is to be expected for all raw materials, utilities, and product, regardless of location.

A key point of the Directors' interest involves the potential similarities and differences between facilities using woody biomass compared to molasses and cane juice, and sugar liberated from corn grain, including but not limited to, capital investment, overall process sustainability, and profitability. Your business director has determined that the process facilities and equipment should produce at a 400 MMlb per year capacity, using the technology documented in the patents, patent applications, and references listed below as an initial basis. Your para-xylene product must meet the minimum industry purity and quality standards for polymer intermediate grade material, as the expected end use is in bio-PET production. Given the recent volatility of petroleum markets and pricing, your marketing organization is unsure if this material will be able to command any premium above market pricing. Therefore, your business director believes sensitivity analyses are necessary to understand the potential exposure to market fluctuations, and any benefit that a market premium could provide.

This technology has potential use in the U. S. Corn Belt, where water is an extremely limited resource and a large area of concern for any potential plant site. Therefore, your plant and process design will need to use the minimum amount of water necessary for the technology, with the goal of being a zero-discharge plant (meaning that all process water is recycled within the plant). The current benchmark for total water use in a fuel-ethanol plant is about 3 gal/gal of product, and you should strive to meet or exceed this benchmark, regardless of raw biomass source.

Your plant design should be as environmentally friendly as possible, and satisfy the required state and federal emissions legislation. It is expected that the facility will include emission-control equipment as a part of the process design. Recover and recycle process materials to the maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. Your plant design must be controllable and safe to operate. As the process technology integration and design team, you will participate in the start-up and will have to live with any of your poor design decisions.

Undoubtedly, you will need additional data beyond that given here and listed in the references below. Cite any literature data used. If required, make reasonable assumptions, state them, and identify whether your design or economics are sensitive to the assumptions you have made.

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http://www.fs.fed.us/woodybiomass/whatis.shtml, http://www.fs.fed.us/woodybiomass/state.shtml, &
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U. S. Patent Application 20,090,124,839, Dumesic, J. A., et al., "Production of Liquid Alkanes in the Jet Fuel Range (C8-C15) From Biomass-Derived Carbohydrates", May 14, 2009.

U. S. Patent 5,763,713, Blommel, et al., "Process for the Isomerization of Benzene Containing Feed Streams", June 9, 1998.

U. S. Patent 5,962,755, Blommel, et al., "Process for the Isomerization of Benzene

Containing Feed Streams", October 5, 1999.

Cortright, R. A., et al., "Hydrogen from catalytic reforming of biomass-derived hydrocarbons in liquid water," *Nature*, **418**, 964-967, Aug. 29, 2002.

The Renewable Fuels Association web site has a good description of the fuel-ethanol process and industry, which may be helpful in understanding the corn dry-grind process. http://www.ethanolrfa.org

A good model for much of the dry-grind ethanol process is discussed on http://www.intelligen.com/literature.shtml, which links to a paper by Kwiatkowski et al. This includes a SUPERPRO DESIGNER model that works with their evaluation version of the software. Note, however, that SUPERPRO DESIGNER does not handle VLE rigorously, and thus, is not suitable for designing this process.

Web resources for sugar and sugar solution properties (including molasses), with references for items common to the sugar and ethanol industries.
http://www.sugartech.co.za/matlprop/index.php
www.ams.usda.gov

Appendix B: Sample Calculations

SC-000: Molasses Storage Requirements

The basic requirements for molasses storage are as follows: 1) molasses must be supplied at 1.245 Mlb/h, 2) there must be enough storage capacity to last three months, or 2208 h without replenishment, and 3) no one tank can exceed 20,000,000 gal. Additionally, given that the capacity should be within a "reasonable" range, the residence time is the key (least specified) variable of design. Vessel prices are estimated according to PPDP Table 22.32, with adjustments for the CE index change, C_E. The residence time is specified at six days, to permit active usage of five tanks at a time with once monthly deliveries.

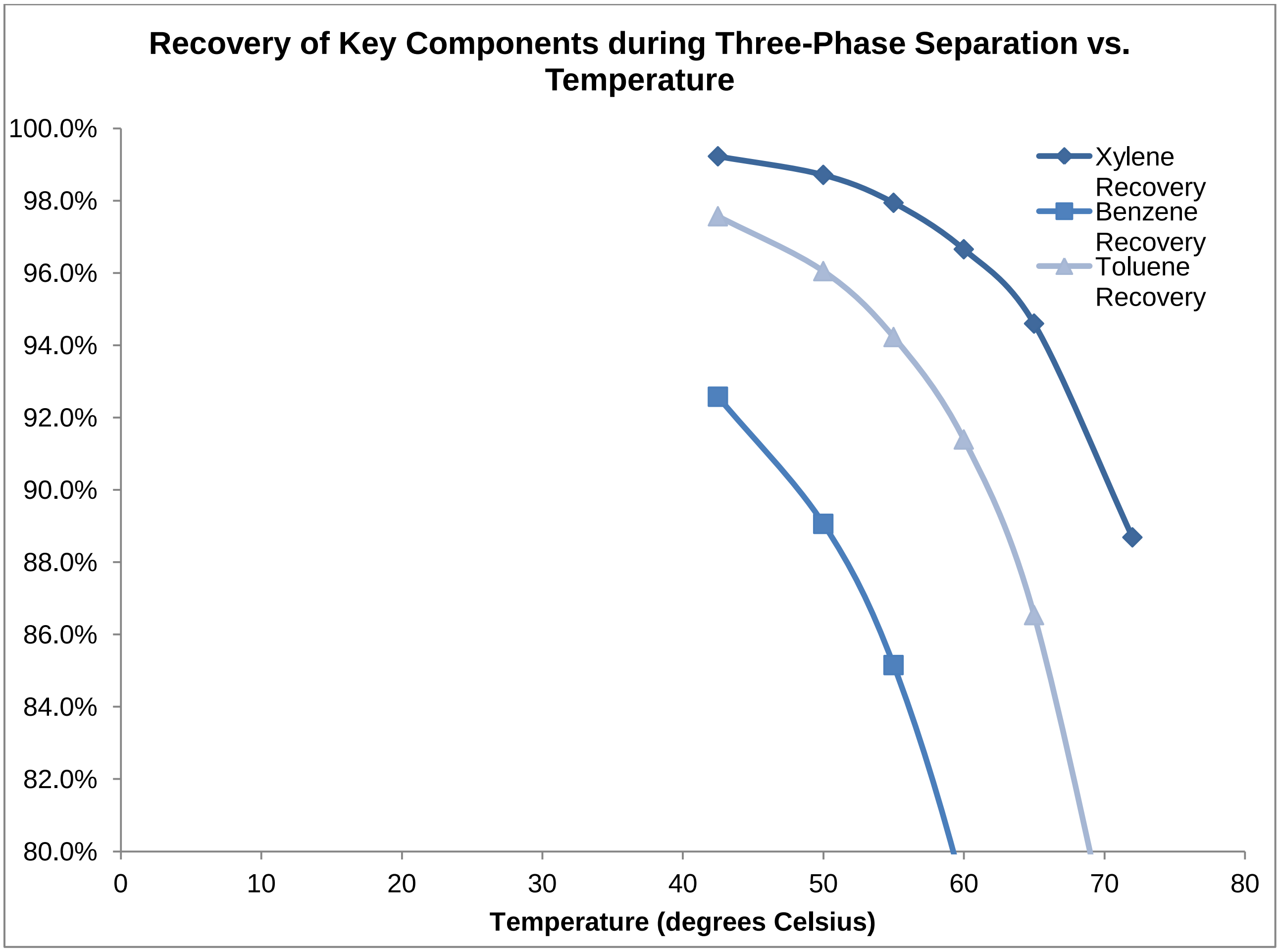
Equations

$$V = \frac{F\tau}{\rho_{mol}*u};\ C = C_E * 265V^{0.51}$$ (CS spherical , 0-30psig)

Example

$$C = \frac{680}{500} * 265\left(\frac{1245000*144}{11.75*0.76}\right)^{0.51} = \$1{,}906{,}822$$

SC-500: Three Phase Separation



SC-501: Crystallization Utilities

The crystallizer must remove 2,293,914.1 BTU per hour in order to chill the mixed xylenes to -22 °F from 60°F. Additionally, the crystallizer requires 69.347 BTU per pound p-xylene to account for the latent heat of crystallization, and with 50,321.7 pounds per hour p-xylene product. This means 3,489,658.93 BTU per hour is required to crystallize the p-xylene. Therefore a total of 5,783,573.03 BTU per hour of refrigeration is used by the crystallizer unit.

At a cost of $10.867 per million BTU of heat removed for -90°F refrigerant, the total crystallization utilities are $62.85 per hour, or about $500,000 per year.

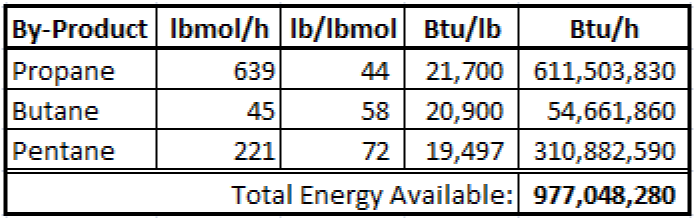
SC-700: Combustion Energy Availability

The amount of energy available from combustion is estimated from the flow rates and enthalpies of combustion of the major by-product species. Although there are many more hydrocarbon species in the process output, the light alkanes alone provide enough energy to cover the steam utility requirements. Therefore, this brief calculation (results tabulated in Figure 23) lends confidence to the notion that no outside steam would be necessary during normal operation.

<u>Equations</u>

$$\dot{Q} = \dot{m}\Delta\bar{H}_{comb}$$

Figure 23



By-Product	lbmol/h	lb/lbmol	Btu/lb	Btu/h
Propane	639	44	21,700	611,503,830
Butane	45	58	20,900	54,661,860
Pentane	221	72	19,497	310,882,590
			Total Energy Available:	**977,048,280**

SC-701: Sizing and Pricing for Heating Fluid Storage Vessels

The amount of heating fluid required is directly related to the net duty and the storage vessel residence. Net duties (Q) are calculated from ASPEN – these in turn are converted to mass flow rates via latent heat information (ΔH). The residence time (τ) for a storage vessel is a key determinant of how much fluid is required to be purchased up front. τ are chosen from recommendations or from the literature specifications. Capacity utilization (u) was taken at a conservative 70% for these units. Vessel prices are estimated according to PPDP Table 22.32, with adjustments for materials (F_M) according to PPDP p.580. The CE index change is accounted for by the multiplicative factor, C_E. Equations for all cases and an example calculation for Dowtherm A (ST-700), are shown below.

Equations

$V = \frac{\left(\frac{\dot{Q}}{\Delta H_v}\right)\tau}{u}$; $C_P = 265V^{0.51}$ (CS cone roof); $C_P = 47V^{0.78}$ (CS spherical, 30-200 psig); $C = F_M C_P C_E$

Example

Q = 532 MBtu/h, $\Delta H_v(700^0 C) = 102$ Btu/lb, τ = 0.1 h, u = 70%, P = 94 psig, low-alloy

$$C_P = 47 * \left(\frac{\left(\frac{532*10^6}{102}\right)*0.1}{0.70}\right)^{0.78} = \$441{,}074 \rightarrow C = 1.2 * \$441{,}074 * \left(\frac{680}{500}\right) = \$719{,}833.$$

SC-702: Pricing of Fired Heaters

Fired heaters are priced using Table 22.32 of PPDP and the desired heat duties, Q. The equations for all cases and an example for the molten salt heater are provided below. One source of concern is that the specified duties for the Dowtherm A and the steam boiler significantly exceed the specified range for the given equations. Prices were adjusted for the chemical engineering index and the material chosen.

Equations

$C_P = 12.32Q^{0.64}$ (molten salt); $C_P = 12.74Q^{0.65}$ (Dowtherm A); $C_P = 0.367Q^{0.77}$(CS reboiler, P <20 atm); $C = F_M C_P C_E$

Example

Q = 62 MBtu/h, molten salt, stainless steel

$$C_P = 12.32(62 * 10^6)^{0.64} = \$1{,}196{,}028 \rightarrow C = 2.0 * \$1{,}196{,}028 * \left(\frac{680}{500}\right) = \$3{,}253{,}196.$$

SC-U00: Heating Fluid Requirements and Costs

Heat duties from ASPEN (Q) and materials information from the supplier (P, ΔH_{vap}) Appendix D provides the necessary information for these calculations, given a specified or assumed residence time (τ).

Equations

$m = \dot{m}\tau$, $\dot{m} = \frac{\dot{Q}}{\Delta\hat{H}_{vap}}$ (condensing), $\dot{m} = \frac{\dot{Q}}{c\Delta T}$ (simple), $C = \hat{P}m$

Example

Q = 532 MBtu/h, condensing, $\Delta\hat{H}_{vap}(700^0F)$ =101Btu/lb, τ = 0.10 h, $\hat{P}$ = \$7.13/lb

$$m = \frac{532*10^6}{101} * 0.10 = 532{,}000 \text{ lb} \rightarrow C = \$7.13 * 532{,}000 = \$3{,}793{,}160.$$

SC-U01: Utility Savings Calculations

Utilities savings were calculated in two steps: 1) baseline utility requirements and 2) calculation of differential savings from substitution. From ASPEN, unit heat duties and temperatures are used to specify what utility is necessary, and how much. Pricing for baseline requirements is done using Table 23.1 in PPDP. Given the baseline, appropriate substitutes are sought from the process excess production, by-products, or integration opportunities. The substitutes are also priced according to Table 23.1. After annualizing, the difference in cost between baseline and substitute is the savings. An example is shown for steam, but an analogous procedure was followed for cooling and boiler feed water. Results for steam are shown in Figure 24.

Equations

$\dot{m} = \frac{\dot{Q}}{\Delta\hat{H}_{vap}}$ (condensing) $C = \dot{m}\hat{P}$

Example: RB-500

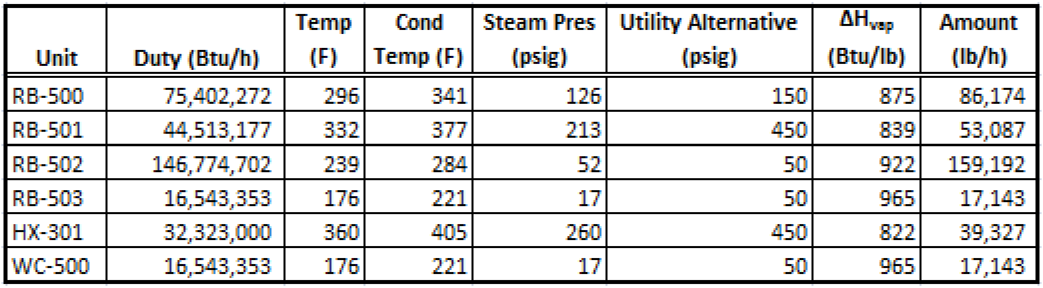
Given Q = 75.4 MBtu/h, T = 296^0F; Found P^s= 126 psig (X-Eng Tables), $\Delta\hat{H}_{vap}(296^0F)$ =875 Btu/lb; Assumed $\hat{P}$ = \$4.80/1000 lb (Table 23.1, PPDP)

$\dot{m} = \frac{75.4*10^6}{875} = 86{,}174$ lb/h → $C = \$4.80 * 8.6174 * 7920 = \$3{,}134{,}780$/yr.

Substituting boiler feed water: $\hat{P}_{sub} = \$1.80/1000$ gal. Ignoring density changes as function of temperature, $V = \frac{\dot{m}}{\rho} = \frac{8.6174}{8.32} * 7920 = 82{,}000$ kgal/yr → $C = \$1.80 * 82{,}000 = \$147{,}600$

Savings: \$3.13M - \$0.15M = \$2.99M/yr

Figure 24



Unit	Duty (Btu/h)	Temp (F)	Cond Temp (F)	Steam Pres (psig)	Utility Alternative (psig)	ΔH_{vap} (Btu/lb)	Amount (lb/h)
RB-500	75,402,272	296	341	126	150	875	86,174
RB-501	44,513,177	332	377	213	450	839	53,087
RB-502	146,774,702	239	284	52	50	922	159,192
RB-503	16,543,353	176	221	17	50	965	17,143
HX-301	32,323,000	360	405	260	450	822	39,327
WC-500	16,543,353	176	221	17	50	965	17,143

SC-C00

WHSV = mass of reactant fed per hour / mass catalyst = 13.5/7 ≈ 1.93 hr^{-1}

Mass of catalyst needed = 625000*453.6/1.93 = 147,000,000 grams of catalyst

Price of catalyst = 12/16 * 1.47E8 * price of H_4SiO_4 per gram + 1/16 * 1.47E8 * price of Na_2AlO_2 per gram + 3/16 * 1.47E8 * price of $(NH_4)_2SiF_6$ per gram = \$2.49 million *0.25 = \$0.62 million

Mass of deactivated catalyst per hour = 13.29 * 1818.58 = 24,169 grams.

Yearly price = (12/16 * 24,169 * price of H_4SiO_4 per gram + 1/16 * 24,169 * price of Na_2AlO_2 per gram + 3/16 * 24,169 * price of $(NH_4)_2SiF_6$ per gram)* 24 * 365 = \$3.52 million * 0.25 = \$0.88 million

SC-C01

“VHSV” = 300/40 = 7.5

SUF = 17378.7*28.3/0.04/7.5 = 1640368.8

Toluene scale up = 300 * SUF = 492.11 million ml

Ruthenium (III) Acetylacetonate scale up = 2.907 * SUF = 4.77 million grams

Al_2O_3 scale up = 73 * SUF = 119.75 million grams

Price = Toluene scale up * Toluene density * Toluene price + Ruthenium (III) Acetyl Acetonate scale up * Ruthenium (III) Acetyl Acetonate price + Al_2O_3 scale up * Al_2O_3 price = \$229.7 million *0.25 = \$57.4 million

Ruthenium (III) Acetyl Acetonate wt% = 101/398 = 0.254

Mass of Ru in Ruthenium (III) Acetyl Acetonate scale up = Ruthenium (III) Acetyl Acetonate scale up * 0.254 = 1.21 million grams

Mass of catalyst needed = Mass of Ru in Ruthenium (III) Acetyl Acetonate scale up / 0.05 = 24.2 million grams

Price of catalyst = price of similar catalyst * mass of catalyst needed = \$47.5 million * 0.25 = \$11.9 million.

SC-C02

Mass of catalyst needed = 175,659 *453.6 / 1.8 = 44.27 million grams

Number of batches needed = 44.27 million / 19.875 = 2.46 million

Price of catalyst = (Rhodium (III) Nitrate price * Rhodium (III) Nitrate batch mass + Perrhenic acid price * Perrhenic acid batch mass + Cerium (III) Nitrate price * Cerium (III) Nitrate batch mass) * 2.46 million = \$686 million

Number batches needed = 44.27 million / 13.28 = 3.33 million

Price of catalyst = (Rhodium market price * Rhodium batch mass + Rhenium market price * Rhenium batch mass + Cerium market price * Cerium batch mass + Titanium market price *

Titanium batch mass + Activated Carbon market price * Activated Carbon batch mass) * 3.33 million = \$240.9 million * 0.25 = \$60.2 million

SC-C03

Mass of catalyst needed = 530,125*453.6/1.93 = 120.2 million grams of catalyst

Price of catalyst = 30/31 * 120.2 million * price of H_4SiO_4 per gram + 1/31 * 120.2 million * price of Na_2AlO_2 per gram = \$2.41 million *0.25 = \$0.60 million

Mass of deactivated catalyst per hour = 13.29 * 2910 = 38,674 grams

Yearly price = (30/31 * 38,674 * price of H_4SiO_4 per gram + 1/31 * 38,674 * price of Na_2AlO_2 per gram) * 24 * 365 = \$6.80 million * 0.25 = \$1.70 million

SC-C04

WHSV = 12 (ml fed per hour in patent) * 0.8669 (density of toluene) / 2 (mass of catalyst in patent) = 5.2 hr^{-1}

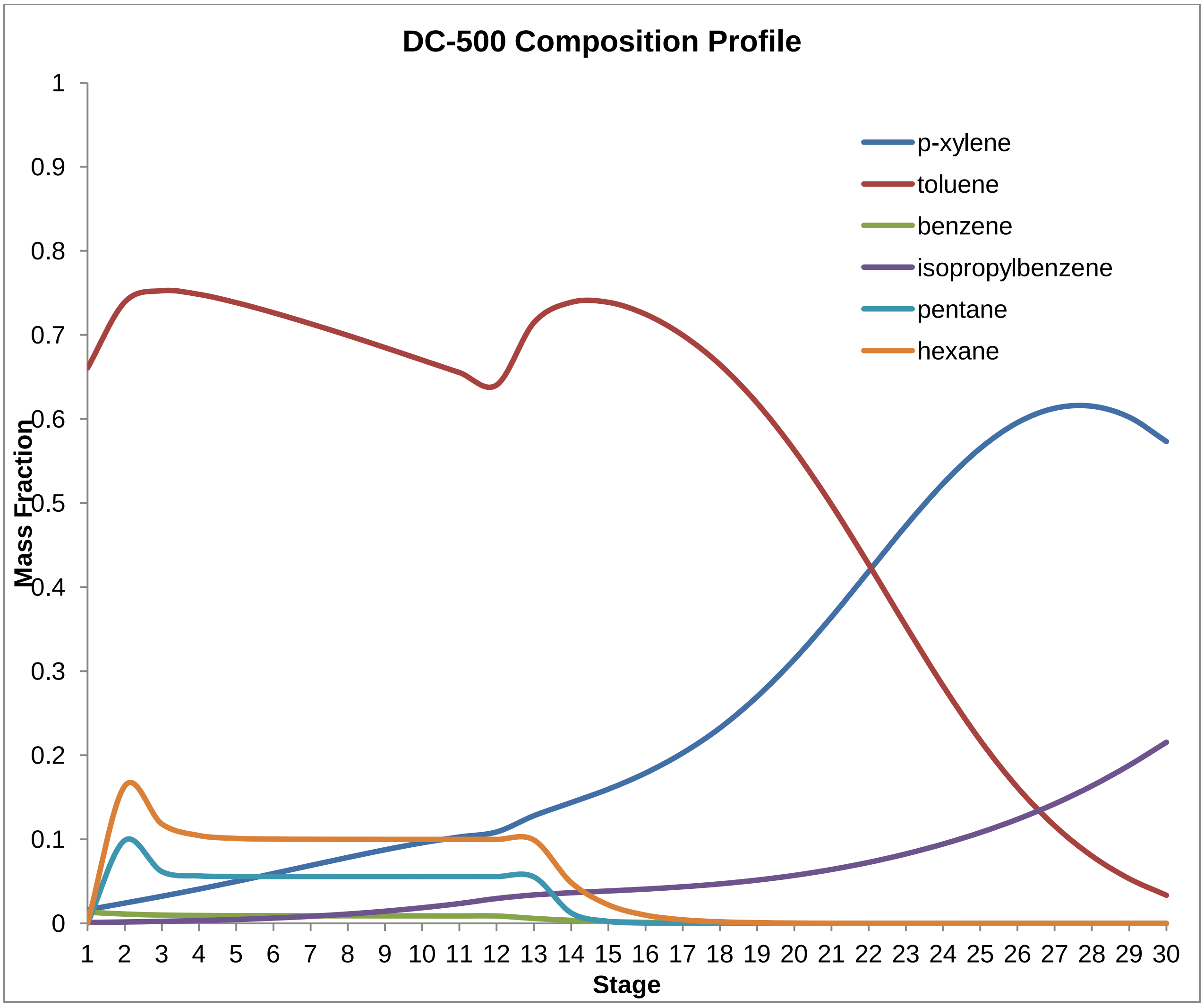
Mass of catalyst needed = 144,783*453.6/1.93 = 12.6 million grams of catalyst

Price of catalyst = 70/71 * 12.6 million * price of H_4SiO_4 per gram + 1/71 * 12.6 million * price of Na_2AlO_2 per gram = \$0.25 million *0.25 = \$0.06 million

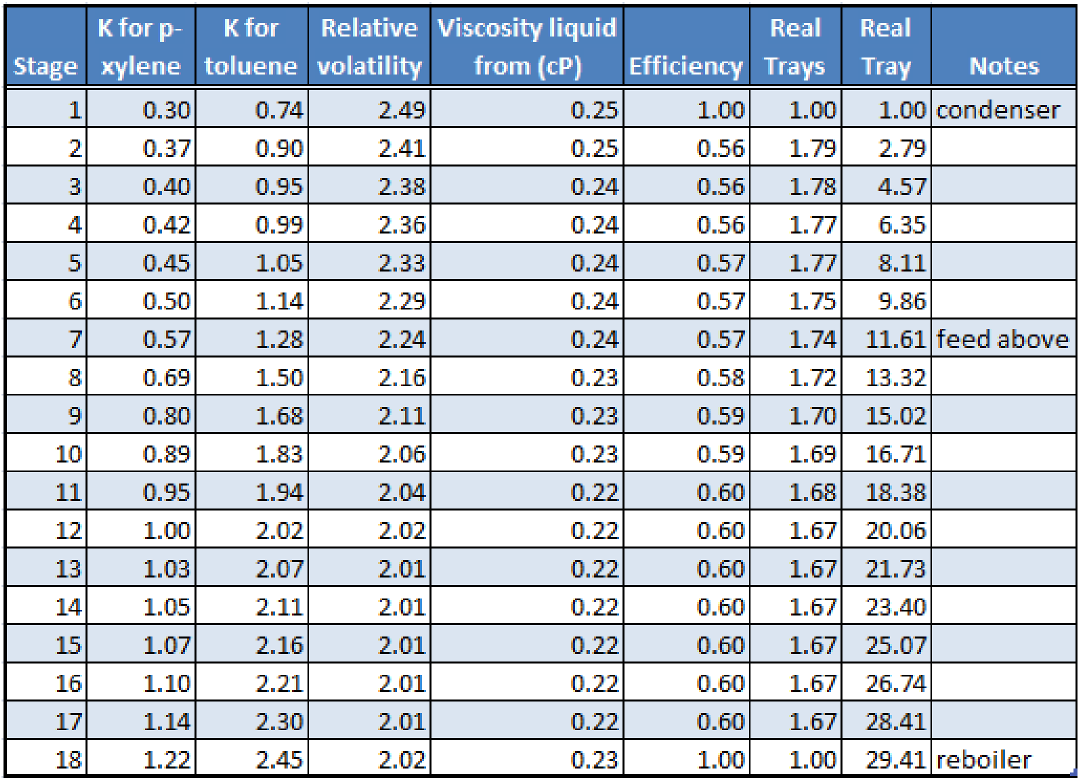
Mass of deactivated catalyst per hour = 13.29 * 1571.33 = 38,674 grams

Yearly price = (70/71 * 38,674 * price of H_4SiO_4 per gram + 1/71 * 38,674 * price of Na_2AlO_2 per gram) * 24 * 365 = \$3.67 million * 0.25 = \$0.92 million

DC-500 Concentration Profile

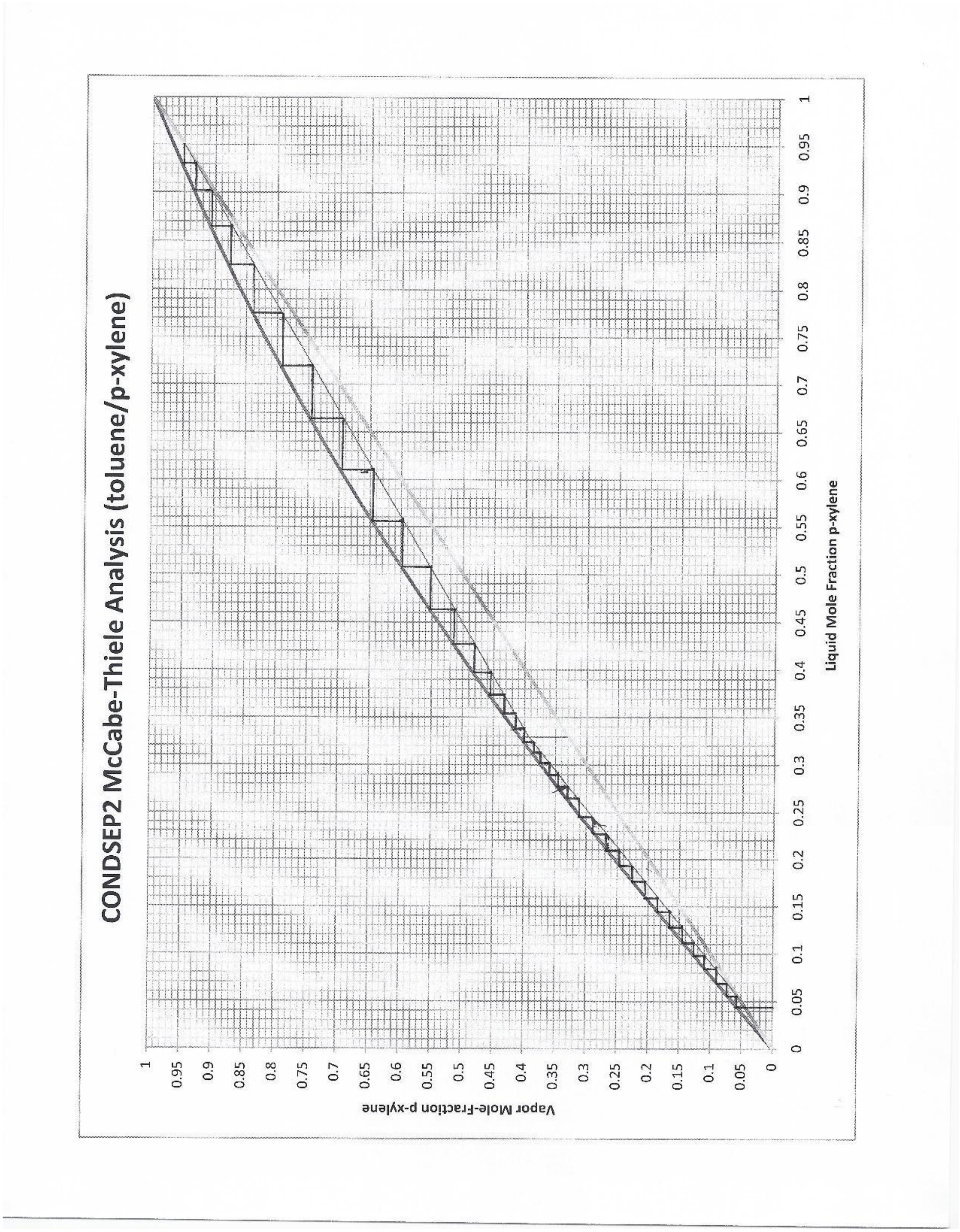


DC-500 Real Tray Efficiency Calculations

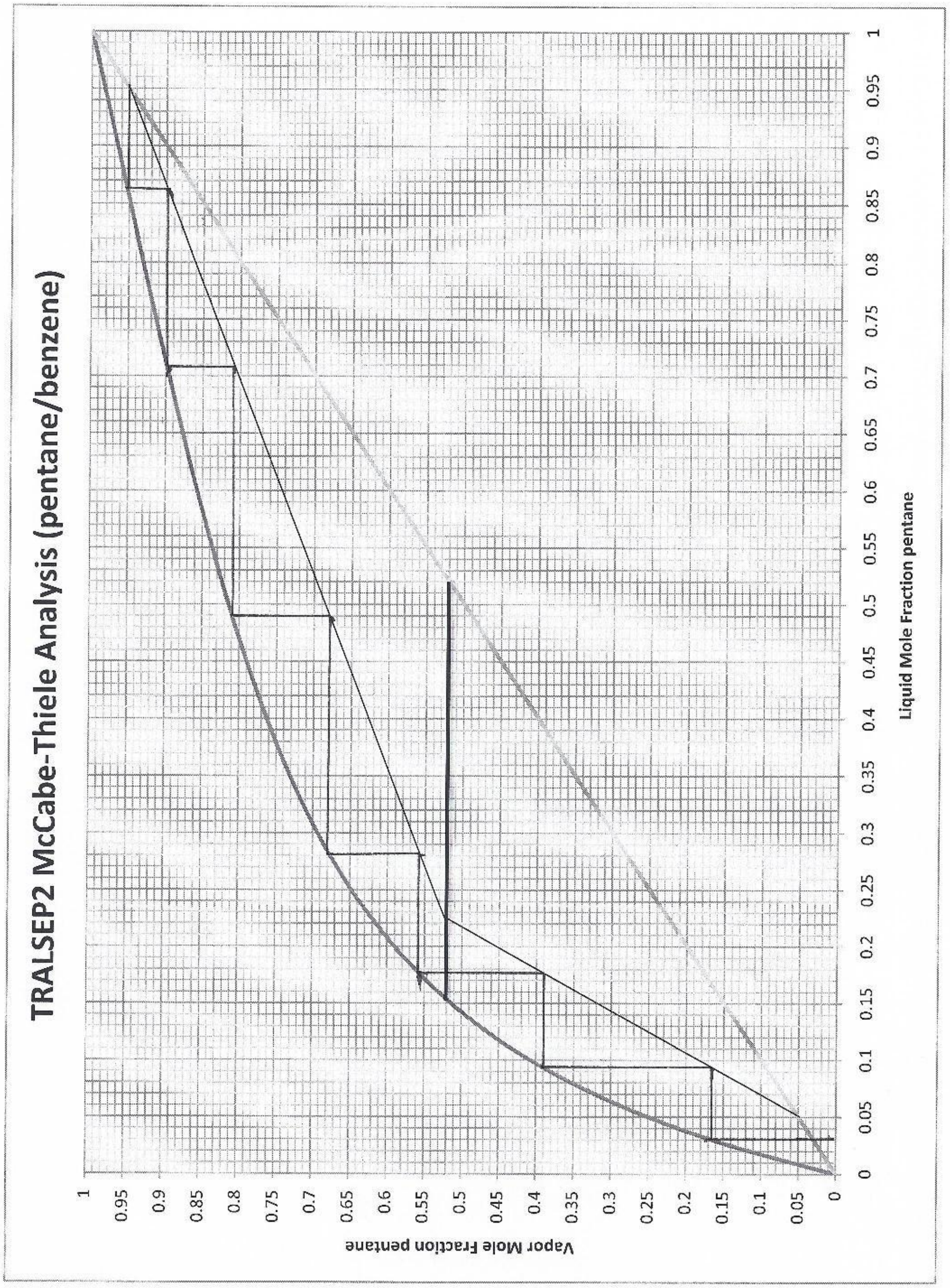


Stage	K for p-xylene	K for toluene	Relative volatility	Viscosity liquid from (cP)	Efficiency	Real Trays	Real Tray	Notes
1	0.30	0.74	2.49	0.25	1.00	1.00	1.00	condenser
2	0.37	0.90	2.41	0.25	0.56	1.79	2.79	
3	0.40	0.95	2.38	0.24	0.56	1.78	4.57	
4	0.42	0.99	2.36	0.24	0.56	1.77	6.35	
5	0.45	1.05	2.33	0.24	0.57	1.77	8.11	
6	0.50	1.14	2.29	0.24	0.57	1.75	9.86	
7	0.57	1.28	2.24	0.24	0.57	1.74	11.61	feed above
8	0.69	1.50	2.16	0.23	0.58	1.72	13.32	
9	0.80	1.68	2.11	0.23	0.59	1.70	15.02	
10	0.89	1.83	2.06	0.23	0.59	1.69	16.71	
11	0.95	1.94	2.04	0.22	0.60	1.68	18.38	
12	1.00	2.02	2.02	0.22	0.60	1.67	20.06	
13	1.03	2.07	2.01	0.22	0.60	1.67	21.73	
14	1.05	2.11	2.01	0.22	0.60	1.67	23.40	
15	1.07	2.16	2.01	0.22	0.60	1.67	25.07	
16	1.10	2.21	2.01	0.22	0.60	1.67	26.74	
17	1.14	2.30	2.01	0.22	0.60	1.67	28.41	
18	1.22	2.45	2.02	0.23	1.00	1.00	29.41	reboiler

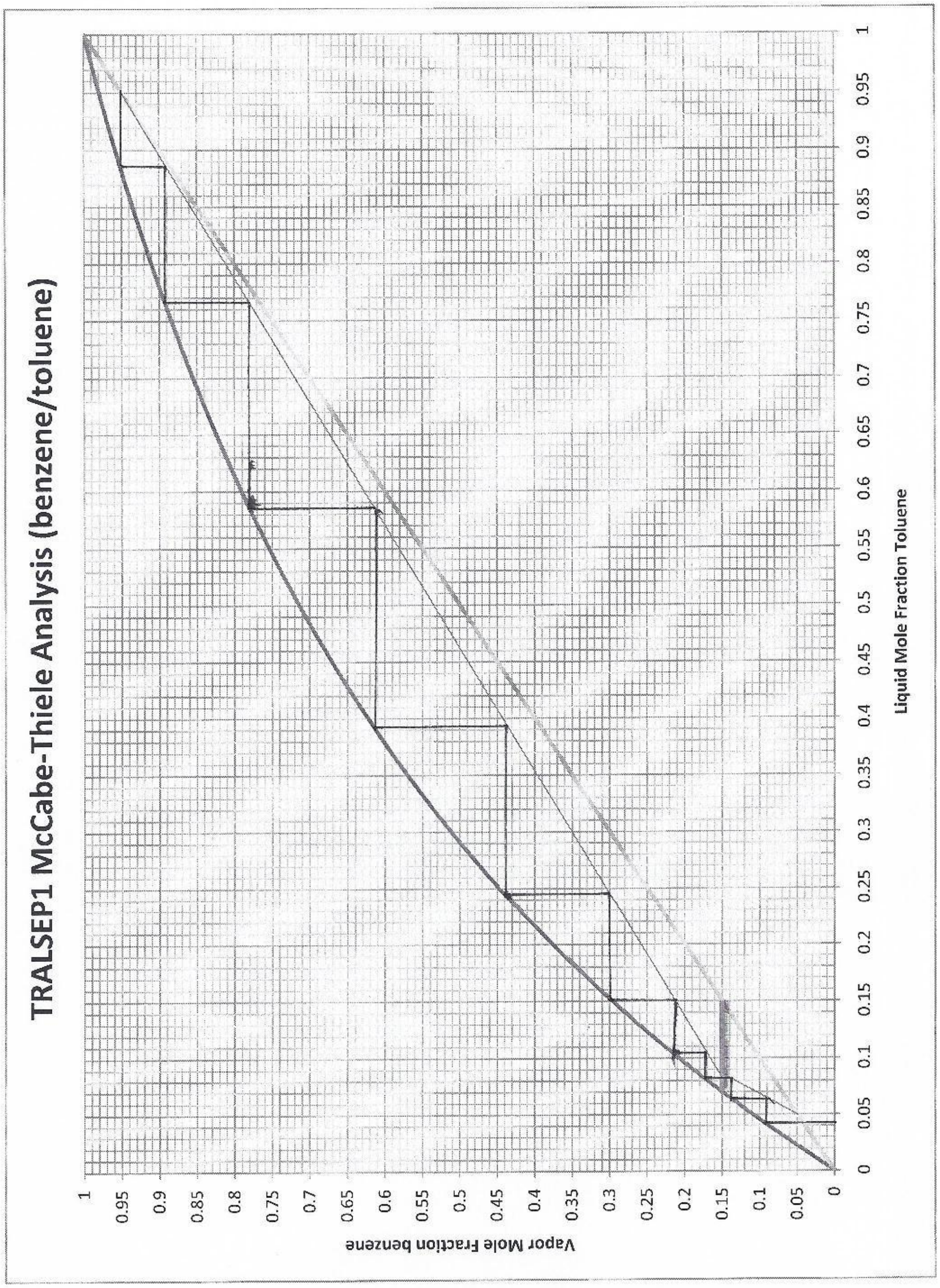
DC-501 McCabe Thiele Analysis



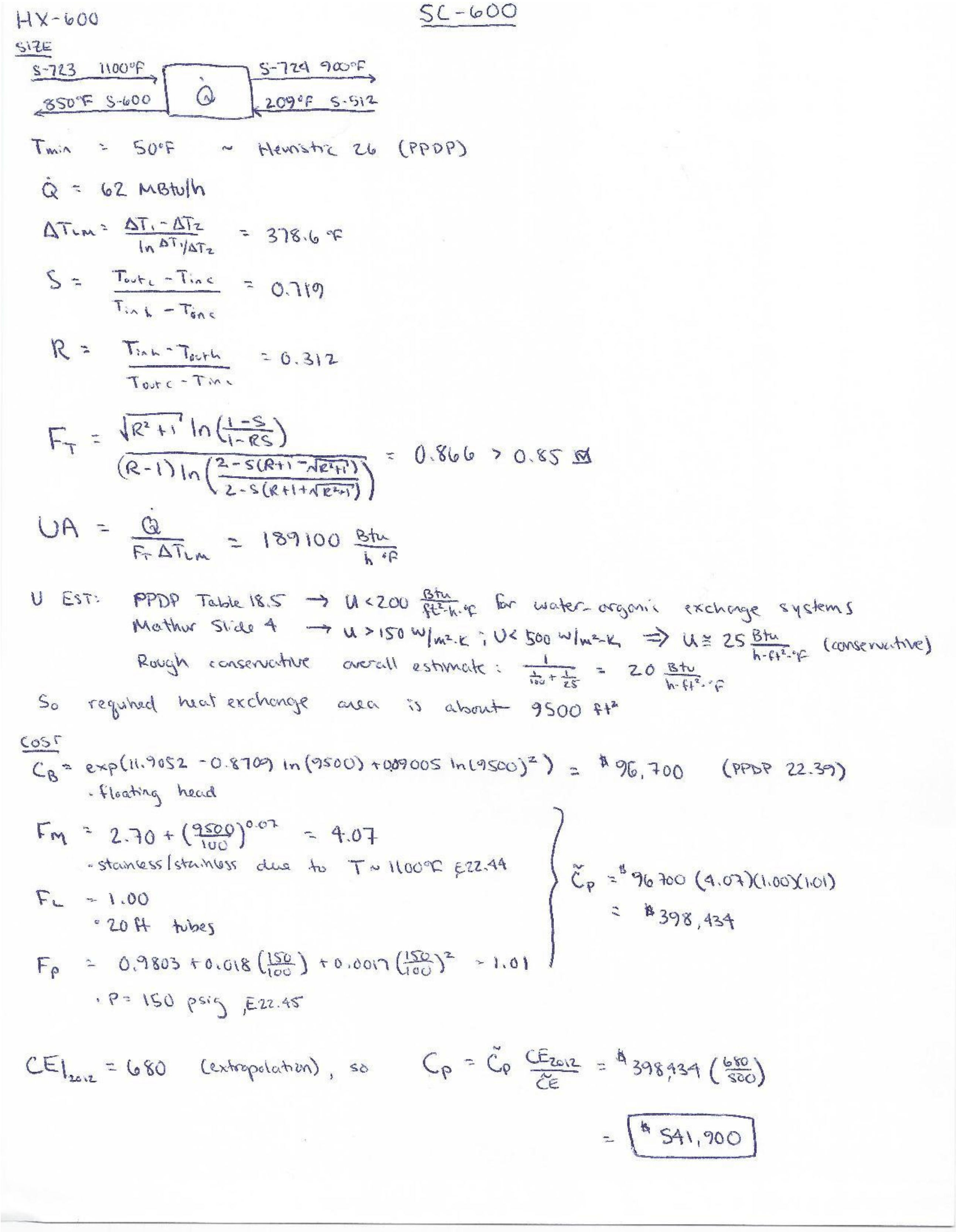
DC-502 McCabe Thiele Analysis



DC-503 McCabe Thiele Analysis



SC-600: Sizing of HX-600



HX-600 SC-600

SIZE

S-723 1100°F → [$\dot{Q}$] → S-724 900°F

850°F S-600 ← [$\dot{Q}$] ← 209°F S-512

$T_{min} = 50°F$ ~ Heuristic 26 (PPDP)

$\dot{Q} = 62$ MBtu/h

$$\Delta T_{LM} = \frac{\Delta T_1 - \Delta T_2}{\ln \Delta T_1/\Delta T_2} = 378.6\ °F$$

$$S = \frac{T_{out\,c} - T_{in\,c}}{T_{in\,h} - T_{in\,c}} = 0.719$$

$$R = \frac{T_{in\,h} - T_{out\,h}}{T_{out\,c} - T_{in\,c}} = 0.312$$

$$F_T = \frac{\sqrt{R^2+1}\,\ln\left(\frac{1-S}{1-RS}\right)}{(R-1)\ln\left(\frac{2-S(R+1-\sqrt{R^2+1})}{2-S(R+1+\sqrt{R^2+1})}\right)} = 0.866 > 0.85\ ☑$$

$$UA = \frac{\dot{Q}}{F_T\,\Delta T_{LM}} = 189100\ \frac{Btu}{h\ °F}$$

U EST: PPDP Table 18.5 → $U < 200\ \frac{Btu}{ft^2\cdot h\cdot °F}$ for water-organic exchange systems

Mathur Slide 4 → $U > 150\ W/m^2\cdot K$; $U < 500\ W/m^2\cdot K$ ⇒ $U \cong 25\ \frac{Btu}{h\cdot ft^2\cdot °F}$ (conservative)

Rough conservative overall estimate : $\frac{1}{\frac{1}{100}+\frac{1}{25}} = 20\ \frac{Btu}{h\cdot ft^2\cdot °F}$

So required heat exchange area is about 9500 ft^2

COST

$C_B = \exp(11.9052 - 0.8709\ \ln(9500) + 0.09005\ \ln(9500)^2) = \$96,700$ (PPDP 22.39)

- floating head

$F_M = 2.70 + \left(\frac{9500}{100}\right)^{0.07} = 4.07$

- stainless/stainless due to T ~ 1100°F E22.44

$F_L = 1.00$

- 20 ft tubes

$F_P = 0.9803 + 0.018\left(\frac{150}{100}\right) + 0.0017\left(\frac{150}{100}\right)^2 = 1.01$

- P = 150 psig, E22.45

$\tilde{C}_P = \$96700\,(4.07)(1.00)(1.01)$

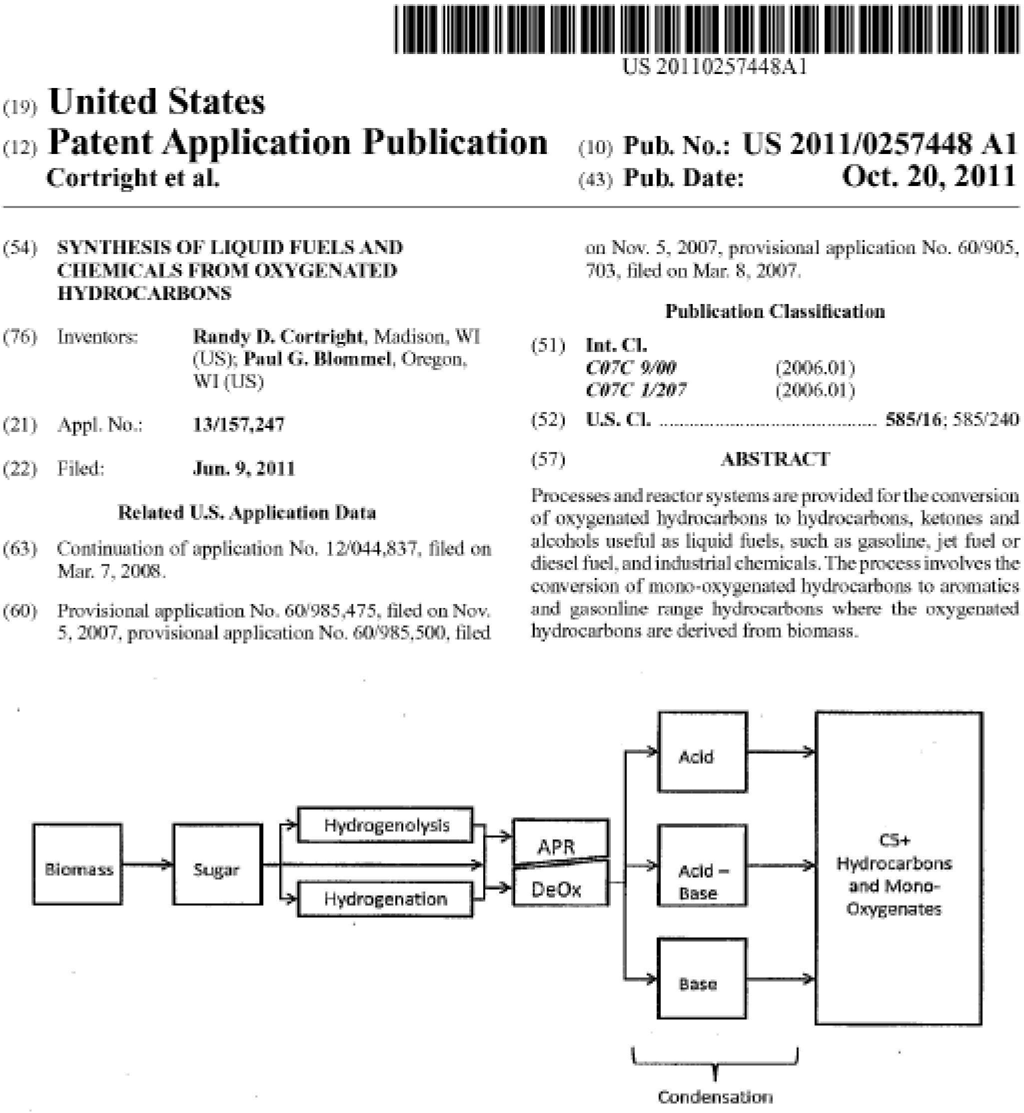
$= \$398,434$

$CEI|_{2012} = 680$ (extrapolation), so $C_P = \tilde{C}_P\,\frac{CE_{2012}}{\tilde{CE}} = \$398,434\left(\frac{680}{500}\right)$

$= \boxed{\$541,900}$

Appendix C: Patents

US2011/0257448-A1



US 20110257448A1

(19) **United States**

(12) **Patent Application Publication**

Cortright et al.

(10) **Pub. No.: US 2011/0257448 A1**

(43) **Pub. Date: Oct. 20, 2011**

(54) **SYNTHESIS OF LIQUID FUELS AND CHEMICALS FROM OXYGENATED HYDROCARBONS**

(76) Inventors: **Randy D. Cortright**, Madison, WI (US); **Paul G. Blommel**, Oregon, WI (US)

(21) Appl. No.: **13/157,247**

(22) Filed: **Jun. 9, 2011**

Related U.S. Application Data

(63) Continuation of application No. 12/044,837, filed on Mar. 7, 2008.

(60) Provisional application No. 60/985,475, filed on Nov. 5, 2007, provisional application No. 60/985,500, filed on Nov. 5, 2007, provisional application No. 60/905,703, filed on Mar. 8, 2007.

Publication Classification

(51) **Int. Cl.**

C07C 9/00	(2006.01)
C07C 1/207	(2006.01)

(52) **U.S. Cl.** **585/16**; 585/240

(57) **ABSTRACT**

Processes and reactor systems are provided for the conversion of oxygenated hydrocarbons to hydrocarbons, ketones and alcohols useful as liquid fuels, such as gasoline, jet fuel or diesel fuel, and industrial chemicals. The process involves the conversion of mono-oxygenated hydrocarbons to aromatics and gasonline range hydrocarbons where the oxygenated hydrocarbons are derived from biomass.

preparation was dried overnight in a vacuum oven and subsequently calcined in a stream of flowing air at 400° C.

Example 51

[0270] The same procedure used for preparing the catalyst of Example 50 was followed with the exception that the target rhenium loading was 1.8%.

Example 52

[0271] An 80:1 SiO_2:Al_2O_3 ratio ZSM-5 zeolite (Zeolyst International, CBV 8014) was mixed with a 1:1 molar ratio of ZnO and Al_2O_3 powders so that the ZnO and Al_2O_3 (Dispal 18N4-80, Sasol North America, Houston, Tex.) combined comprised 30 weight % of the total solids. Dilute nitric acid was added at a level of 2 weight % HNO_3 to the combined ZnO and Al_2O_3. The dough consistency was adjusted with water addition to form a workable dough suitable for extrusion and the mixture was extruded using a laboratory scale extruder. The extrudates were dried overnight under vacuum at 100° C. and subsequently calcined at 600° C. under flowing air.

Example 53

[0272] An aqueous solution of gallium nitrate was added to the material of Example 52, with particle sizes restricted to those that were maintained on a 60 mesh screen after passing through an 18 mesh screen, using an incipient wetness technique to target a gallium loading of 1.2 weight %. The preparation was dried overnight in a vacuum oven and subsequently calcined in a stream of flowing hydrogen at 400° C.

Example 54

[0273] An aqueous solution of nickel nitrate was added to the material of Example 52, with particle sizes restricted to those that were maintained on a 60 mesh screen after passing through an 18 mesh screen, using an incipient wetness technique to target a nickel loading of 1.0 weight %. The preparation was dried overnight in a vacuum oven and subsequently calcined in a stream of flowing hydrogen at 400° C.

Example 55

[0274] The catalyst systems referenced in Examples 6, 46, 48, 49, 51, 53, and 54 were investigated for the conversion of glycerol, sorbitol, sucrose, and xylose to hydrocarbons using the reactor configuration described in Example 2. The studies were conducted using two 21.2 mm internal diameter stainless steel tube reactors shown in Example 4, with an analysis completed as described in Example 5. Tungstated zirconia (NorPro-Saint Gobain, product code SZ61143, with particle sizes restricted to those that were maintained on a 60 mesh screen after passing through an 18 mesh screen) was placed on top of the condensation catalyst installed in the second reactor to provide for a zone for vaporization of the first reactor effluent prior to entering the condensation catalyst.

[0275] Table 13 shows the results of these investigations. For Experiment NN (38% Sucrose+7% Xylose), a stream of hydrogen with a targeted flow rate equal to 3 times the moles of sucrose plus 1.5 times the moles of xylose was combined with the feed prior to entering the reactor. The other experiments were conducted without externally supplied hydrogen. Heaters external to the reactor, shown in FIG. **9** as **10***a*, **10***b*, **10***c*, **10***d*, **23***a*, **23***b*, **23***c*, and **23***d*, were used to maintain the reactor wall temperatures, as indicated in Table 13. The hydrocarbon products of these studies, disclosed in Table 13, were grouped into a C_{4-} fraction, which are predominately present in the gas phase at ambient temperature and pressure, and a C_{5+} fraction, which are generally suitable for incorporation into liquid fuels. The results show that a variety of sugars and polyhydric alcohols may be readily converted to C_{5+} hydrocarbons by the processes described here. The products contained mainly paraffin and aromatic constituents. The breakdown of paraffins and aromatics within this sample is shown in FIG. **17**.

TABLE 13

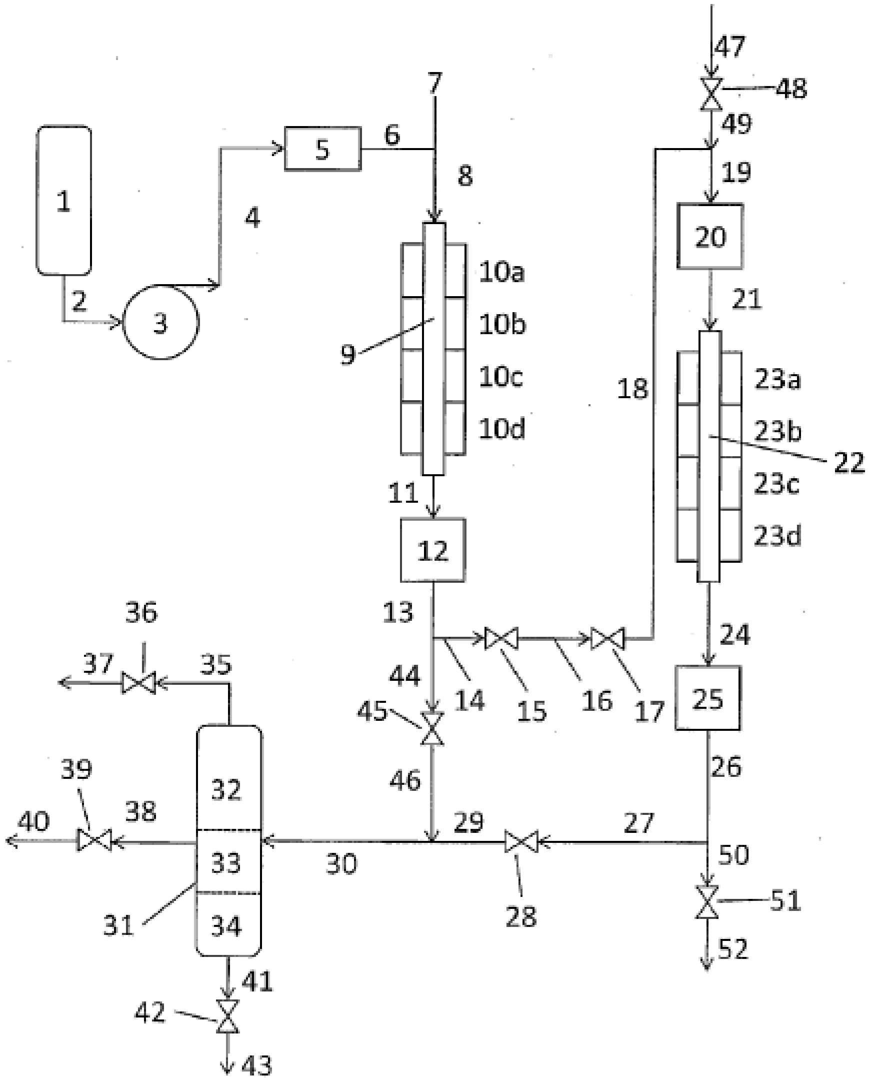
Conversion of Sugars and Polyhydric Alcohols to C5+ Hydrocarbons

Experiment		NN	OO	PP	QQ
Catalyst Descriptions					
Hydrogenation		Example 6	None	None	None
APR/Deoxygenation		Example 48	Example 51	Example 51	Example 50
Condensation		Example 49	Example 53	Example 46	Example 54
Catalyst Loadings					
Hydrogenation	grams	10	—	—	—
APR/Deoxygenation	grams	40	52	60	60
Tungstated Zirconia	grams	71	60	~60	58
Condensation	grams	62	60	60	60
Heater Block Temperature Ranges, Inlet of Catalyst Bed - Outlet of Catalyst Bed					
Hydrogenation	° C.	100-150	—	—	—
APR/Deoxygenation	° C.	245-265	250-270	335-365	275-285
Tungstated Zirconia	° C.	250-375	370-370	395-375	395-375
Condensation	° C.	375-375	385-385	375-375	375-375
Pressures					
First Reactor Outlet	psig	625	625	625	625
2nd Reactor Outlet	psig	625	350	250	350
Feed		38% Sucrose + 7% Xylose	50% Glycerol	50% Glycerol	50% Sorbitol

TABLE 13-continued

Conversion of Sugars and Polyhydric Alcohols to C5+ Hydrocarbons

Experiment		NN	OO	PP	QQ
Hydrogen production	mol/mol feed	−2.85	0.73	0.57	0.50
WHSV	$wt_{feed}/(wt_{catalyst}\,hr)$	1.6	1.9	2.0	2.0
	Reactor Outlet Yield Distribution				
C_{4-} Alkanes	wt % of feed carbon	21.2	26.9	8.1	13.0
C_{4-} Olefins	wt % of feed carbon	1.1	1.4	1.3	5.2
Total C_{4-} Hydrocarbons	wt % of feed carbon	22.3	28.3	9.4	18.1
C_{5+} Paraffins	wt % of feed carbon	20.0	7.9	9.5	11.3
C_{5+} Olefins	wt % of feed carbon	0.8	1.9	1.2	7.8
Naphthenes	wt % of feed carbon	1.9	1.4	1.6	1.2
Aromatics	wt % of feed carbon	25.0	17.8	48.4	22.3
Other C_{5+} Hydrocarbons	wt % of feed carbon	0.0	1.1	0.2	3.4
Total C_{5+} Hydrocarbons	wt % of feed carbon	47.7	30.1	61.0	46.1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10a
10b
10c
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FIG 9

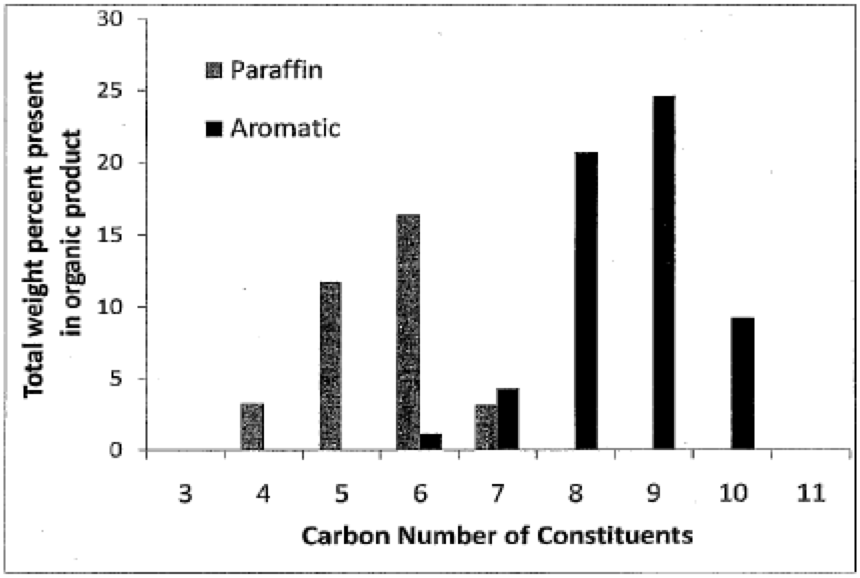
30
25
20
15
10
5
0
▨ Paraffin
■ Aromatic
Total weight percent present in organic product
3
4
5
6
7
8
9
10
11
Carbon Number of Constituents

FIG 17

US5730837

US005730837A

United States Patent [19]

Black et al.

[11] **Patent Number: 5,730,837**

[45] **Date of Patent: Mar. 24, 1998**

[54] **METHOD OF SEPARATING LIGNOCELLULOSIC MATERIAL INTO LIGNIN, CELLULOSE AND DISSOLVED SUGARS**

[75] Inventors: **Stuart K. Black**, Denver; **Bonnie R. Hames**, Westminster; **Michele D. Myers**, Dacono, all of Colo.

[73] Assignee: **Midwest Research Institute**, Kansas City, Mo.

[21] Appl. No.: **348,469**

[22] Filed: **Dec. 2, 1994**

[51] **Int. Cl.**^{6} **D21C 3/20**

[52] **U.S. Cl.** **162/16**; 162/72; 162/77; 127/37

[58] **Field of Search** 162/72, 76, 77, 162/29, 16; 127/37

[56] **References Cited**

U.S. PATENT DOCUMENTS

1,594,389	8/1926	Theillier .	
1,888,025	11/1932	Bent .	
2,024,689	12/1935	Groombridge .	
2,037,001	4/1936	Aronovsky .	
2,042,705	6/1936	Dreyfus .	
3,585,104	6/1971	Kleinert	162/77
3,932,207	1/1976	Fogarassy .	
3,951,734	4/1976	DeHaas	162/72
4,520,105	5/1985	Sinner .	
4,594,130	6/1986	Chang .	

FOREIGN PATENT DOCUMENTS

0211558	of 1987	European Pat. Off. .

Primary Examiner—Steven Alvo
Attorney, Agent, or Firm—Edna M. O'Connor; Ruth Eure

[57] **ABSTRACT**

A method for separating lignocellulosic material into (a) lignin, (b) cellulose, and (c) hemicellulose and dissolved sugars. Wood or herbaceous biomass is digested at elevated temperature in a single-phase mixture of alcohol, water and a water-immiscible organic solvent (e.g., a ketone). After digestion, the amount of water or organic solvent is adjusted so that there is phase separation. The lignin is present in the organic solvent, the cellulose is present in a solid pulp phase, and the aqueous phase includes hemicellulose and any dissolved sugars.

8 Claims, No Drawings

METHOD OF SEPARATING LIGNOCELLULOSIC MATERIAL INTO LIGNIN, CELLULOSE AND DISSOLVED SUGARS

CONTRACTUAL ORIGIN OF THE INVENTION

The United States Government has rights in this invention under Contract No. DE-AC36-83CH10093 between the United States Department of Energy and the National Renewable Energy Laboratory, a Division of the Midwest Research Institute.

BACKGROUND OF THE INVENTION

1. Field of the Invention

The present invention relates to methods and techniques for the fractionation of wood and herbaceous biomass. More particularly, this invention relates to methods and techniques for separating wood and biomass into three major components for further processing.

2. Description of the Prior Art

Pulping processes have previously been used for separating cellulose from lignin and other components of lignocellulosic materials. For example, various types of inorganic chemicals in water have been used to modify lignin to render it water soluble. Those processes, however, present problems in recovering or destroying the inorganic chemicals.

Other processes have been proposed using organic solvents for dissolving the lignin from the lignocellulosic material. Such processes can be expensive because of the cost of solvent recovery.

Still other processes have involved combinations of acids and alcohols with water. However, the presence of excess water can be detrimental to the process, and use of high concentrations of acid require costly recovery systems.

U.S. Pat. No. 2,037,001 (Aronovsky) describes an extraction process involving a two component aqueous alcoholic liquor. Lignin is separated from the aqueous stream by cooling the pulping liquid to ambient temperature following digestion and allowing the liquor to phase separate. The dissolved lignin is carried with the alcohol while any dissolved sugars remain in the aqueous liquor. The purity of lignin products isolated from processes using alcohols is not as high as is desired. An impure lignin isolated from alcohol requires extensive and expensive purification. Also, use of cooling temperatures for phase separation of the liquor could lead to re-deposition of lignin on the fibers.

U.S. Pat. No. 1,594,389 (Thellier) deals with the removal of extractives from flax and similar plants using a water/hydrocarbon mixture. This extraction would not remove any of the structural components of the flax nor would it result in the fractionation of the material due to the low concentration of the hydrocarbon which would remain soluble in the water.

U.S. Pat. No. 1,888,025 (Bent) describes a process in which wood or lignocellulosic material is extracted with aqueous organic solvents followed by the recovery of relatively hydrophobic extractives into an immiscible hydrophobic solvent. The patent deals with the removal of rosin from wood—essentially an extractive in pine wood—with an aqueous alcoholic solvent followed by a liquid/liquid extraction of the rosin from the solvent rather than the separation of biomass into structural polymer components.

U.S. Pat. No. 2,024,689 (Groombridge) refers to the use of mixtures of organic compounds with water for the separation of cellulose from the noncellulosic material in lignocellulosic feedstocks. However, there is no description of the use of a water-immiscible organic compound, water and a water-soluble organic compound to effect this separation.

U.S. Pat. No. 2,042,705 (Dreyfus) describes a process very similar to Groombridge, above, with the addition of water to the solvent mixture. There is no description of the separation of the pulping liquor into a lignin-rich component and a hemicellulose-rich component.

U.S. Pat. No. 3,932,207 (Fogarassy) describes a process in which, prior to cooking, fragments of raw lignocellulosic material are impregnated with a solution of a lignin-solubilizing reactant in an organic solvent with a boiling point higher than the cooking temperature. Then the impregnated material is immersed in a liquid which is immiscible with the solvent of the solution.

U.S. Pat. No. 4,520,105 (Sinner) describes a process involving a chemical pretreatment with a mixture of water and lower alcohols or acetone, after which the residue is separated and then treated with a similar solvent mixture at elevated temperature. However, alcohol or acetone mixtures with water cannot be separated into two phases. Also, separation of the lignin from dissolved sugars would require further processing through extensive washing.

U.S. Pat. No. 4,594,130 (Chang) describes a cooking process, in the absence of oxygen, at elevated temperatures with a neutral or acidic mixture of alcohol and water containing a magnesium, calcium or barium salt as a catalyst. The catalyst is for the purpose of aiding retention of the hemicellulose in the cellulosic cake.

European Patent Application 86305606.5 (Biodyne) describes a process for digesting lignocellulosic material with an ester, an organic lignin solvent and water. The lignin solvent is either an organic acid or alcohol or mixtures thereof, and it is miscible in both the ester and the water. Cooling of the liquor apparently results in some phase separation, but a centrifuge is also required.

There has not heretofore been described an efficient process involving the use of a single phase cooking liquor which can be readily separated into two liquid phases when desired.

SUMMARY OF THE INVENTION

It is an object of the invention to provide a process for separating wood and herbaceous biomass into its three major components for further processing.

It is an object of the invention to provide a convenient and efficient process for separating lignocellulosic material into lignin, cellulose, hemicellulose and sugars.

It is another object of the invention to provide a process for separating lignocellulosic material into its three major components using either a batch process or a continuous process.

It is yet another object of the invention to provide a very pure lignin stream in a process for fractionating lignocellulosic material.

It is still another object of this invention to provide a cellulose stream free of re-precipitated lignin in a process for fractionating lignocellulosic material.

Additional objects, advantages, and novel features of the invention shall be set forth in part in the description that follows and in part will become apparent to those skilled in the art upon examination of the following or may be learned by the practice of the invention. The objects and the advantages of the invention may be realized and attained by means of the instrumentalities and in combinations particularly pointed out in the appended claims.

To achieve the foregoing and other objects and in accordance with the purpose of the present invention, as embodied and broadly described herein, the improved methods may comprise separating lignocellulosic material into lignin, (b) cellulose, and (c) hemicellulose and sugars. In one embodiment the method comprises:

(a) digesting the lignocellulosic material in a single-phase mixture of alcohol, water and a water-immiscible organic solvent selected from the group consisting of ketones;

(b) adjusting the amount of water in said mixture to cause phase separation;

(c) separating said mixture into first, second and third phases; wherein said first phase comprises lignin and said organic solvent, said second phase comprises solid cellulosic cake, and said third phase is an aqueous alcoholic mixture and comprises hemicellulose and dissolved sugars.

The methods and techniques provided by this invention enable wood or herbaceous biomass to be fractionated very efficiently in a single phase, after which the pulping mixture can be separated into separate phases wherein the lignin is present in a homogeneous organic phase, the hemicellulose and sugars are present in the aqueous phase, and cellulose is present as a solid cellulosic cake. The organic phase can be separated, and the lignin can be isolated by evaporation of the organic solvent. The isolated lignin is substantially free of sugars.

The separate components of the wood and herbaceous biomass can be used for further desired processing. For example, the cellulose can be used for making paper and paperboard products or ethanol. It can also be used for making cellulose derivatives such as cellulose esters. The lignin can be used as a feedstock for phenolics, enhanced oil recovery surfactants, or fuel additives. The hemicellulose can be used making ethanol or other chemicals.

Other advantages of the methods of this invention will be apparent from the following detailed description.

DETAILED DESCRIPTION OF THE INVENTION

The improved methods of this invention involve placing the lignocellulosic material (e.g., wood or herbaceous biomass) in a suitable reactor, after which a mixture of solvents and water are added. It is necessary to obtain a single phase mixture.

A water-insoluble or water-immiscible organic solvent is used which is a ketone. A water-soluble or miscible alcohol and water are also used. Preferably the ketone is an aliphatic ketone having at least 4 carbon atoms (and may have as many as 10 carbon atoms). The alcohol preferably has less than about 4 carbon atoms to assure that it will be water-miscible.

Useful aliphatic ketones include, for example, methyl ethyl ketone, methyl isopropyl ketone, methyl propyl ketone, methyl butyl ketone, methyl isobutyl ketone, methyl isoamylketone, diethyl ketone, ethyl isopropyl ketone, ethyl propyl ketone, and ethyl isobutyl ketone. Useful alcohols include methanol, ethanol, propanol, isopropanol and butanol.

Typically the ketone is present in the solvent system in an amount of about 7 to 65% by weight, and water is present in an amount of about 10 to 65% by weight. The alcohol is typically present in an amount of about 25 to 35% by weight. The weight ratio of ketone to water is preferably in the range of about 1:9 to 6.5:1, so long as a single phase of digesting liquid is obtained.

Typically, the weight ratio of liquor to wood or biomass is at least about 4:1 and could be much greater if desired, e.g., 8:1 or 10:1.

The digestion is preferably carried out at an elevated temperature. Typically the digestion mixture is heated in the reactor to a temperature in the range of about 100° to 220° C. Some types of biomass can be digested more quickly than other types. If desired, a concept called severity may be used to determine the length of time required to obtain complete digestion of a particular biomass. The term severity involves use of an empirically derived equation relating time at temperature and the temperature above a base temperature at which reaction does not occur. The concept and the equation are explained in *Organosolv Pretreatment for Enzymatic Hydrolysis of Poplars. 2. Catalyst Effects and the Combined Severity Parameter,* H. L. Chum, D. K. Johnson, and S. K. Black, I & EC Research, 1990, 29, 156–162, incorporated herein by reference.

After the digestion has been completed, the single phase can be easily converted into two liquid phases upon the addition of either water or water-immiscible solvent. The two phases have very little cross-contamination of components from one phase into the other. The lignin stream is very pure and is easily isolated by evaporation of the organic solvent which is water-immiscible. The cellulosic stream obtained is free of re-precipitated lignin because the lignin and other dissolved materials remain in solution at all temperatures of the reaction. The lignin and hemicellulose are dissolved away from the wood chips leaving an insoluble cellulosic cake.

An acid catalyst is added to reduce the reaction temperature from about 200° C. for uncatalyzed cooks to 140° C. for a catalyzed cook. It also reduces the amount of time required. The catalysts used are mineral acids such as sulfuric or phosphoric acid. Nitric acid may also be used but it is not as effective. The amount of catalyst used varies with the feedstock but is generally in the range of 0.025M to 0.2M (0.2 to 2 wt % of the liquor used).

The processes of this invention are useful for fractionating all types of lignocellulosic material into separate components. For example, the processes may be used in connection with wood and herbaceous derived materials such as sugar cane bagasse, switch grass, and legumes.

EXAMPLE 1

Poplar wood chips (13.7 g oven-dried equivalent) were charged into a 200 ml batch reactor. A single phase pulping liquor composed of 24% water, 44% methyl isobutyl ketone (MIBK) and 32% ethanol with a 0.05 M H_2SO_4 catalyst was added in a ratio of 10 parts liquor to 1 part wood. The reactor was placed in a preheated heating block. The reactor was held at 140° C. for 56 minutes after a 34 minute heat-up time. Severity of the reaction was 4.3. The resulting pulp was fiberized in a Waring blender and washed with fresh neutral liquor. The oven-dried equivalent yield of pulp was 64%. Kappa number for this pulp was measured at 72.

Water was added to the liquor in a ratio of 1.3 parts water to 1 part liquor to cause phase separation of the insoluble MIBK component. Lignin was isolated from the MIBK phase by evaporation with a yield of 18%. Klason lignin analysis of this lignin gave a 88% purity.

Dissolved sugars composed mostly of hemicellulose were contained in the combined alcohol-aqueous fraction in a 18% yield based on the wood charged.

EXAMPLE 2

Under the same conditions as above, 14.4 g of oven-dried equivalent weight poplar was charged into a batch reactor. A

H_2SO_4 catalyst at a 0.1M concentration was added. The yield of pulp was 53% with a Kappa number of 46. The lignin yield was 23% with a purity of 92%. The yield of the hemicellulose fraction was 24%.

EXAMPLE 3

Aspen chips (193 g, oven-dried equivalent) were charged into a 1.7 liter percolation reactor. The reactor was filled with a MIBK/ethanol/water mixture containing 16% MIBK, 34% ethanol and 50% water containing 0.025M H_2SO_4. The reactor was heated to 140° C. over 34 minutes without flow of solvent. When the pulping temperature was reached, pulping solvent of the same composition was pumped through the chip bed at a flow rate of 28 ml/min. for 56 minutes. The chips were then washed in the reactor with neutral solvent at the same flow rate for 60 minutes without heating. Total severity for the reaction was 4.27. The reactor was drained, the chips fiberized and the lignin separated as described above. The pulp yield was 52% with a Kappa of 28. Lignin was isolated in a 17% yield. Hemicellulose yield was 31%.

EXAMPLE 4

Poplar chips from undebarked logs (189 g, oven-dried equivalent) were pulped under the same conditions as example 3 except for a 0.1 M H_2SO_4 catalyst concentration. Severity for this run was 4.27. The pulp yield was 45% with a Kappa of 42. Lignin was isolated in a 22% yield at a purity of 93%. Hemicellulose yield was 33%.

EXAMPLE 5

Depithed sugar cane bagasse (72 g, oven-dried equivalent) was pulped under the same conditions as example 4. The solvent mixture used was the same as that of example 1. Severity was 4.23. The yield of pulp was 49% with a Kappa of 8. The yield of lignin was 32%. Yield of hemicellulose was 19%.

The foregoing is considered as illustrative only of the principles of the invention. Further, since numerous modifications and changes will readily occur to those skilled in the art, it is not desired to limit the invention to the exact construction and operation shown and described. Accordingly, all suitable modifications and equivalents may be resorted to falling within the scope of the invention as defined by the claims which follow. The embodiments of the invention in which an exclusive property or privilege is claimed are defined as follows:

What is claimed is:

1. A method for separating lignocellulosic material into lignin, cellulose, and dissolved sugars composed mostly of hemicellulose and sugars, the method comprising: the steps of:

(a) digesting the solid lignocellulosic material in a single phase mixture of an alcohol, water and a water-immiscible ketone having at least 4 carbon atoms to solubilize lignin and hemicellulose and leave a cellulosic solid phase; said water being present in said single phase mixture in an amount of about 10 to 65 percent by weight, and said water-immiscible ketone being present in an amount of about 7 to about 65% by weight;

(b) adjusting the amount of water in said single liquid phase mixture to cause phase separation into two liquid phases of a lignin water-immiscible ketone stream and a stream of dissolved sugars composed mostly of hemicellulose; and

(c) separating said mixture into first, second and third phases; wherein said first phase is a liquid and comprises high purity lignin by evaporating water-immiscible ketone; said second phase comprises high purity cellulose in a solid phase; and said third phase is aqueous and comprises hemicellulose and dissolved sugars.

2. A method in accordance with claim **1**, wherein said digesting is carried out at a temperature in the range of about 135° C. to 220° C.

3. A method in accordance with claim **1**, wherein said ketone is selected from the group consisting of methyl isobutyl ketone, methyl isopropyl ketone methyl isoamyl ketone.

4. A method in accordance with claim **1**, wherein said alcohol has 1–4 carbon atoms.

5. A method in accordance with claim **1**, wherein said single phase mixture further comprises an acid catalyst.

6. A method in accordance with claim **5**, wherein said acid catalyst comprises a mineral acid which is present in an amount about 0.2 to 2% by weight.

7. A method in accordance with claim **6**, wherein said catalyst is selected from the group consisting of sulfuric acid and phosphoric acid.

8. A method for separating lignocellulosic material into lignin, cellulose, and dissolved sugars composed mostly of hemicellulose and sugars, the method comprising: the steps of:

(a) digesting lignocellulosic material in a single phase mixture of an alcohol, water and a water-immiscible ketone having at least 4 carbon atoms to solubilize lignin and hemicellulose and leave a cellulose solid phase; said water being present in said single phase mixture in an amount of about 10 to 65 percent by weight, and said water-immisible ketone being present in an amount of about 7 to about 65% by weight;

(b) adjusting the amount of said ketone in said single liquid phase mixture to cause phase separation into two liquid phases of a lignin water-immiscible ketone stream and a stream of dissolved sugars composed mostly of hemicellulose; and

(c) separating said mixture into first, second and third phases; wherein said first phase is liquid and comprises high purity lignin by evaporating water immiscible ketone said second phase comprises high purity cellulose in a solid phase; and said third phase is an aqueous alcohol mixture and comprises hemicellulose and dissolved sugars.

* * * * *

US6323381

US006323381B1

(12) **United States Patent**
Nacamuli et al.

(10) **Patent No.: US 6,323,381 B1**
(45) **Date of Patent: Nov. 27, 2001**

(54) **MANUFACTURE OF HIGH PURITY BENZENE AND PARA-RICH XYLENES BY COMBINING AROMATIZATION AND SELECTIVE DISPROPORTIONATION OF IMPURE TOLUENE**

(75) Inventors: **Gerald J. Nacamuli**, Mill Valley; **Robert A. Innes**, San Rafael; **Arnold J. Gloyn**, Walnut Creek, all of CA (US)

(73) Assignee: **Chevron Corporation**, San Ramon, CA (US)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 0 days.

(21) Appl. No.: **08/273,933**

(22) Filed: **Jul. 12, 1994**

Related U.S. Application Data

(63) Continuation-in-part of application No. 08/120,632, filed on Sep. 13, 1993, now abandoned, which is a continuation of application No. 07/952,312, filed on Sep. 28, 1992, now abandoned, which is a continuation of application No. 07/900,857, filed on Jun. 18, 1992, now abandoned.

(51) **Int. Cl.**^{7} **C07C 6/00**; C07C 15/04; C07C 15/08

(52) **U.S. Cl.** **585/475**; 585/312; 585/322

(58) **Field of Search** 585/475, 312, 585/322

(56) **References Cited**

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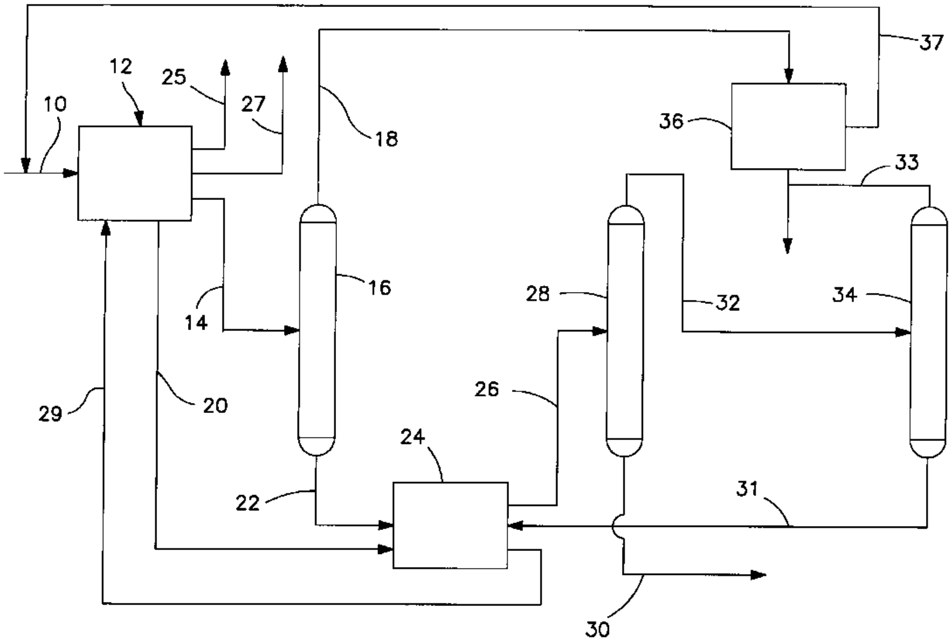
(57) **ABSTRACT**

A process is set forth for reacting impure toluene to obtain benzene, toluene and a para-rich xylene stream, which are substantially free of close-boiling non-aromatics. The impure toluene comprises at least 70 wt % toluene and between about 0.2 wt % and about 5 wt % close-boiling non-aromatics. The process may also comprise aromatizing a naphtha over a non-acidic catalyst. The impure toluene from the aromatization step is passed over an acidic intermediate pore zeolite to produce a para-rich xylene stream and chemically pure benzene.

19 Claims, 3 Drawing Sheets



The present invention will be more clearly understood by reference to the following examples.

EXAMPLE 1

Comparison Example with Non-selectivated Catalyst

Debutanized reformate prepared by reforming of a full boiling range naphtha feedstock over a catalyst comprising platinum on alumina and was distilled to obtain light and heavy fractions. The heavy reformate was further distilled to a 30% cut point. The overhead product of the second distillation, comprising about 92 wt % toluene and about 5 wt % nonaromatics, was vaporized, blended with hydrogen, and passed through a tubular fixed-bed reactor charged with acidic but not selectivated ZSM-5 catalyst. The reaction was carried out at 1000° F. (538° C.), 150 psig, and 5.7 liquid toluene feed weight hourly space velocity (WHSV). The added hydrogen:toluene molar ratio was about 3:1.

Feed and product analyses were obtained by capillary gas-liquid chromatography after nine hours on stream, as shown in Table 1. The gas chromatograph was equipped with a flame ionization detector and a polar column that eluted nonaromatics before aromatics.

TABLE 1

Components	Feed Area %	Product Area %	Difference
Nonaromatics:			
C1–C5	0.008	5.536	5.536
isohexanes	0.002	0	−0.002
n-hexane	0.001	0	−0.001
C6–C7 nonaromatics	0.092	0	−0.092
n-heptane	0.334	0	−0.334
C7–C8 nonaromatics	2.044	0.009	−2.035
n-octane	0.933	0	−0.933
C8–C9 nonaromatics	1.423	0.116	−1.307
C9 + nonaromatics	0.431	0.037	−0.394
Aromatics:			
Benzene	0.05	25.25	25.20
Toluene	91.69	42.03	−49.66
Ethylbenzene	1.38	1.07	−0.31
p-Xylene	0.53	4.94	4.41
m-Xylene	0.97	10.75	9.78
O-Xylene	0.11	5.05	4.94
C9 + aromatics	0	5.21	5.21
Total	99.998	99.998	0.008

$$\text{p-Xylene\%} = \frac{\text{p-Xylene} \times 100\%}{\text{p-Xylene} + \text{m-Xylene} + \text{o-Xylene}} = \frac{4.94 \times 100\%}{4.94 + 10.75 + 5.05} = 24\%$$

The analyses show that the toluene disproportionated to make benzene and xylenes, while nonaromatic impurities in the same boiling range were substantially eliminated by cracking to form light ends. Para-xylene comprised 24 wt % of the xylenes produced.

This example demonstrates the elimination of close boiling nonaromatics and the preparation of chemically pure benzene and xylene using a non-para-selective catalyst whereby only 24 wt % of the xylene fraction was para-xylene.

EXAMPLE 2

Aromatization Followed by Selectivated Para-Xylene Production

A C_6–C_7 naphtha was aromatized over a non-acidic platinum L-zeolite catalyst by being fed via line 10 (refer to FIG. **1**) to an aromatization unit 12. The aromatization was run to maximize yield of benzene whereby the resulting liquid product contained only a small amount of unreacted C_{7+} naphtha components. The C_{6+} product stream was collected. It was then taken, as represented by line 14 and was separated in a distillation column 16 into a benzene-rich fraction (removed as represented by line 18) and a C_{7+} bottoms fraction, both having close-boiling nonaromatics. Most of the unreacted paraffins, olefins and naphthenes were found in the benzene overhead fraction rather than the toluene and heavy aromatics C_{7+} fraction after distillation. As a result the feed (bottoms fraction) to the toluene disproportionation step which followed contained about 0.4 wt % close boiling non-aromatics. The benzene fraction was sent as represented by line 37 to aromatics extraction unit 36.

The conditions during the aromatization process were as follows:

Naphtha WHSV=1.0, feed molar ratio H_2/naphtha=5.0, temperature=890° F., pressure=70 psig.

The C_{7+} bottoms fraction, along with some of the hydrogen from the aromatization unit 12 introduced as represented by line 20, was fed via line 22 to a disproportionation zone 24 wherein it was contacted with a selectivated intermediate pore size zeolite catalyst whereby para-xylene was selectively produced and close boiling non-aromatics were converted to materials which boil generally outside of the benzene and xylene ranges. Excess hydrogen was removed from the aromatization unit 12 via line 25 and light hydrocarbons were removed via line 27. The toluene fraction was reacted over an acidic, large crystallite size (0.5–2.0) HZSM-5 (Silica to alumina ratio of 70:1) catalyst, which had previously been selectivated by passing toluene and nitrogen over the catalyst at 1100° F. and 150 psig for 27 hours. 12 mL/h of toluene feed and 75 CC—STP of hydrogen were passed over 2 grams of catalyst at 850° F. and 150 psig. Table 2 shows the analysis of the toluene fraction of the aromatization product and of the product of the selectivated conversion of toluene to benzene and para-xylene.

TABLE 2

Reaction of C_7 + Aromatization Product over Para-Selective Catalyst

Composition, Wt %	Feed	Product	Difference
Light Ends	0.00	0.71	0.71
C6 non-aromatics	0.00	0.00	0.00
Benzene	1.01	10.35	9.33
C7 non-aromatics	0.11	0.02	−0.09
Toluene	83.79	68.36	−15.42
C8 + non-aromatics	0.32	0.06	−0.26
Ethylbenzene	1.57	0.32	−1.25
p-Xylene	1.90	9.78	7.88
m-Xylene	1.86	3.02	1.16
o-Xylene	2.41	1.51	−0.90
Heavy aromatics	7.02	5.86	−1.16
Total	99.99	100.00	0.01

Catalyst: 'Selectivated Large Crystal HZSM-5'
Conditions:

TABLE 2-continued

Reaction of C_7 + Aromatization Product over Para-Selective Catalyst			
Composition, Wt %	Feed	Product	Difference

Catalyst Weight = 2.0 Grams
Liquid Feed Rate = 12 mL/h
H_2 Feed Rate = 75 cc/min
Temperature = 850° F.
Pressure = 150 psig

$$\text{p-Xylene } \% = \frac{\text{p-Xylene} \times 100\%}{\text{p-Xylene} + \text{m-Xylene} + \text{o-Xylene}}$$

$$= \frac{9.78 \times 100}{9.78 + 3.02 + 1.51} 68.3\%$$

Better than 80% of the close boiling non-aromatic material in the toluene fraction was converted to light or heavy ends in the toluene disproportionation reactor leaving only 0.02 wt % C_7 non-aromatics in the final product relative to 10.35 wt % benzene and 0.06 wt % C_{8+} non-aromatics relative to 14.31 wt % xylenes. Thus the benzene stream has a purity of 99.8 wt %. About 80% of the ethylbenzene and a proportion of the ortho-xylene and heavy aromatics in the original feed were converted yielding even more benzene and para-xylene. The para-xylene proportion of the xylene fraction was 68.3 wt %.

Hydrogen and light hydrocarbons from the disproportionation zone 24 are recycled via line 29 to the aromatization unit 12. The rest of the product from the disproportionation zone 24 is conducted via line 26 to distillation column 28 where it is distilled to provide a bottom fraction having C_{8+} aromatics and being enriched in para-xylene which is removed via line 30 and an overhead fraction containing C_6 and C_7 aromatics. The C_{8+} aromatics stream is sent to a para-xylene plant for the recovery of para-xylene and the isomerization of ortho- and meta-xylenes to para-xylene. operating costs in the para-xylene plant are significantly reduced because the toluene disproportionation unit produces a xylene stream which 1) is substantially free of nonaromatics, 2) is rich in the para-xylene isomer and 3) contains a reduced amount of ethylbenzene.

The C_6/C_7 aromatics fraction is conducted via line 32 to a further distillation column 34 where it is further distilled to provide toluene for sending via line 31 to the disproportionation zone 24 (or for recovery as a chemically pure product) and to provide high purity benzene as an overhead. This benzene is combined via line 33 with the high purity benzene obtained from the aromatics extraction unit 36. The benzene product is chemically pure and the xylene product is substantially free of non-aromatics. The xylene product is enriched in para-xylene. The para-xylene proportion of the xylene fraction is 60 to 80 wt %.

This example demonstrates the production of high purity benzene and a para-enriched xylenes stream from a C_6–C_7 naphtha. The process comprises aromatization of a C_6–C_7 naphtha followed by para-selective disproportionation of impure toluene.

EXAMPLE 3

Process Starting with C_7 Naphtha

A C_7 naphtha is fed via line 38 (see FIG. 2) to an aromatization reactor 40 along with hydrogen gas which may be fed via line 42. The aromatics and close-boiling non-aromatics contained in the product from the reactor are fed via line 44 to a disproportionation zone 46 containing an acidic intermediate pore size zeolite catalyst which has been selectivated for para-xylene production. Hydrogen is separated from the product of the disproportionation zone 46 in flash drum 48 and removed via line 47. All or a portion of the hydrogen can be recycled, for example, via compressor 49, to the aromatization reactor 40 via line 42. The remainder of the product is fed via line 50 to a stabilizer column 52 wherein light hydrocarbons are stripped off and removed via line 51. The bottoms fraction from the stabilizer column is fed via line 54 to a benzene recovery column 56 wherein an overhead fraction of chemically pure benzene is removed via line 58. The bottoms fraction from the benzene recovery column contains C_7 and C_{8+} aromatics and is substantially free of close-boiling nonaromatics. The bottoms fraction is fed via line 60 to a toluene recycle column 62 wherein toluene is removed as the overhead via line 64 and sent to the disproportionation zone 46 (or recovered as a chemically pure product). The bottom fraction from the toluene recycle column contains chemical grade C_{8+} aromatics enriched in para-xylene. The para-xylene proportion of the xylene fraction is 60 to 80 wt %.

This example demonstrates high para-xylene yield with the product being of chemical grade quality starting with a C_7 naphtha.

EXAMPLE 4

Process Starting with C_5–C_{11} Naphtha

FIG. **3** illustrates this example which is similar to the embodiment of FIG. **1**. A C_5–C_{11} full boiling range naphtha is fed to aromatization unit 12 via line 10. Hydrogen and light hydrocarbons are removed via lines 25 and 27. The remainder of the aromatization product is fed via line 14 to distillation column 16. The overhead from column 16 contains benzene and lighter components. It is fed to benzene extractor 36. The raffinate from extractor 36 is cycled to the aromatization unit 12 via line 37. A chemically pure benzene product is removed via line 57.

The bottoms fraction from column 16 is delivered via line 22 to a distillation column 60. C_{9+} is removed from column 60 via line 62 and can be used as a heavy gasoline blending stock. The C_6–C_8 overhead from column 60 is led via line 64 to a further distillation column 66.

Distillation column 66 separates the C_6–C_8 overhead from column 60 into a C_8 product which is removed via line 30 and into a C_6–C_7 overhead which is further separated in distillation column 34 into chemically pure benzene and into toluene which is sent to disproportionation unit 24 via line 31 (or is recovered as chemically pure toluene). The chemically pure benzene from unit 34 is combined with the chemically pure benzene from unit 34. The toluene stream is disproportionated to yield chemically pure benzene, toluene and para-rich-xylenes. The toluene disproportionation product then proceeds to the distillation train via line 26 and high purity benzene, toluene and C_8 aromatics are removed as described above.

The above examples demonstrate the wide applicability of the process of the present invention for the production of para-xylene enriched xylenes along with high purity benzene from full boiling range naphthas and from toluene-rich feedstocks which can be prepared from such naphthas.

INDUSTRIAL APPLICABILITY

The present invention provides the capability of synthesizing chemical grade benzene and para-xylene enriched

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(81) **Designated States** *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

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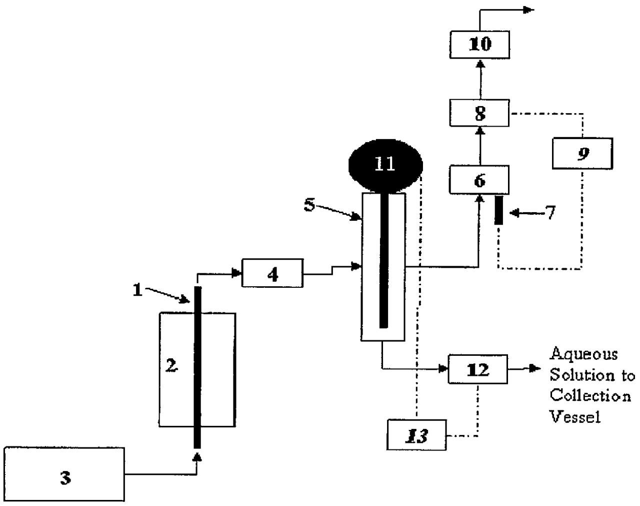
[Continued on next page]

(54) Title: CATALYSTS AND METHODS FOR REFORMING OXYGENATED COMPOUNDS



(57) Abstract: Disclosed are catalysts and methods that can reform aqueous solutions of oxygenated compounds such as ethylene glycol, glycerol, sugar alcohols, and sugars to generate products such as hydrogen and alkanes. In some embodiments, aqueous solutions containing at least 20 wt% of the oxygenated compounds can be reformed over a catalyst comprising a Group VIII transition metal and a Group VIIB transition metal, preferably supported on an activated carbon-supported catalyst. In other embodiments, catalysts are provided for the production of hydrogen or alkanes at reaction temperatures less than 300°C.

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Example 30

[0118] Functionalized carbon surfaces were modified by impregnation of metal oxides prior to impregnation of catalyst precursors. Titanium n-butoxide, 1.95g, was diluted to 12mL with anhydrous isopropanol. This solution was added by incipient wetting to air oxidation functionalized carbon (see Example 26 above), 10g. The wetted carbon was dried under vacuum at 100°C overnight.

Example 31 (RhReCe catalyst, 5% wt. Rh, 1:1:1 molar ratio Re:Rh:Ce)

[0119] Rhodium(III) Nitrate, 3.86g, Perrhenic Acid, 1.64g, and Cerium(III) Nitrate hexahydrate, 2.21g, were dissolved in enough DI water to make 12mL of solution. This solution was added by incipient wetting to Titania modified carbon from Example 30, and then dried under vacuum at 100°C overnight.

Example 32

[0120] The catalysts of Examples 25 through 31 were pretreated under flowing hydrogen at 250°C, before the liquid feed containing oxygenated compounds were introduced to the catalyst at the desired reaction temperature. Table 5 shows the results of reforming the different solutions over these catalysts. When compared to the results for the conversion of higher concentrations of glycerol presented in Example 24, Table 5 shows that the combination of rhenium and Group VIII metals supported on activated carbon significantly enhances the activity for the reforming of higher concentrations of oxygenated compounds.

Table 7. Effect of Addition of Base to Feed on Activity and Selectivity for APR Catalysts.

Feedstock	Catalyst	Ex.	Base	Wt % M	Molar Ratios (Re:Rh:Ce or Re:Pt)	WHSV $(hr^{-1})^a$	Conversion to Gas (%)	Gas Composition		
								H_2 (%)	Alkanes (%)	CO_2 (%)
30% Sorbitol	RhReCe	NA[b]	none	5% Rh	1:1:1	1.8	70%	47%	12%	40%
30% Sorbitol	RhReCe	b	0.5% NaOH	5% Rh	1:1:1	1.7	71%	53%	8%	39%
30% Sorbitol	RhReCe	b	1.25% NaOH	5% Rh	1:1:1	1.8	78%	57%	8%	37%
30% Sorbitol	RhReCe	b	1.5% NaOH	5% Rh	1:1:1	1.8	75%	56%	8%	34%
30% Sorbitol	RhReCe	b	1.65% NaOH	5% Rh	1:1:1	1.8	73%	56%	8%	34%
30% Sorbitol	PtRe	28	none	5% Pt	2.5:1	2.2	57%	36%	12%	47%
30% Sorbitol	PtRe	28	2.5% KOH	5% Pt	2.5:1	2.2	64%	55%	7%	36%
50% Sorbitol	RhReCe	31	none	5% Rh	1:1:1	1.8	81%	49%	19%	35%
50% Sorbitol	RhReCe	31	1.65% NaOH	5% Rh	1:1:1	1.8	75%	57%	12%	33%

[a] Weight hour space velocities (WHSV) are based on feed rate of oxygenated substrate.

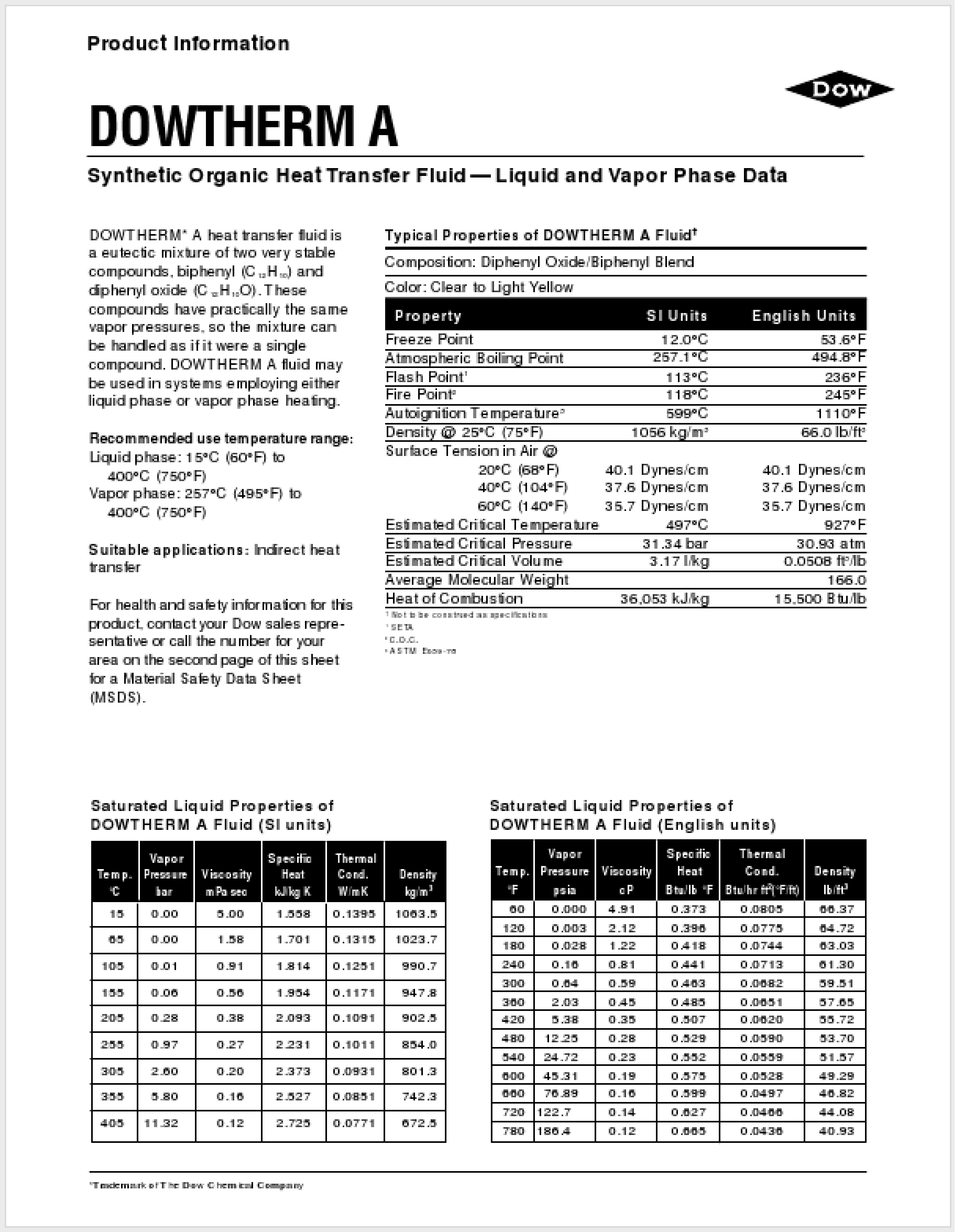
[b] preparation of this catalyst (on H_2O_2 vanadium modified carbon) was not described in any example, but the procedure was similar to example 34.

Example 37

[0125] A 3 wt% platinum catalyst supported on activated carbon was prepared according to the general method of Example 1. An aqueous solution, approximately 9.5mL, containing 0.75g of dihydrogen hexachloroplatinate (IV) hexahydrate (Alfa Aesar, 39.85% Pt) and 1.22g of perrhenic acid solution (Alfa Aesar, 79.18% $HReO_4$) was added to 10.0g peroxide functionalized carbon (Calgon UU, sieved to 60-120 mesh functionalized using the method of Example 20). The mixture was dried at 100°C under vacuum.

Appendix D: Materials

Dowtherm A Specifications



Product Information

DOWTHERM A

Synthetic Organic Heat Transfer Fluid — Liquid and Vapor Phase Data

DOWTHERM* A heat transfer fluid is a eutectic mixture of two very stable compounds, biphenyl ($C_{12}H_{10}$) and diphenyl oxide ($C_{12}H_{10}O$). These compounds have practically the same vapor pressures, so the mixture can be handled as if it were a single compound. DOWTHERM A fluid may be used in systems employing either liquid phase or vapor phase heating.

Recommended use temperature range:
Liquid phase: 15°C (60°F) to 400°C (750°F)
Vapor phase: 257°C (495°F) to 400°C (750°F)

Suitable applications: Indirect heat transfer

For health and safety information for this product, contact your Dow sales representative or call the number for your area on the second page of this sheet for a Material Safety Data Sheet (MSDS).

Typical Properties of DOWTHERM A Fluid[†]

Composition: Diphenyl Oxide/Biphenyl Blend

Color: Clear to Light Yellow

Property	SI Units	English Units
Freeze Point	12.0°C	53.6°F
Atmospheric Boiling Point	257.1°C	494.8°F
Flash Point[1]	113°C	236°F
Fire Point[2]	118°C	245°F
Autoignition Temperature[3]	599°C	1110°F
Density @ 25°C (75°F)	1056 kg/m³	66.0 lb/ft³
Surface Tension in Air @		
20°C (68°F)	40.1 Dynes/cm	40.1 Dynes/cm
40°C (104°F)	37.6 Dynes/cm	37.6 Dynes/cm
60°C (140°F)	35.7 Dynes/cm	35.7 Dynes/cm
Estimated Critical Temperature	497°C	927°F
Estimated Critical Pressure	31.34 bar	30.93 atm
Estimated Critical Volume	3.17 l/kg	0.0508 ft³/lb
Average Molecular Weight		166.0
Heat of Combustion	36,053 kJ/kg	15,500 Btu/lb

[†] Not to be construed as specifications
[1] SETA
[2] C.O.C.
[3] ASTM E659-78

Saturated Liquid Properties of DOWTHERM A Fluid (SI units)

Temp. °C	Vapor Pressure bar	Viscosity mPa sec	Specific Heat kJ/kg K	Thermal Cond. W/m K	Density kg/m³
15	0.00	5.00	1.558	0.1395	1063.5
65	0.00	1.58	1.701	0.1315	1023.7
105	0.01	0.91	1.814	0.1251	990.7
155	0.06	0.56	1.954	0.1171	947.8
205	0.28	0.38	2.093	0.1091	902.5
255	0.97	0.27	2.231	0.1011	854.0
305	2.60	0.20	2.373	0.0931	801.3
355	5.80	0.16	2.527	0.0851	742.3
405	11.32	0.12	2.725	0.0771	672.5

Saturated Liquid Properties of DOWTHERM A Fluid (English units)

Temp. °F	Vapor Pressure psia	Viscosity cP	Specific Heat Btu/lb °F	Thermal Cond. Btu/hr ft²(°F/ft)	Density lb/ft³
60	0.000	4.91	0.373	0.0805	66.37
120	0.003	2.12	0.396	0.0775	64.72
180	0.028	1.22	0.418	0.0744	63.03
240	0.16	0.81	0.441	0.0713	61.30
300	0.64	0.59	0.463	0.0682	59.51
360	2.03	0.45	0.485	0.0651	57.65
420	5.38	0.35	0.507	0.0620	55.72
480	12.25	0.28	0.529	0.0590	53.70
540	24.72	0.23	0.552	0.0559	51.57
600	45.31	0.19	0.575	0.0528	49.29
660	76.89	0.16	0.599	0.0497	46.82
720	122.7	0.14	0.627	0.0466	44.08
780	186.4	0.12	0.665	0.0436	40.93

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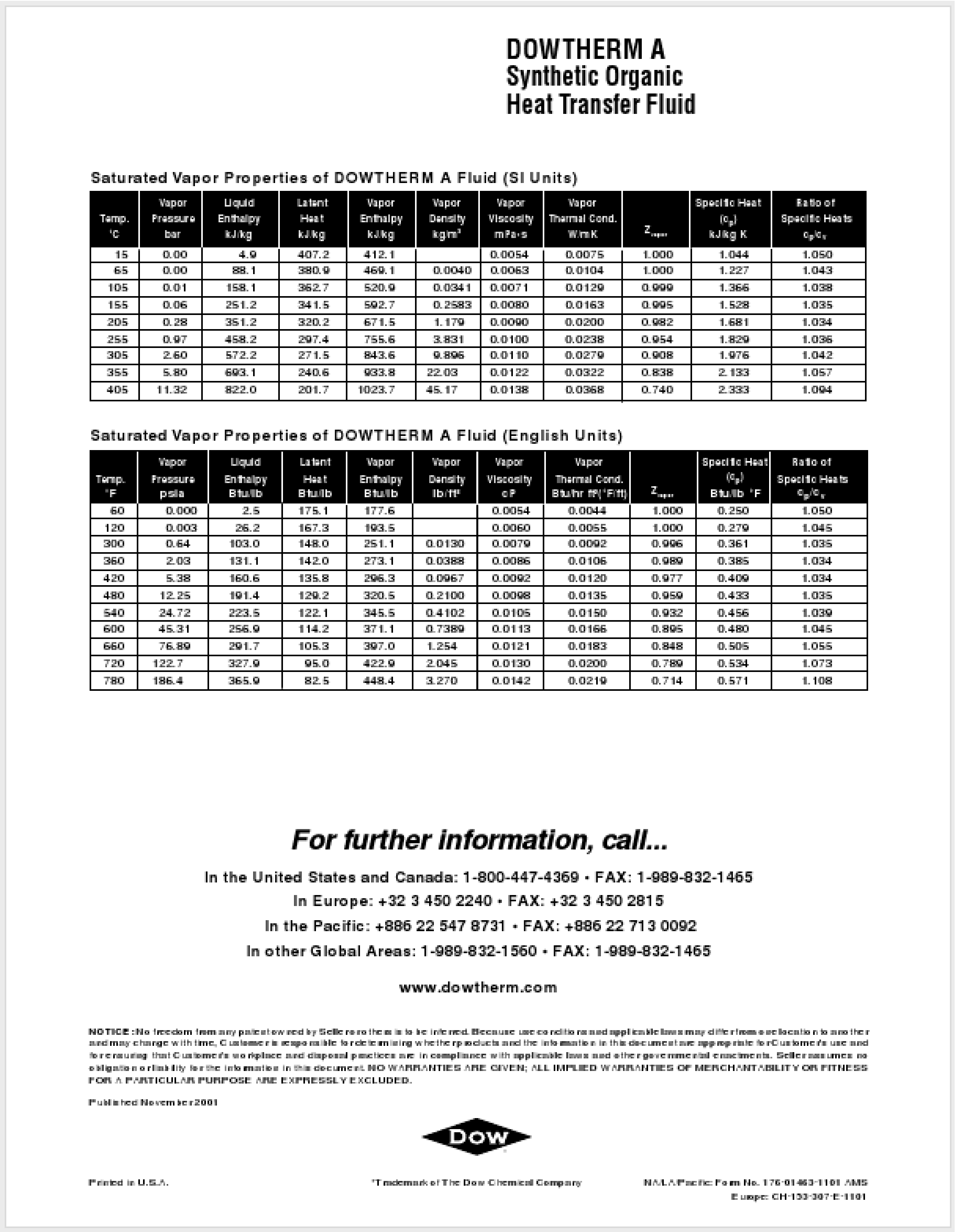

DOWTHERM A
Synthetic Organic Heat Transfer Fluid

Saturated Vapor Properties of DOWTHERM A Fluid (SI Units)

Temp. °C	Vapor Pressure bar	Liquid Enthalpy kJ/kg	Latent Heat kJ/kg	Vapor Enthalpy kJ/kg	Vapor Density kg/m³	Vapor Viscosity mPa·s	Vapor Thermal Cond. W/mK	Z_{vapor}	Specific Heat (c_p) kJ/kg K	Ratio of Specific Heats c_p/c_v
15	0.00	4.9	407.2	412.1		0.0054	0.0075	1.000	1.044	1.050
65	0.00	88.1	380.9	469.1	0.0040	0.0063	0.0104	1.000	1.227	1.043
105	0.01	158.1	362.7	520.9	0.0341	0.0071	0.0129	0.999	1.366	1.038
155	0.06	251.2	341.5	592.7	0.2583	0.0080	0.0163	0.995	1.528	1.035
205	0.28	351.2	320.2	671.5	1.179	0.0090	0.0200	0.982	1.681	1.034
255	0.97	458.2	297.4	755.6	3.831	0.0100	0.0238	0.954	1.829	1.036
305	2.60	572.2	271.5	843.6	9.896	0.0110	0.0279	0.908	1.976	1.042
355	5.80	693.1	240.6	933.8	22.03	0.0122	0.0322	0.838	2.133	1.057
405	11.32	822.0	201.7	1023.7	45.17	0.0138	0.0368	0.740	2.333	1.094

Saturated Vapor Properties of DOWTHERM A Fluid (English Units)

Temp. °F	Vapor Pressure psia	Liquid Enthalpy Btu/lb	Latent Heat Btu/lb	Vapor Enthalpy Btu/lb	Vapor Density lb/ft³	Vapor Viscosity cP	Vapor Thermal Cond. Btu/hr ft²(°F/ft)	Z_{vapor}	Specific Heat (c_p) Btu/lb °F	Ratio of Specific Heats c_p/c_v
60	0.000	2.5	175.1	177.6		0.0054	0.0044	1.000	0.250	1.050
120	0.003	26.2	167.3	193.5		0.0060	0.0055	1.000	0.279	1.045
300	0.64	103.0	148.0	251.1	0.0130	0.0079	0.0092	0.996	0.361	1.035
360	2.03	131.1	142.0	273.1	0.0388	0.0086	0.0106	0.989	0.385	1.034
420	5.38	160.6	135.8	296.3	0.0967	0.0092	0.0120	0.977	0.409	1.034
480	12.25	191.4	129.2	320.5	0.2100	0.0098	0.0135	0.959	0.433	1.035
540	24.72	223.5	122.1	345.5	0.4102	0.0105	0.0150	0.932	0.456	1.039
600	45.31	256.9	114.2	371.1	0.7389	0.0113	0.0166	0.895	0.480	1.045
660	76.89	291.7	105.3	397.0	1.254	0.0121	0.0183	0.848	0.505	1.055
720	122.7	327.9	95.0	422.9	2.045	0.0130	0.0200	0.789	0.534	1.073
780	186.4	365.9	82.5	448.4	3.270	0.0142	0.0219	0.714	0.571	1.108

For further information, call...

In the United States and Canada: 1-800-447-4369 • FAX: 1-989-832-1465
In Europe: +32 3 450 2240 • FAX: +32 3 450 2815
In the Pacific: +886 22 547 8731 • FAX: +886 22 713 0092
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www.dowtherm.com

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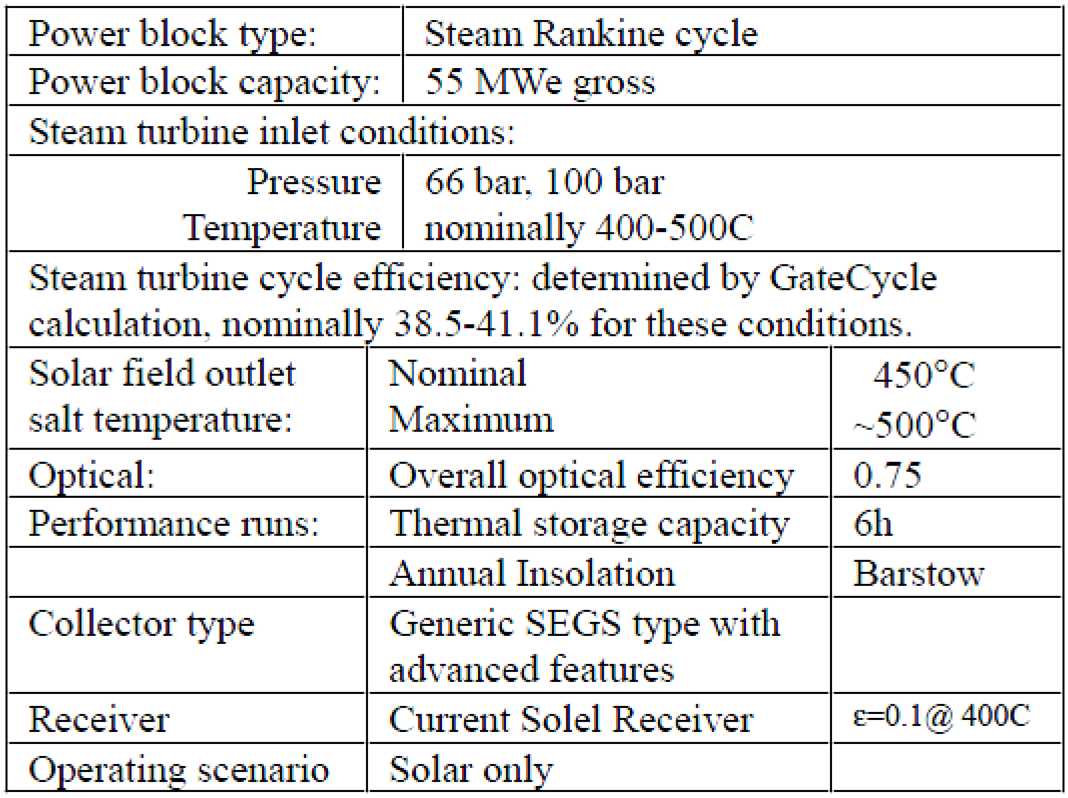
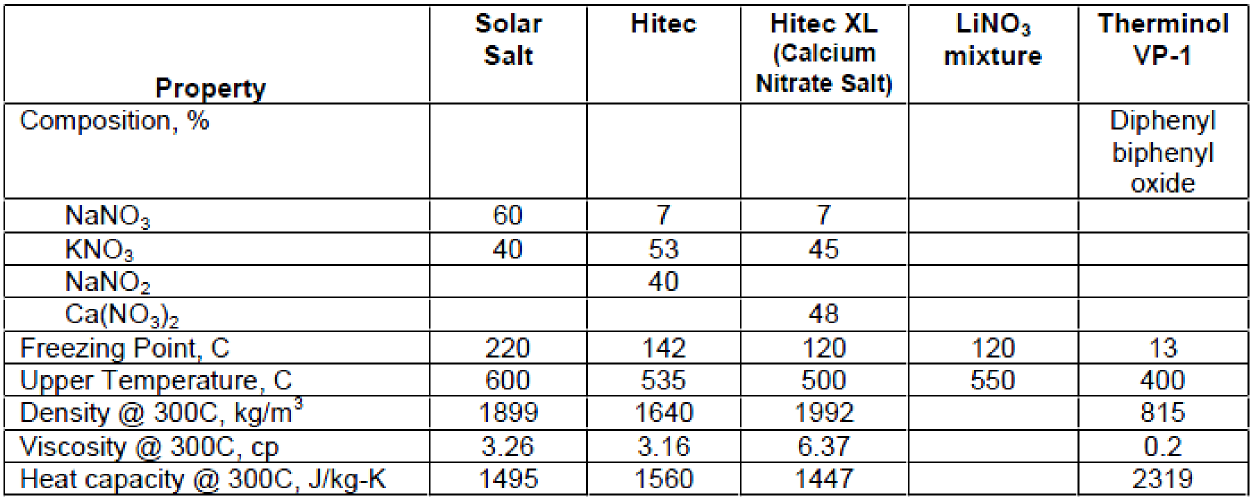
Molten Salts Specifications (Kearney, 2002)

Table 1 Parametric operating conditions for analyses



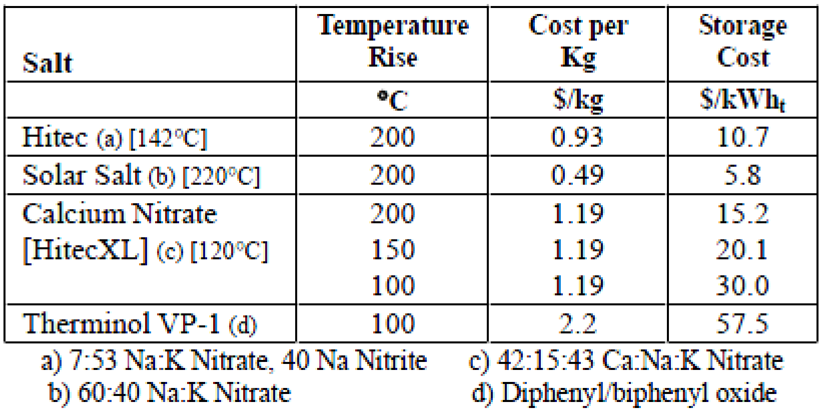
Power block type:	Steam Rankine cycle	
Power block capacity:	55 MWe gross	
Steam turbine inlet conditions:		
Pressure	66 bar, 100 bar	
Temperature	nominally 400-500C	
Steam turbine cycle efficiency: determined by GateCycle calculation, nominally 38.5-41.1% for these conditions.		
Solar field outlet salt temperature:	Nominal Maximum	450°C ~500°C
Optical:	Overall optical efficiency	0.75
Performance runs:	Thermal storage capacity	6h
	Annual Insolation	Barstow
Collector type	Generic SEGS type with advanced features	
Receiver	Current Solel Receiver	ε=0.1@ 400C
Operating scenario	Solar only	

Table 2 Characteristics of the Nitrate Salts and Therminol VP-1



Property	Solar Salt	Hitec	Hitec XL (Calcium Nitrate Salt)	$LiNO_3$ mixture	Therminol VP-1
Composition, %					Diphenyl biphenyl oxide
$NaNO_3$	60	7	7		
KNO_3	40	53	45		
$NaNO_2$		40			
$Ca(NO_3)_2$			48		
Freezing Point, C	220	142	120	120	13
Upper Temperature, C	600	535	500	550	400
Density @ 300C, kg/m^3	1899	1640	1992		815
Viscosity @ 300C, cp	3.26	3.16	6.37		0.2
Heat capacity @ 300C, J/kg-K	1495	1560	1447		2319

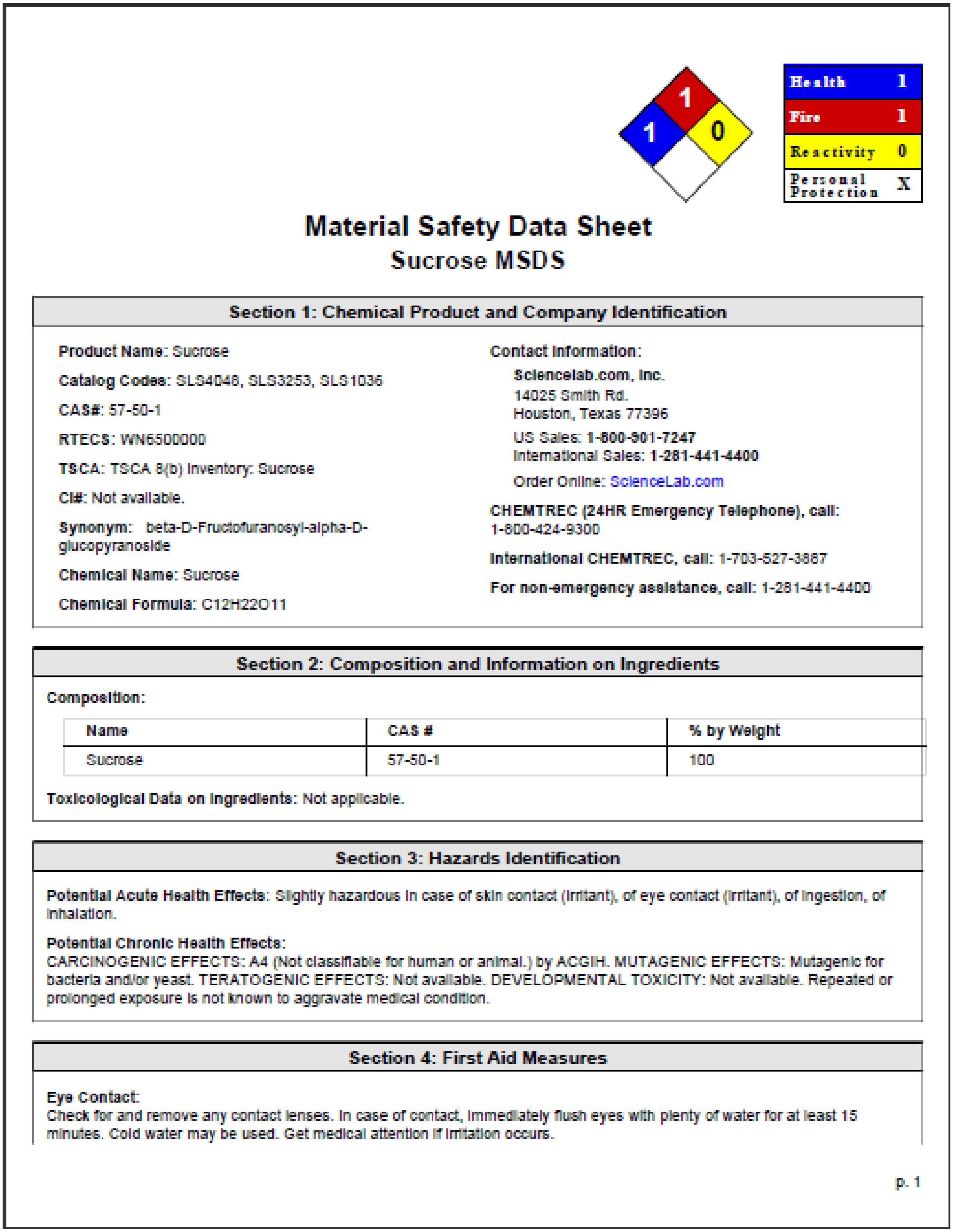
Table 3 Effective Storage Fluid Cost



Salt	Temperature Rise	Cost per Kg	Storage Cost
	°C	$/kg	$/kWh$_t$
Hitec (a) [142°C]	200	0.93	10.7
Solar Salt (b) [220°C]	200	0.49	5.8
Calcium Nitrate [HitecXL] (c) [120°C]	200 150 100	1.19 1.19 1.19	15.2 20.1 30.0
Therminol VP-1 (d)	100	2.2	57.5

a) 7:53 Na:K Nitrate, 40 Na Nitrite
b) 60:40 Na:K Nitrate
c) 42:15:43 Ca:Na:K Nitrate
d) Diphenyl/biphenyl oxide

Material Safety Data Sheets



Health	1
Fire	1
Reactivity	0
Personal Protection	X

Material Safety Data Sheet

Sucrose MSDS

Section 1: Chemical Product and Company Identification

Product Name: Sucrose

Catalog Codes: SLS4046, SLS3253, SLS1036

CAS#: 57-50-1

RTECS: WN6500000

TSCA: TSCA 8(b) inventory: Sucrose

CI#: Not available.

Synonym: beta-D-Fructofuranosyl-alpha-D-glucopyranoside

Chemical Name: Sucrose

Chemical Formula: $C_{12}H_{22}O_{11}$

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Sucrose	57-50-1	100

Toxicological Data on Ingredients: Not applicable.

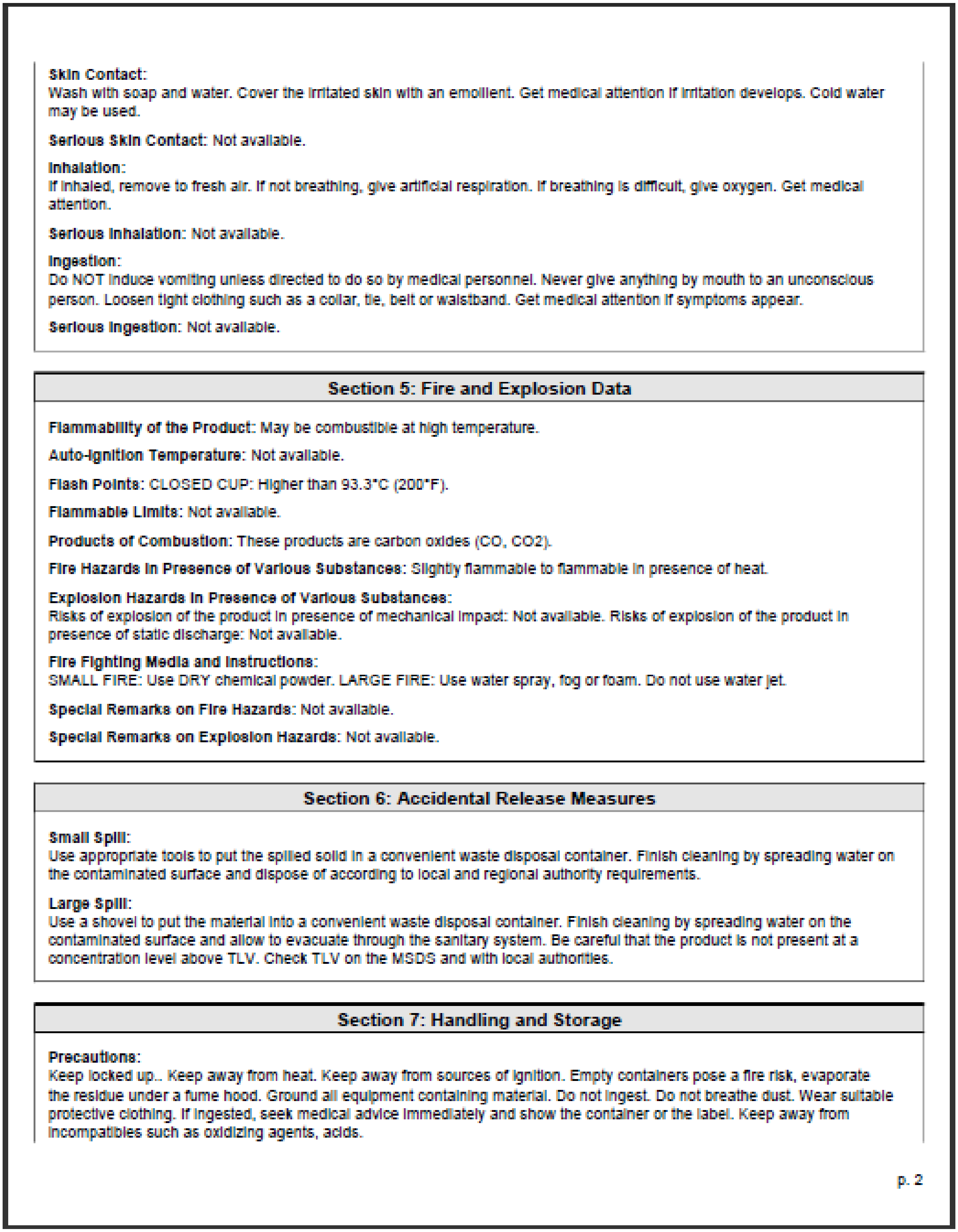
Section 3: Hazards Identification

Potential Acute Health Effects: Slightly hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, of inhalation.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH. MUTAGENIC EFFECTS: Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. Repeated or prolonged exposure is not known to aggravate medical condition.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention if irritation occurs.



Skin Contact:
Wash with soap and water. Cover the irritated skin with an emollient. Get medical attention if irritation develops. Cold water may be used.

Serious Skin Contact: Not available.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation: Not available.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention if symptoms appear.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: May be combustible at high temperature.

Auto-Ignition Temperature: Not available.

Flash Points: CLOSED CUP: Higher than 93.3°C (200°F).

Flammable Limits: Not available.

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Slightly flammable to flammable in presence of heat.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

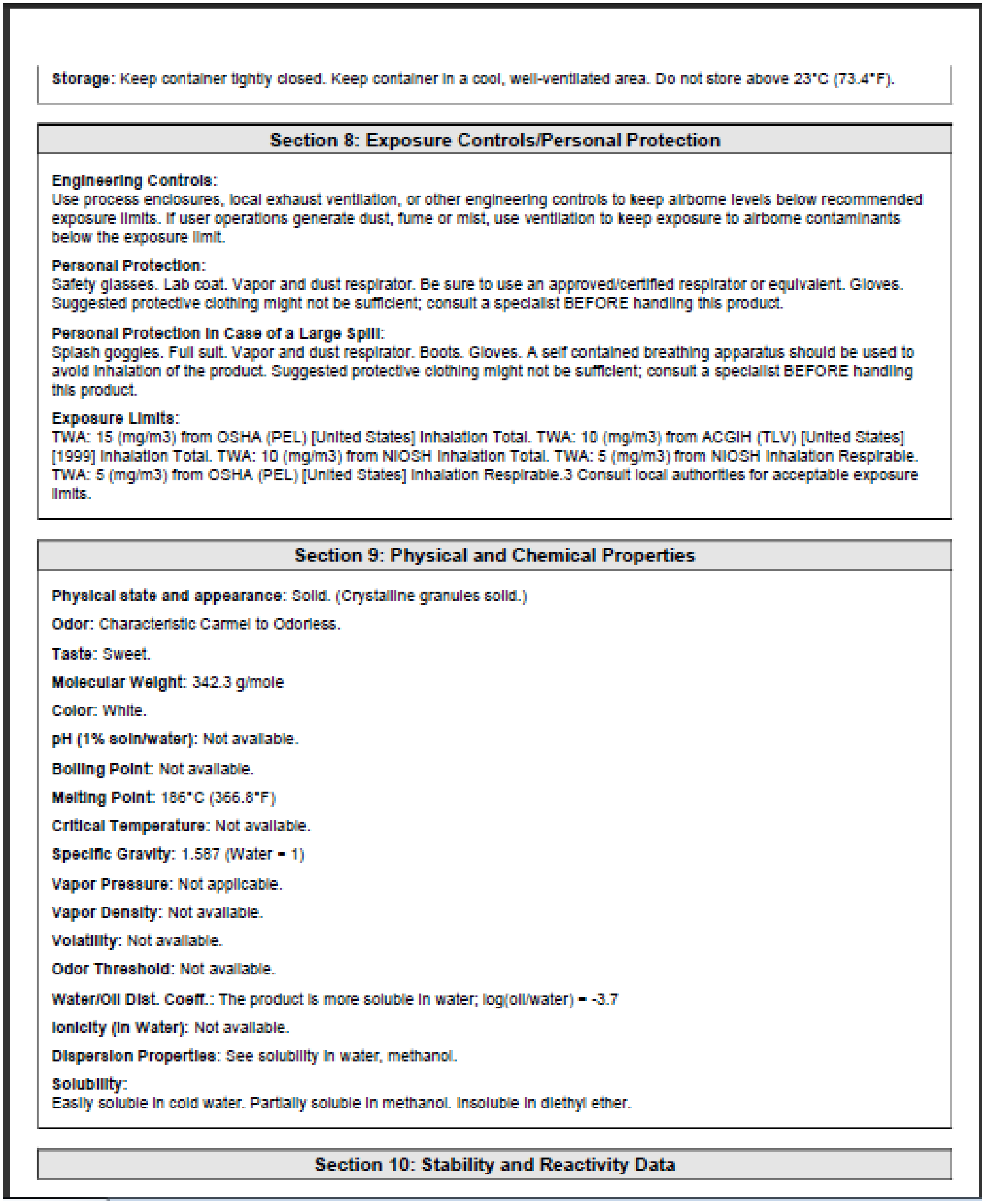
Section 6: Accidental Release Measures

Small Spill:
Use appropriate tools to put the spilled solid in a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and dispose of according to local and regional authority requirements.

Large Spill:
Use a shovel to put the material into a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and allow to evacuate through the sanitary system. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up.. Keep away from heat. Keep away from sources of ignition. Empty containers pose a fire risk, evaporate the residue under a fume hood. Ground all equipment containing material. Do not ingest. Do not breathe the dust. Wear suitable protective clothing. If ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibles such as oxidizing agents, acids.



Storage: Keep container tightly closed. Keep container in a cool, well-ventilated area. Do not store above 23°C (73.4°F).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Safety glasses. Lab coat. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor and dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 15 (mg/m3) from OSHA (PEL) [United States] Inhalation Total. TWA: 10 (mg/m3) from ACGIH (TLV) [United States] [1999] Inhalation Total. TWA: 10 (mg/m3) from NIOSH Inhalation Total. TWA: 5 (mg/m3) from NIOSH Inhalation Respirable. TWA: 5 (mg/m3) from OSHA (PEL) [United States] Inhalation Respirable.3 Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid. (Crystalline granules solid.)

Odor: Characteristic Carmel to Odorless.

Taste: Sweet.

Molecular Weight: 342.3 g/mole

Color: White.

pH (1% soln/water): Not available.

Boiling Point: Not available.

Melting Point: 186°C (366.8°F)

Critical Temperature: Not available.

Specific Gravity: 1.587 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

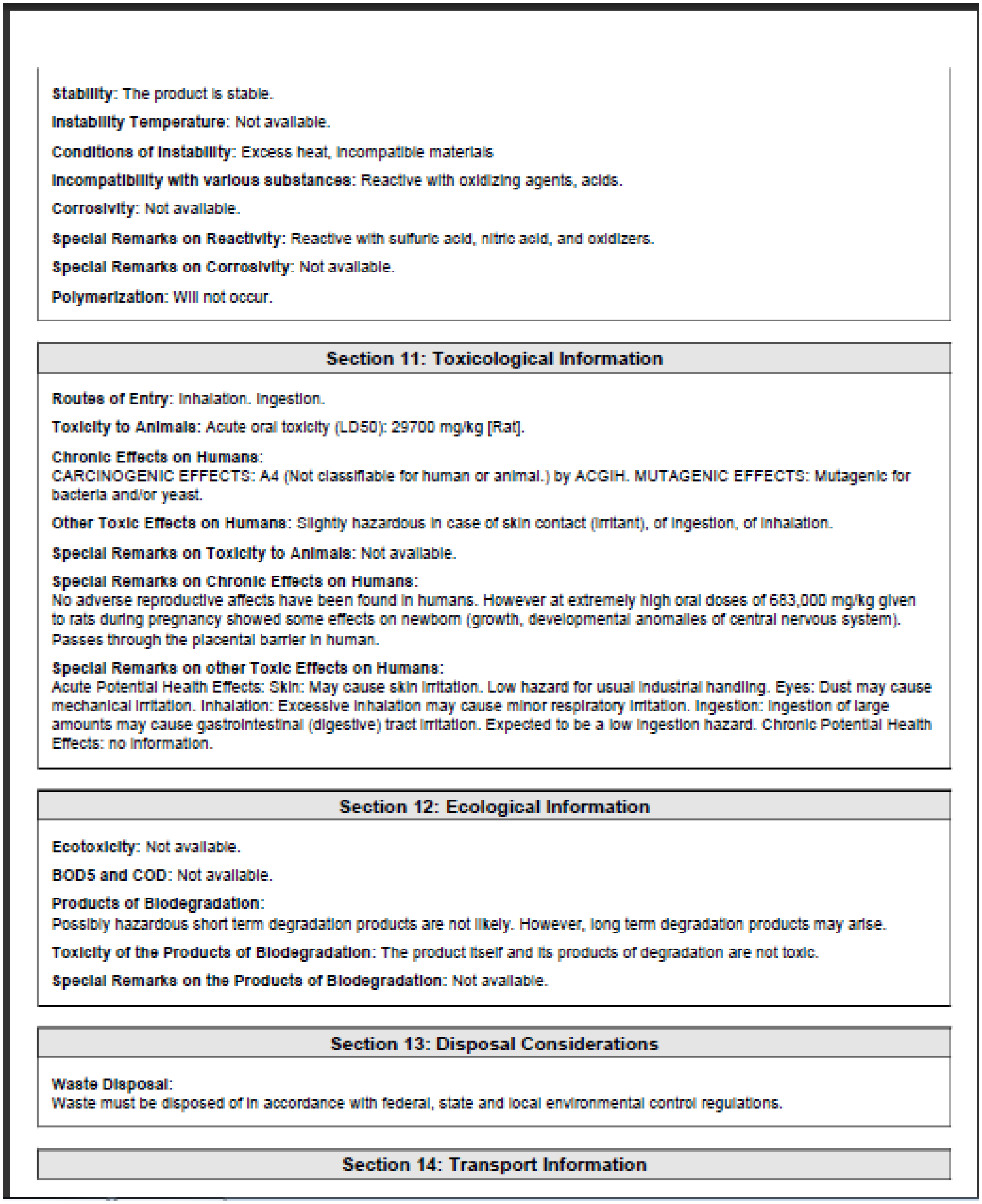
Water/Oil Dist. Coeff.: The product is more soluble in water; log(oil/water) = -3.7

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, methanol.

Solubility:
Easily soluble in cold water. Partially soluble in methanol. Insoluble in diethyl ether.

Section 10: Stability and Reactivity Data



Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Excess heat, incompatible materials

Incompatibility with various substances: Reactive with oxidizing agents, acids.

Corrosivity: Not available.

Special Remarks on Reactivity: Reactive with sulfuric acid, nitric acid, and oxidizers.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Inhalation. Ingestion.

Toxicity to Animals: Acute oral toxicity (LD50): 29700 mg/kg [Rat].

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH. MUTAGENIC EFFECTS: Mutagenic for bacteria and/or yeast.

Other Toxic Effects on Humans: Slightly hazardous in case of skin contact (irritant), of ingestion, of inhalation.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
No adverse reproductive affects have been found in humans. However at extremely high oral doses of 683,000 mg/kg given to rats during pregnancy showed some effects on newborn (growth, developmental anomalies of central nervous system). Passes through the placental barrier in human.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: May cause skin irritation. Low hazard for usual industrial handling. Eyes: Dust may cause mechanical irritation. Inhalation: Excessive inhalation may cause minor respiratory irritation. Ingestion: Ingestion of large amounts may cause gastrointestinal (digestive) tract irritation. Expected to be a low ingestion hazard. Chronic Potential Health Effects: no information.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

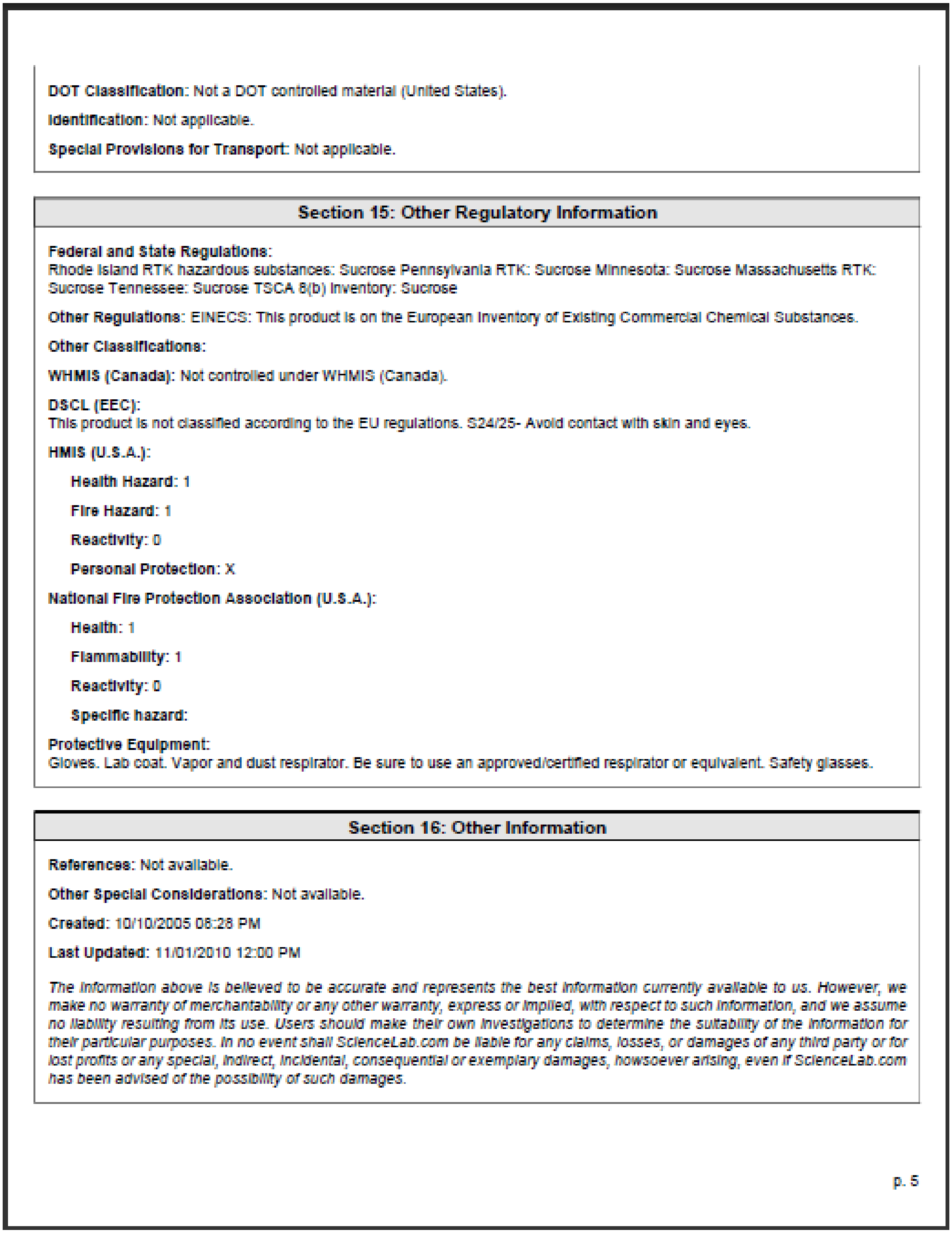
Toxicity of the Products of Biodegradation: The product itself and its products of degradation are not toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information



DOT Classification: Not a DOT controlled material (United States).

Identification: Not applicable.

Special Provisions for Transport: Not applicable.

Section 15: Other Regulatory Information

Federal and State Regulations:
Rhode Island RTK hazardous substances: Sucrose Pennsylvania RTK: Sucrose Minnesota: Sucrose Massachusetts RTK: Sucrose Tennessee: Sucrose TSCA 8(b) inventory: Sucrose

Other Regulations: EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada): Not controlled under WHMIS (Canada).

DSCL (EEC):
This product is not classified according to the EU regulations. S24/25- Avoid contact with skin and eyes.

HMIS (U.S.A.):

Health Hazard: 1

Fire Hazard: 1

Reactivity: 0

Personal Protection: X

National Fire Protection Association (U.S.A.):

Health: 1

Flammability: 1

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Safety glasses.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/10/2005 08:28 PM

Last Updated: 11/01/2010 12:00 PM

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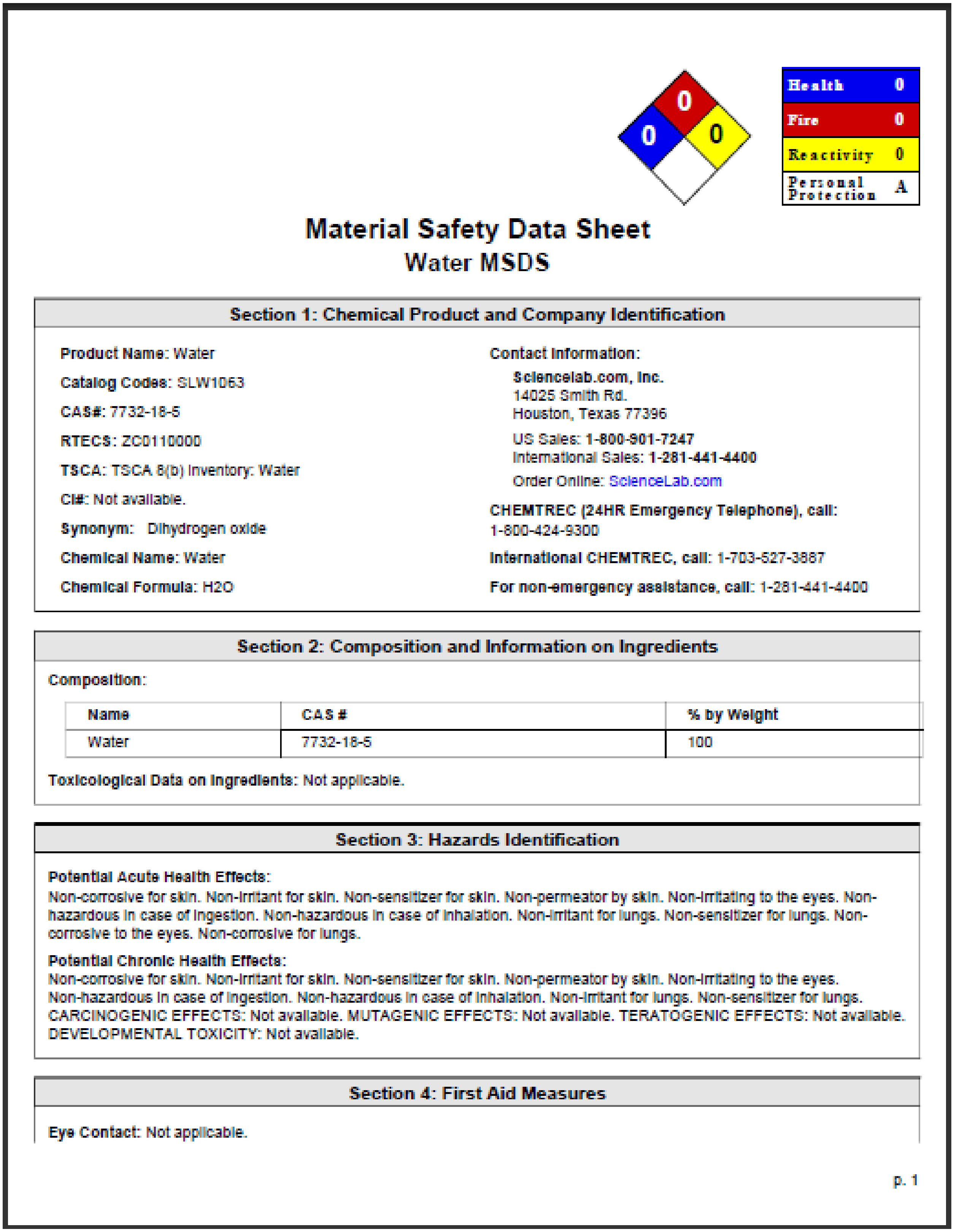
p. 5



Health	0
Fire	0
Reactivity	0
Personal Protection	A

Material Safety Data Sheet
Water MSDS

Section 1: Chemical Product and Company Identification

Product Name: Water

Catalog Codes: SLW1063

CAS#: 7732-18-5

RTECS: ZC0110000

TSCA: TSCA 8(b) inventory: Water

CI#: Not available.

Synonym: Dihydrogen oxide

Chemical Name: Water

Chemical Formula: H_2O

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Water	7732-18-5	100

Toxicological Data on Ingredients: Not applicable.

Section 3: Hazards Identification

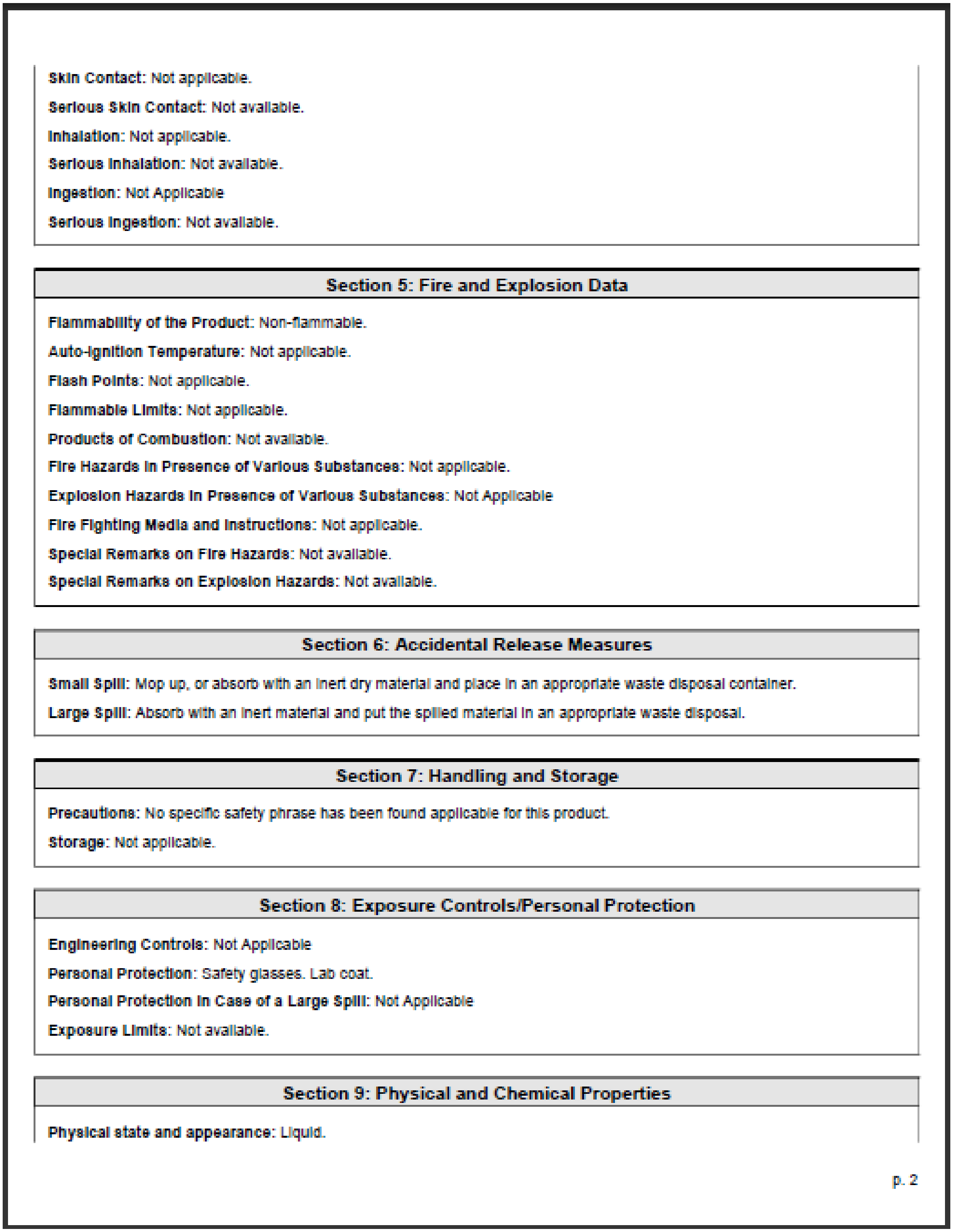
Potential Acute Health Effects:
Non-corrosive for skin. Non-irritant for skin. Non-sensitizer for skin. Non-permeator by skin. Non-irritating to the eyes. Non-hazardous in case of ingestion. Non-hazardous in case of inhalation. Non-irritant for lungs. Non-sensitizer for lungs. Non-corrosive to the eyes. Non-corrosive for lungs.

Potential Chronic Health Effects:
Non-corrosive for skin. Non-irritant for skin. Non-sensitizer for skin. Non-permeator by skin. Non-irritating to the eyes. Non-hazardous in case of ingestion. Non-hazardous in case of inhalation. Non-irritant for lungs. Non-sensitizer for lungs. CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available.

Section 4: First Aid Measures

Eye Contact: Not applicable.

p. 1



Skin Contact: Not applicable.

Serious Skin Contact: Not available.

Inhalation: Not applicable.

Serious Inhalation: Not available.

Ingestion: Not Applicable

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

Fire Hazards in Presence of Various Substances: Not applicable.

Explosion Hazards in Presence of Various Substances: Not Applicable

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Mop up, or absorb with an inert dry material and place in an appropriate waste disposal container.

Large Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Section 7: Handling and Storage

Precautions: No specific safety phrase has been found applicable for this product.

Storage: Not applicable.

Section 8: Exposure Controls/Personal Protection

Engineering Controls: Not Applicable

Personal Protection: Safety glasses. Lab coat.

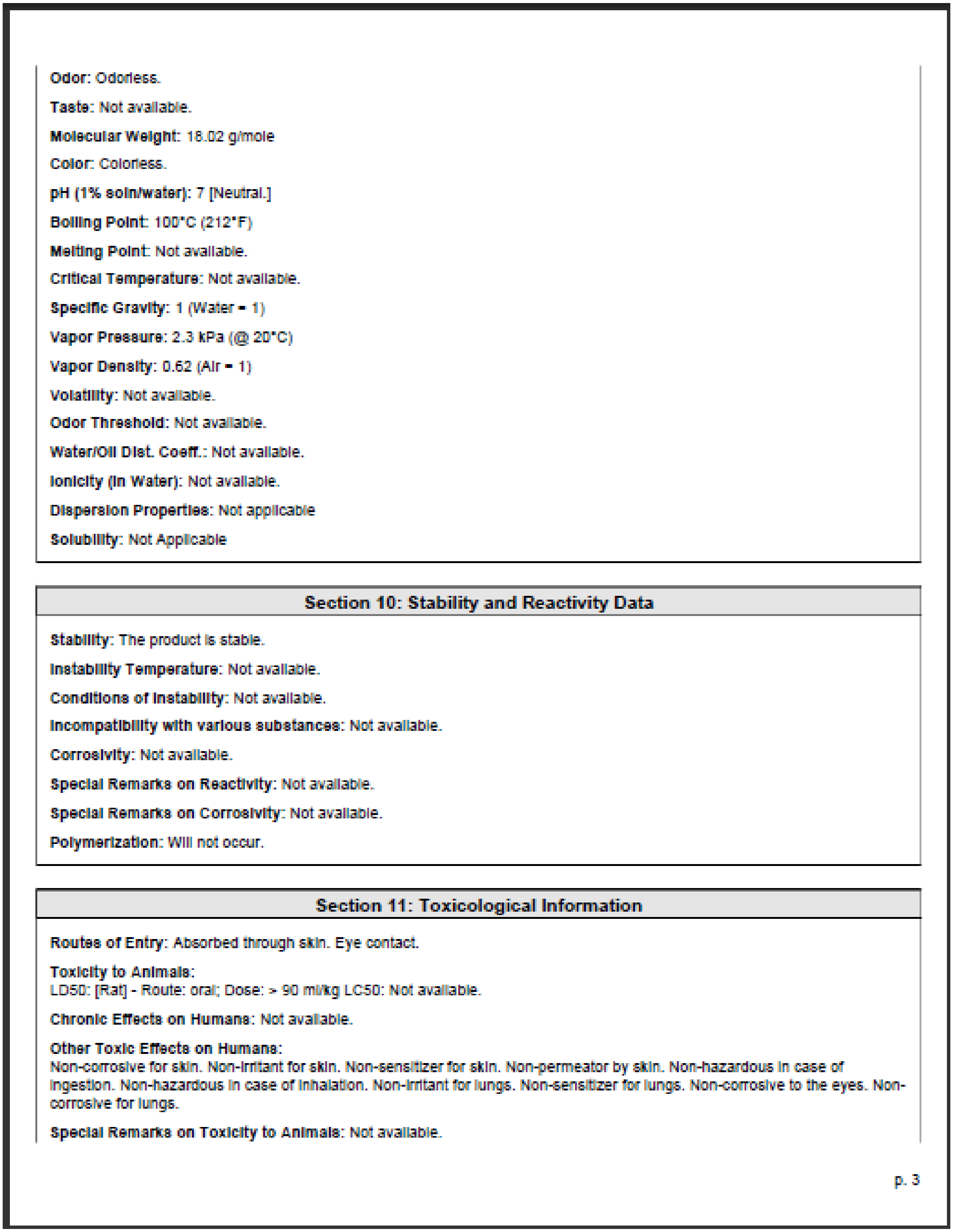
Personal Protection in Case of a Large Spill: Not Applicable

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

p. 2



Odor: Odorless.

Taste: Not available.

Molecular Weight: 18.02 g/mole

Color: Colorless.

pH (1% soln/water): 7 [Neutral.]

Boiling Point: 100°C (212°F)

Melting Point: Not available.

Critical Temperature: Not available.

Specific Gravity: 1 (Water = 1)

Vapor Pressure: 2.3 kPa (@ 20°C)

Vapor Density: 0.62 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: Not applicable

Solubility: Not Applicable

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Not available.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Eye contact.

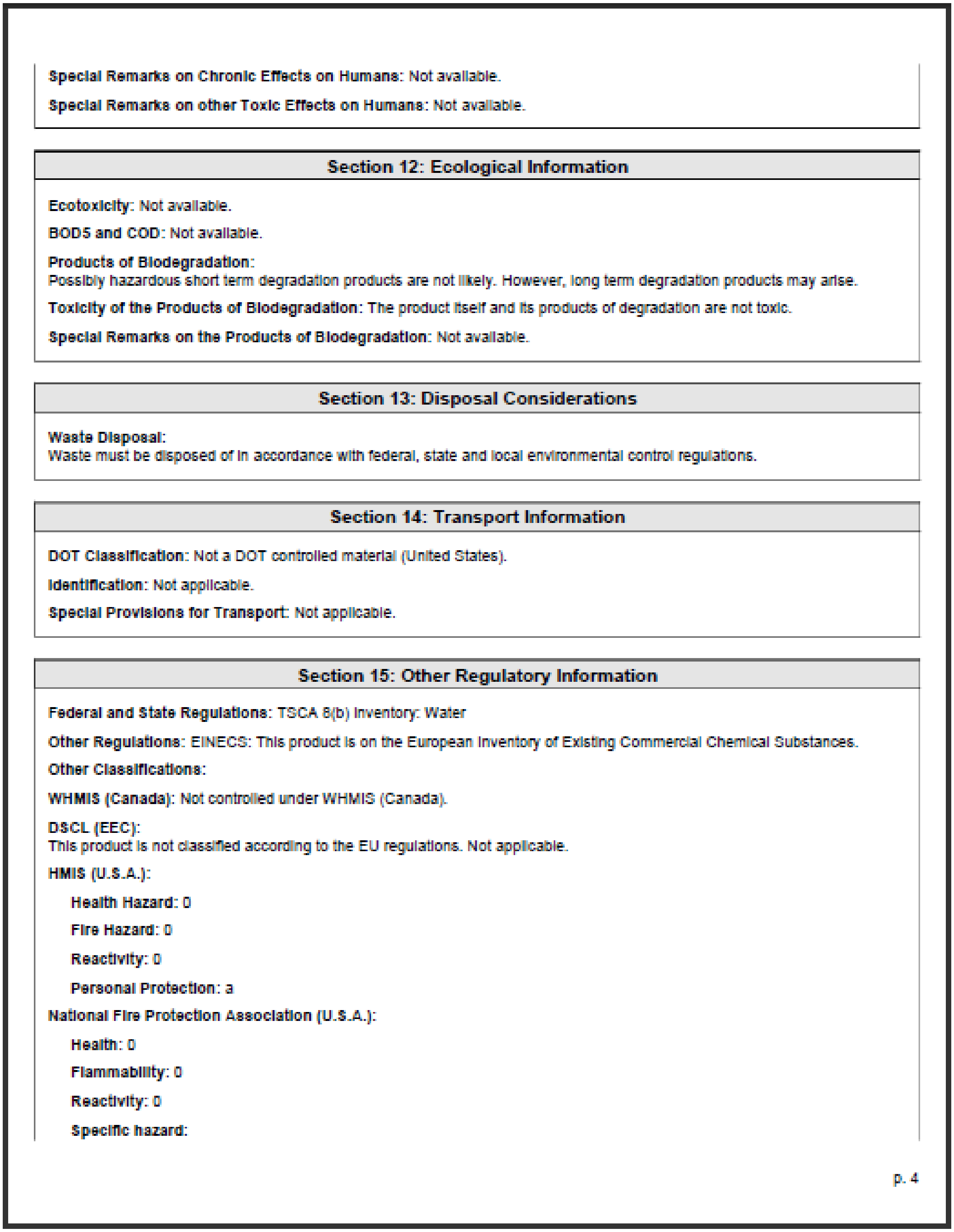
Toxicity to Animals:
LD50: [Rat] - Route: oral; Dose: > 90 ml/kg LC50: Not available.

Chronic Effects on Humans: Not available.

Other Toxic Effects on Humans:
Non-corrosive for skin. Non-irritant for skin. Non-sensitizer for skin. Non-permeator by skin. Non-hazardous in case of ingestion. Non-hazardous in case of inhalation. Non-irritant for lungs. Non-sensitizer for lungs. Non-corrosive to the eyes. Non-corrosive for lungs.

Special Remarks on Toxicity to Animals: Not available.

p. 3



Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The product itself and its products of degradation are not toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: Not a DOT controlled material (United States).

Identification: Not applicable.

Special Provisions for Transport: Not applicable.

Section 15: Other Regulatory Information

Federal and State Regulations: TSCA 8(b) inventory: Water

Other Regulations: EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada): Not controlled under WHMIS (Canada).

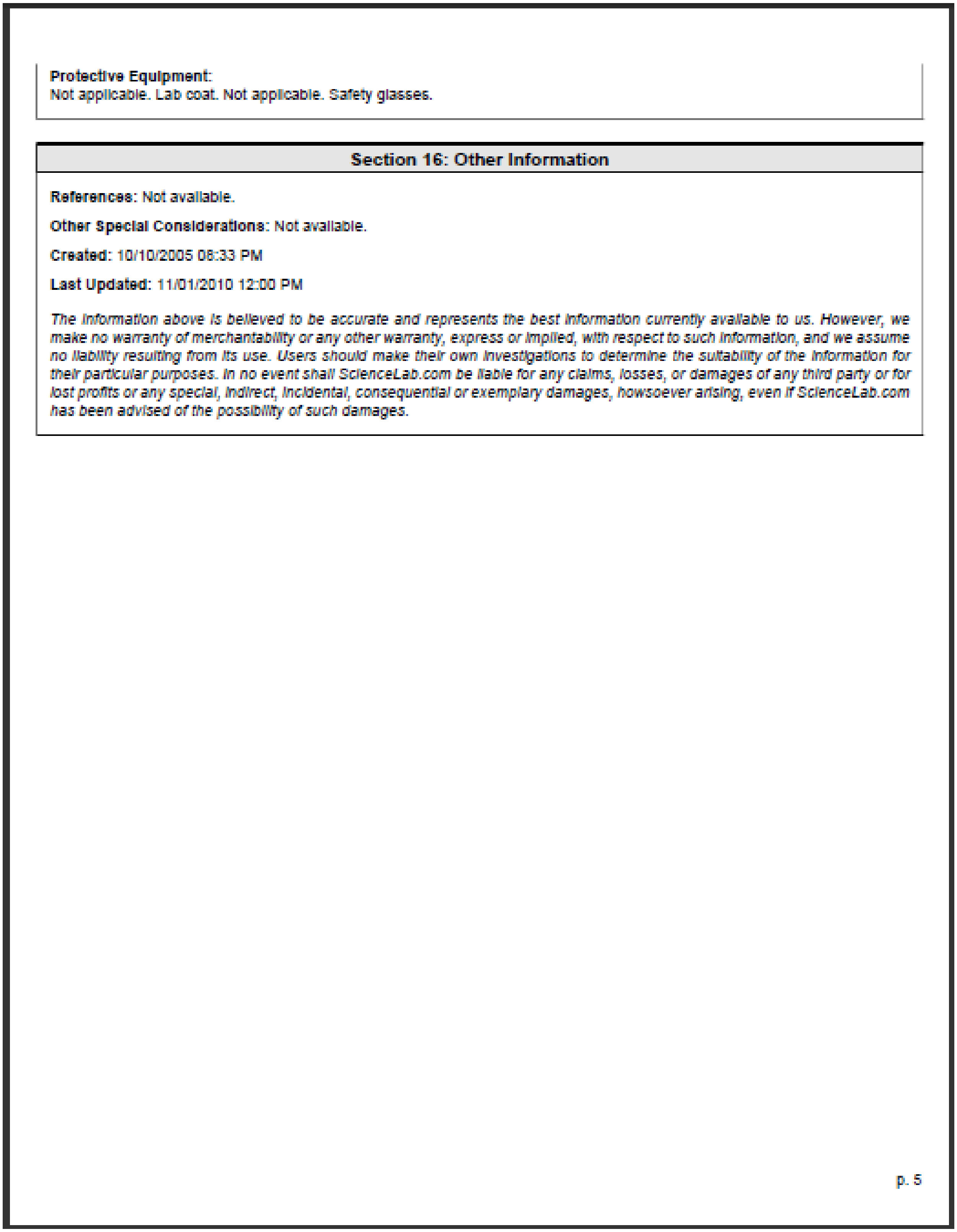
DSCL (EEC):
This product is not classified according to the EU regulations. Not applicable.

HMIS (U.S.A.):

- **Health Hazard:** 0
- **Fire Hazard:** 0
- **Reactivity:** 0
- **Personal Protection:** a

National Fire Protection Association (U.S.A.):

- **Health:** 0
- **Flammability:** 0
- **Reactivity:** 0
- **Specific hazard:**



Protective Equipment:
Not applicable. Lab coat. Not applicable. Safety glasses.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/10/2005 08:33 PM

Last Updated: 11/01/2010 12:00 PM

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Health	1
Fire	1
Reactivity	0
Personal Protection	A

Material Safety Data Sheet
Dextrose anhydrous MSDS

Section 1: Chemical Product and Company Identification

Product Name: Dextrose anhydrous

Catalog Codes: SLD3880, SLD4483

CAS#: 50-99-7

RTECS: LZ6600000

TSCA: TSCA 8(b) inventory: Dextrose anhydrous

CI#: Not available.

Synonym: D-Glucose

Chemical Name: Not available.

Chemical Formula: $C6H12O6$

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Dextrose anhydrous	50-99-7	100

Toxicological Data on Ingredients: Not applicable.

Section 3: Hazards Identification

Potential Acute Health Effects: Slightly hazardous in case of eye contact (irritant), of ingestion, of inhalation.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. Repeated or prolonged exposure is not known to aggravate medical condition.

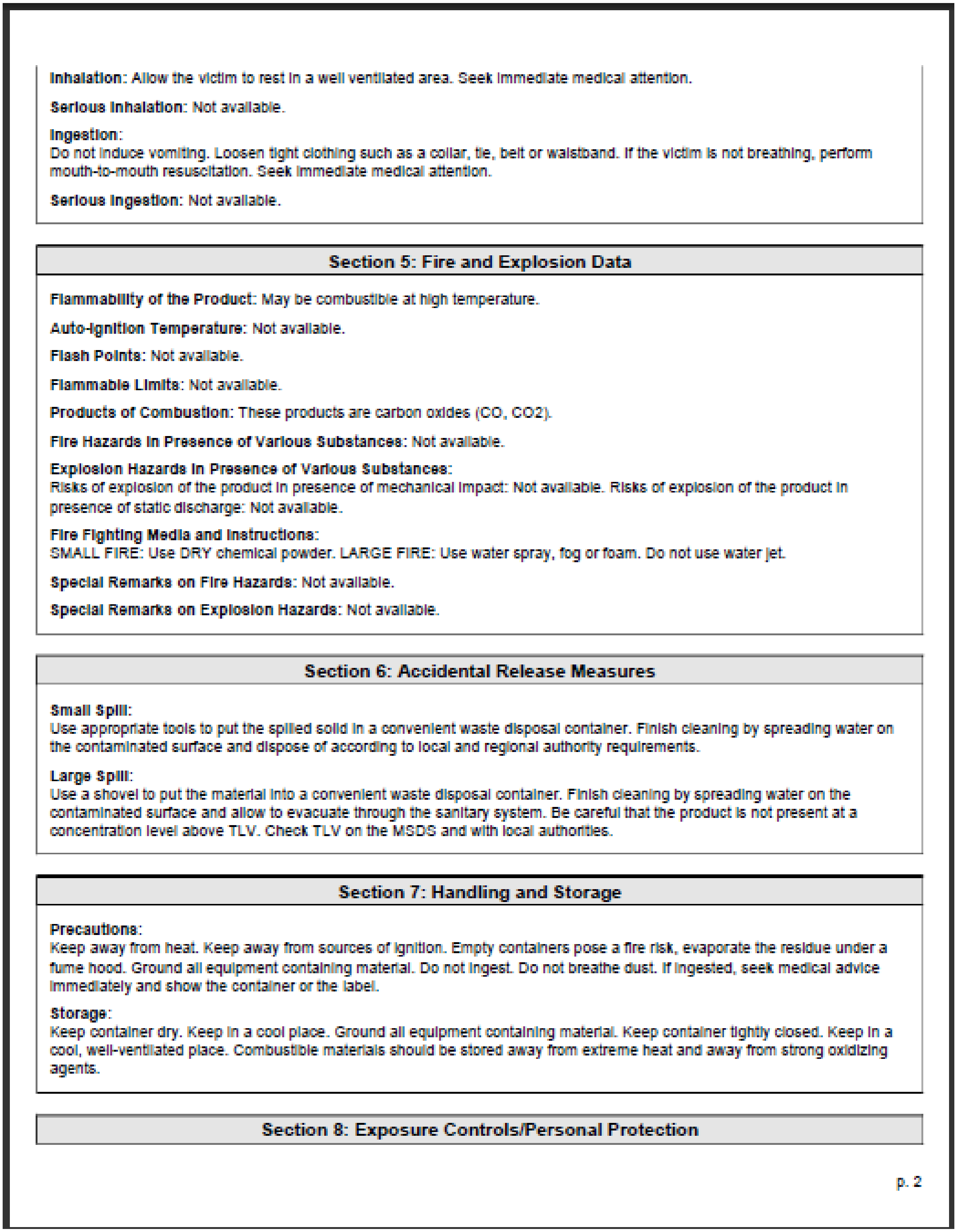
Section 4: First Aid Measures

Eye Contact: Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used.

Skin Contact: No known effect on skin contact, rinse with water for a few minutes.

Serious Skin Contact: Not available.

p. 1



Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate medical attention.

Serious Inhalation: Not available.

Ingestion:
Do not induce vomiting. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: May be combustible at high temperature.

Auto-Ignition Temperature: Not available.

Flash Points: Not available.

Flammable Limits: Not available.

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Not available.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill:
Use appropriate tools to put the spilled solid in a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and dispose of according to local and regional authority requirements.

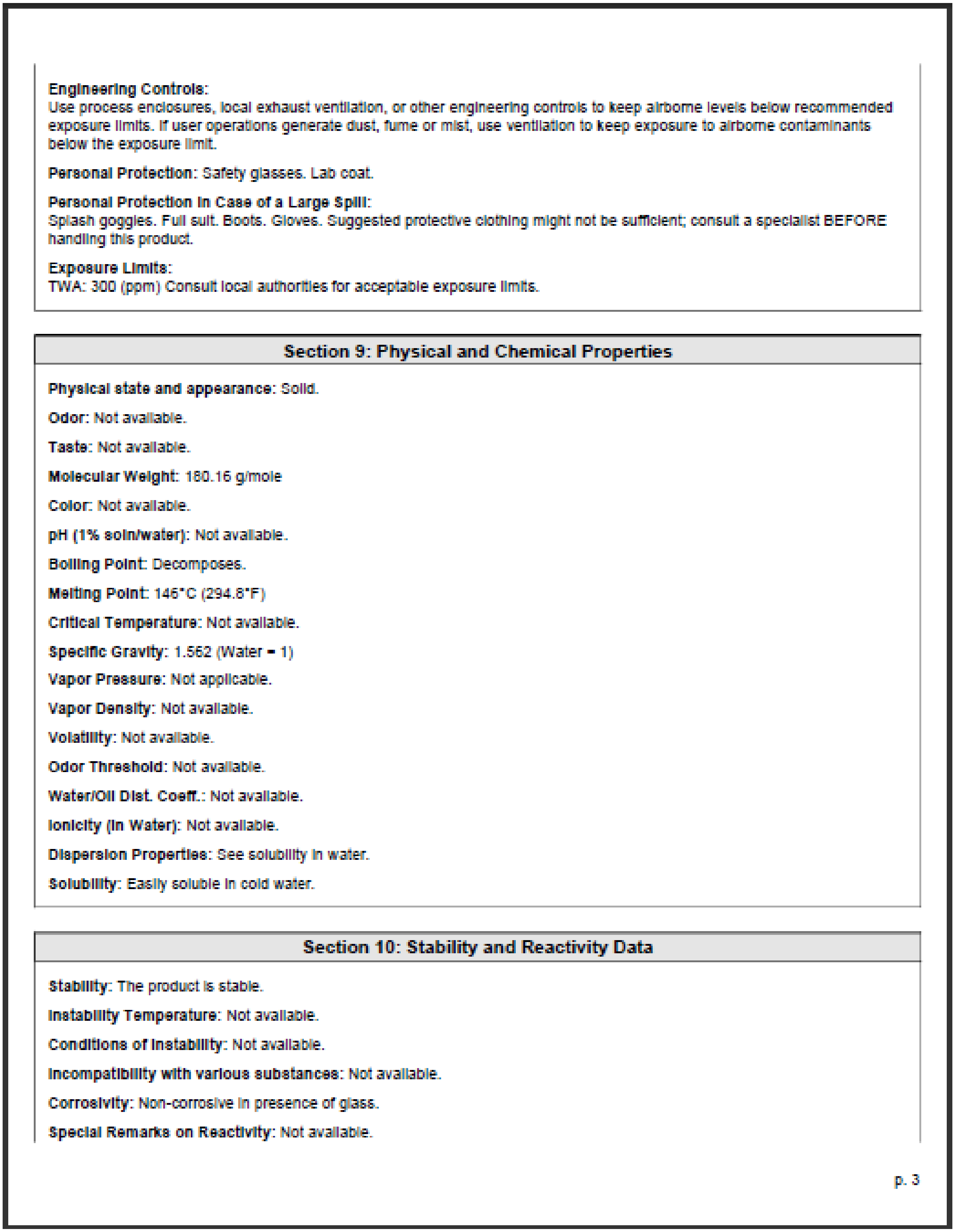
Large Spill:
Use a shovel to put the material into a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and allow to evacuate through the sanitary system. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Empty containers pose a fire risk, evaporate the residue under a fume hood. Ground all equipment containing material. Do not ingest. Do not breathe dust. If ingested, seek medical advice immediately and show the container or the label.

Storage:
Keep container dry. Keep in a cool place. Ground all equipment containing material. Keep container tightly closed. Keep in a cool, well-ventilated place. Combustible materials should be stored away from extreme heat and away from strong oxidizing agents.

Section 8: Exposure Controls/Personal Protection



Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection: Safety glasses. Lab coat.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Boots. Gloves. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 300 (ppm) Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid.

Odor: Not available.

Taste: Not available.

Molecular Weight: 180.16 g/mole

Color: Not available.

pH (1% soln/water): Not available.

Boiling Point: Decomposes.

Melting Point: 146°C (294.8°F)

Critical Temperature: Not available.

Specific Gravity: 1.562 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water.

Solubility: Easily soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

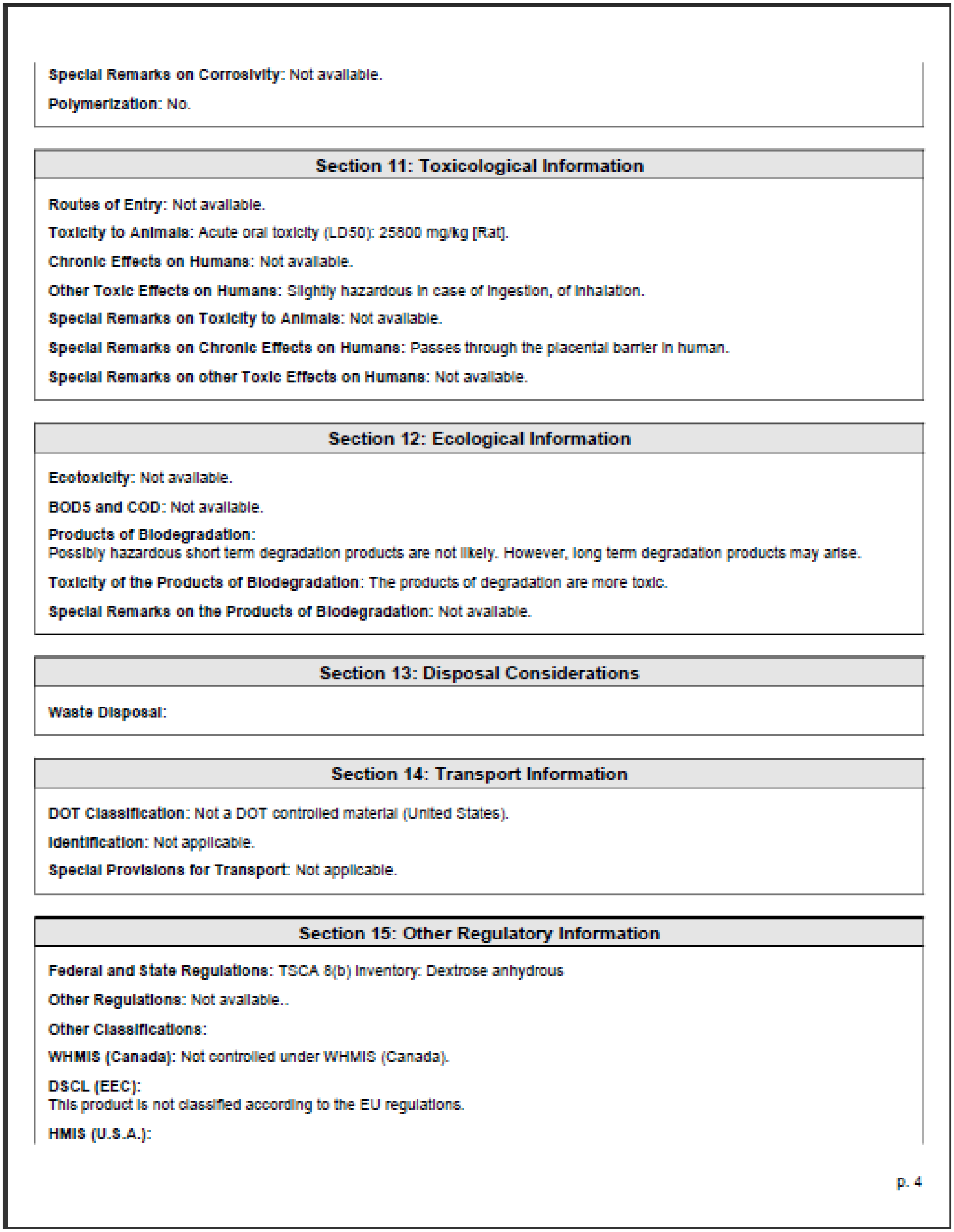
Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

p. 3



Special Remarks on Corrosivity: Not available.

Polymerization: No.

Section 11: Toxicological Information

Routes of Entry: Not available.

Toxicity to Animals: Acute oral toxicity (LD50): 25800 mg/kg [Rat].

Chronic Effects on Humans: Not available.

Other Toxic Effects on Humans: Slightly hazardous in case of ingestion, of inhalation.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Passes through the placental barrier in human.

Special Remarks on other Toxic Effects on Humans: Not available.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are more toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: Not a DOT controlled material (United States).

Identification: Not applicable.

Special Provisions for Transport: Not applicable.

Section 15: Other Regulatory Information

Federal and State Regulations: TSCA 8(b) inventory: Dextrose anhydrous

Other Regulations: Not available..

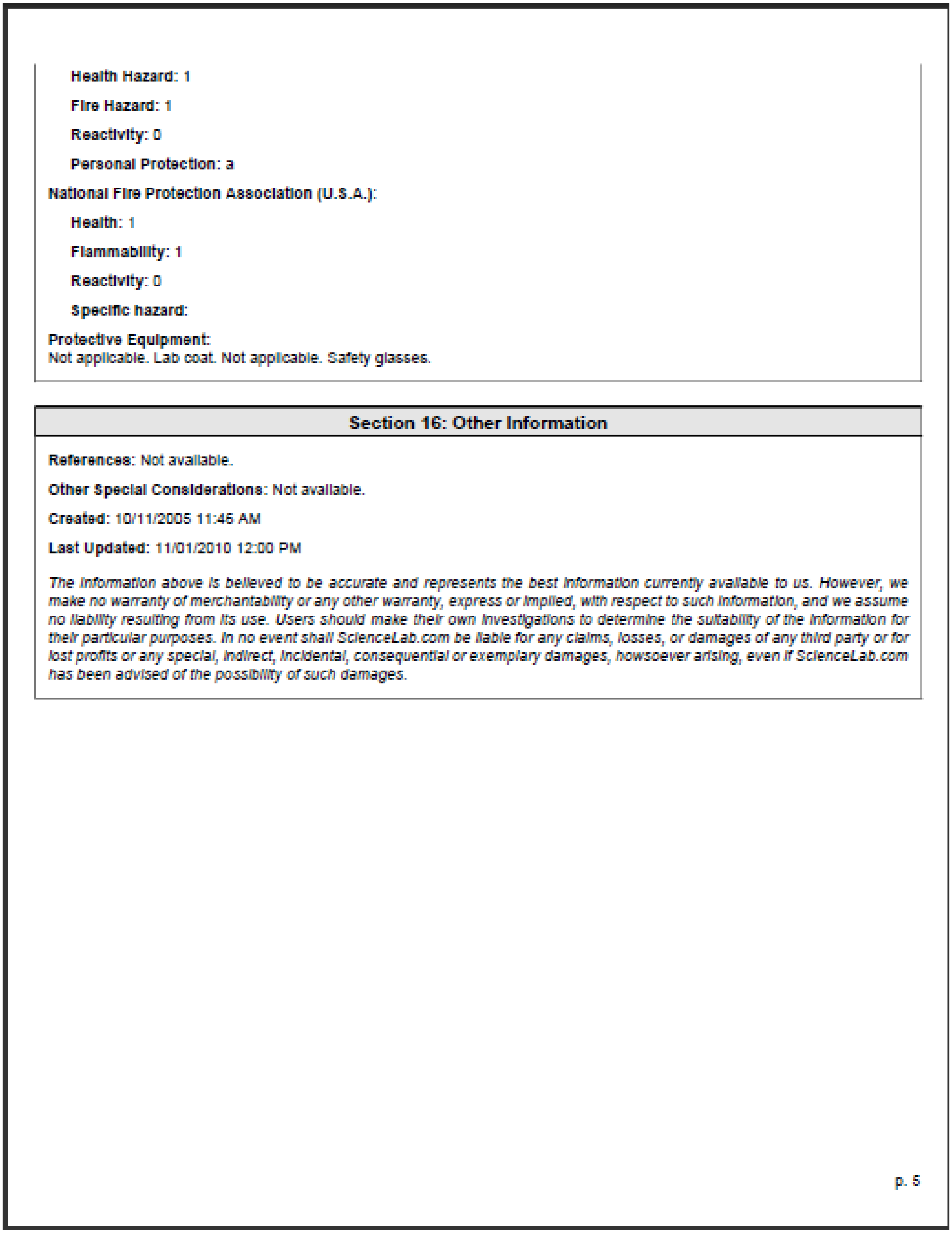
Other Classifications:

WHMIS (Canada): Not controlled under WHMIS (Canada).

DSCL (EEC):
This product is not classified according to the EU regulations.

HMIS (U.S.A.):

p. 4



Health Hazard: 1

Fire Hazard: 1

Reactivity: 0

Personal Protection: a

National Fire Protection Association (U.S.A.):

Health: 1

Flammability: 1

Reactivity: 0

Specific hazard:

Protective Equipment:
Not applicable. Lab coat. Not applicable. Safety glasses.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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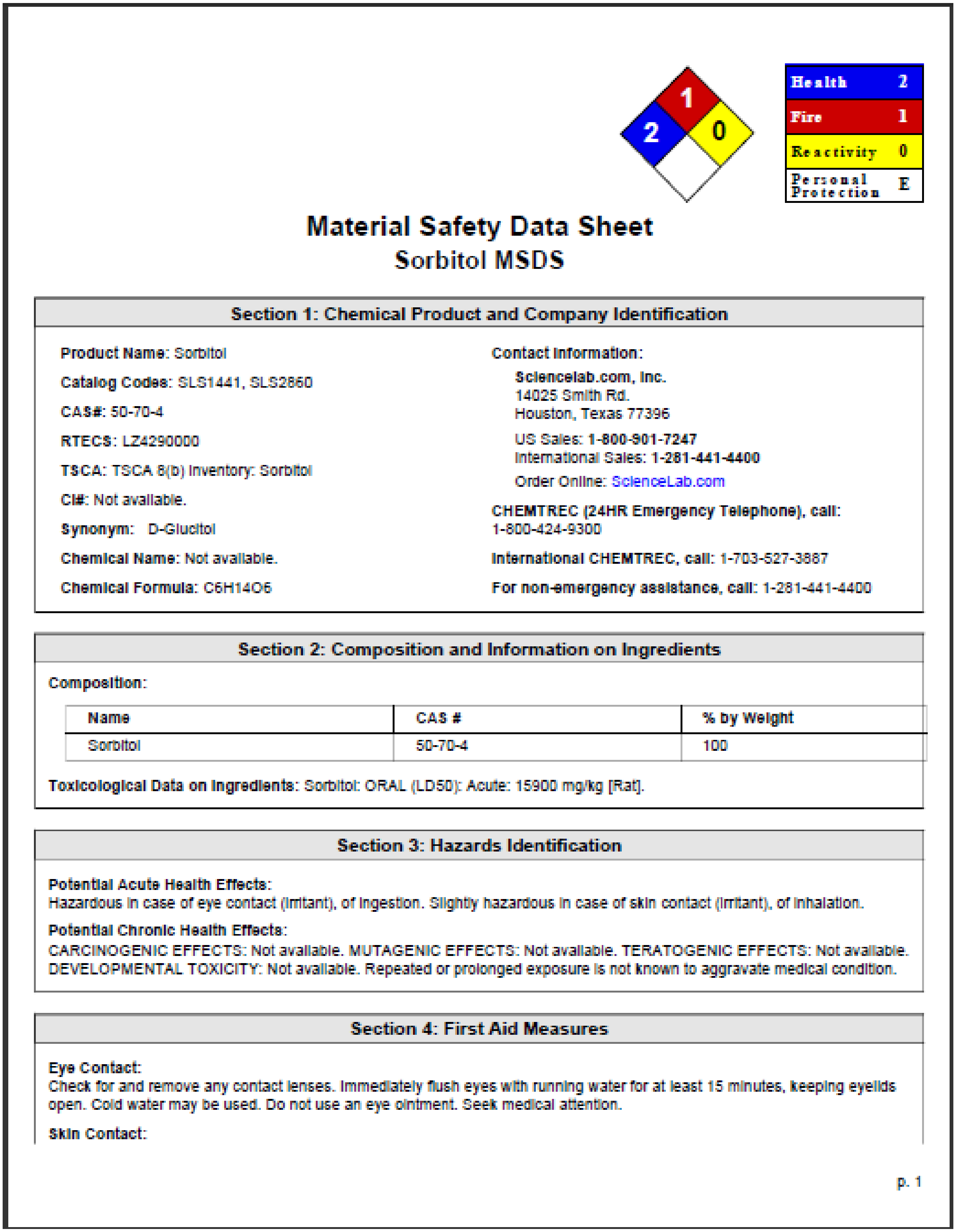


Health	2
Fire	1
Reactivity	0
Personal Protection	E

Material Safety Data Sheet
Sorbitol MSDS

Section 1: Chemical Product and Company Identification

Product Name: Sorbitol

Catalog Codes: SLS1441, SLS2860

CAS#: 50-70-4

RTECS: LZ4290000

TSCA: TSCA 8(b) inventory: Sorbitol

CI#: Not available.

Synonym: D-Glucitol

Chemical Name: Not available.

Chemical Formula: $C_6H_{14}O_6$

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Sorbitol	50-70-4	100

Toxicological Data on Ingredients: Sorbitol: ORAL (LD50): Acute: 15900 mg/kg [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of eye contact (irritant), of ingestion. Slightly hazardous in case of skin contact (irritant), of inhalation.

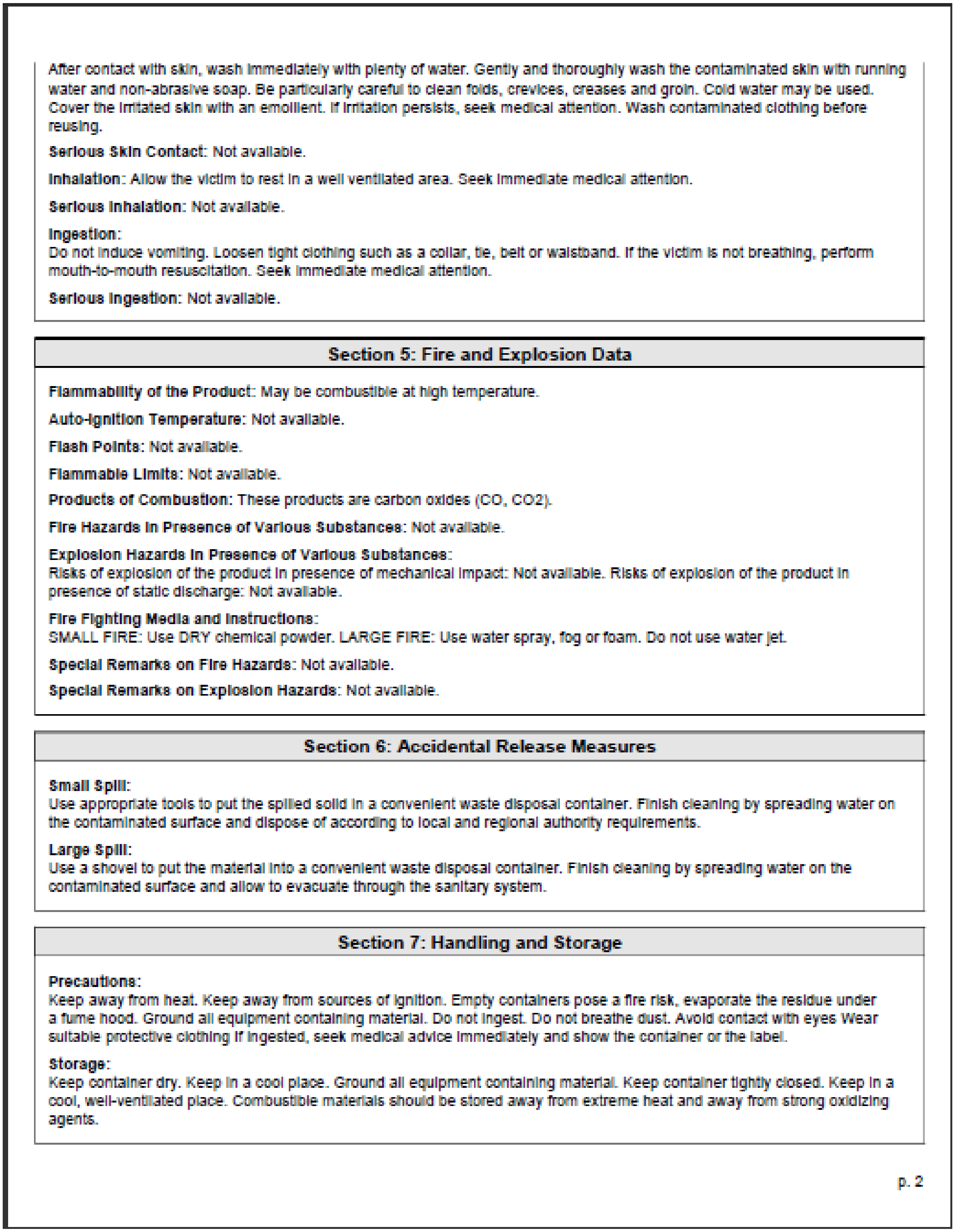
Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. Repeated or prolonged exposure is not known to aggravate medical condition.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Do not use an eye ointment. Seek medical attention.

Skin Contact:

p. 1



After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cold water may be used. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

Serious Skin Contact: Not available.

Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate medical attention.

Serious Inhalation: Not available.

Ingestion:
Do not induce vomiting. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: May be combustible at high temperature.

Auto-Ignition Temperature: Not available.

Flash Points: Not available.

Flammable Limits: Not available.

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Not available.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill:
Use appropriate tools to put the spilled solid in a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and dispose of according to local and regional authority requirements.

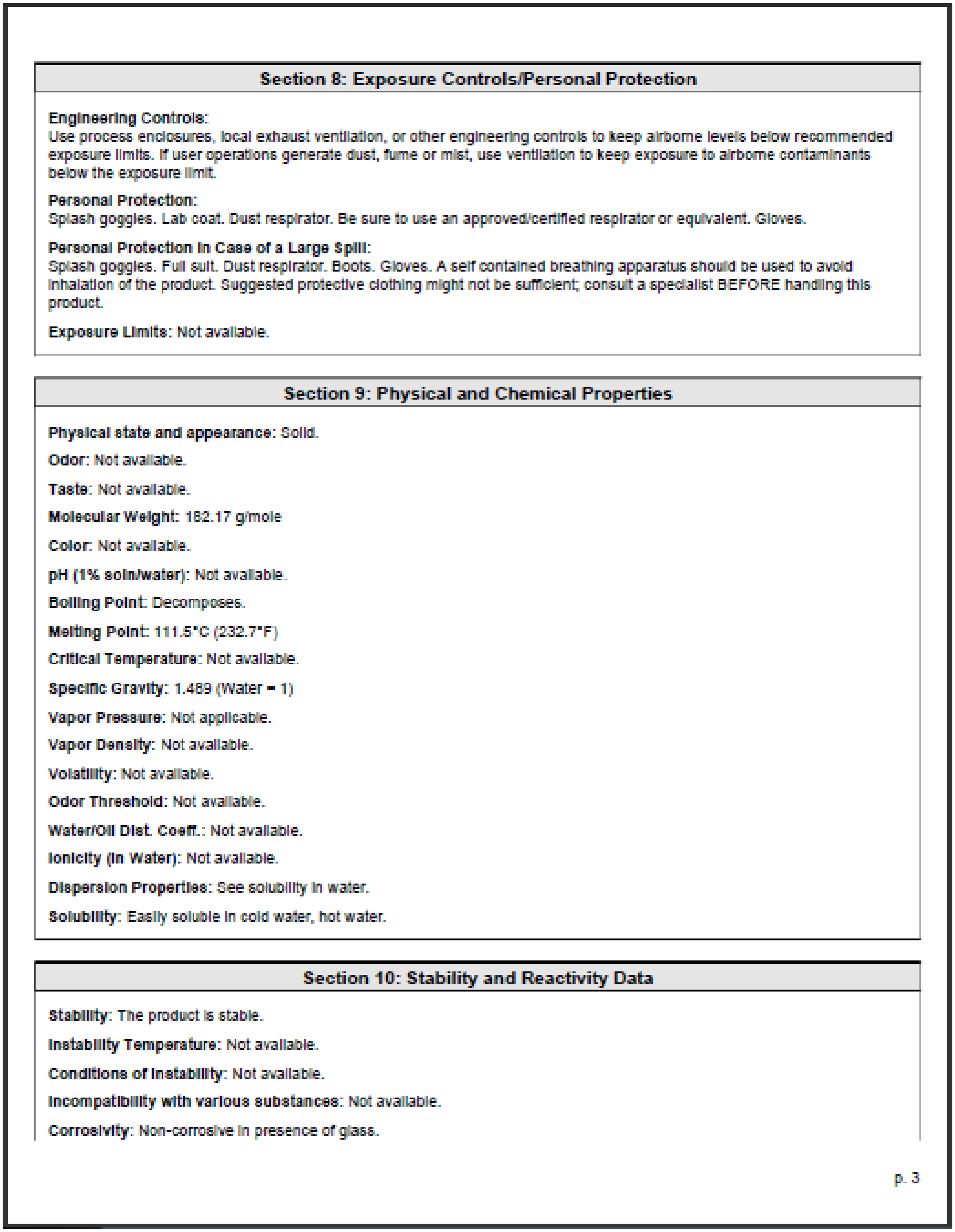
Large Spill:
Use a shovel to put the material into a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and allow to evacuate through the sanitary system.

Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Empty containers pose a fire risk, evaporate the residue under a fume hood. Ground all equipment containing material. Do not ingest. Do not breathe dust. Avoid contact with eyes Wear suitable protective clothing If ingested, seek medical advice immediately and show the container or the label.

Storage:
Keep container dry. Keep in a cool place. Ground all equipment containing material. Keep container tightly closed. Keep in a cool, well-ventilated place. Combustible materials should be stored away from extreme heat and away from strong oxidizing agents.

p. 2



Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid.

Odor: Not available.

Taste: Not available.

Molecular Weight: 182.17 g/mole

Color: Not available.

pH (1% soln/water): Not available.

Boiling Point: Decomposes.

Melting Point: 111.5°C (232.7°F)

Critical Temperature: Not available.

Specific Gravity: 1.489 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water.

Solubility: Easily soluble in cold water, hot water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

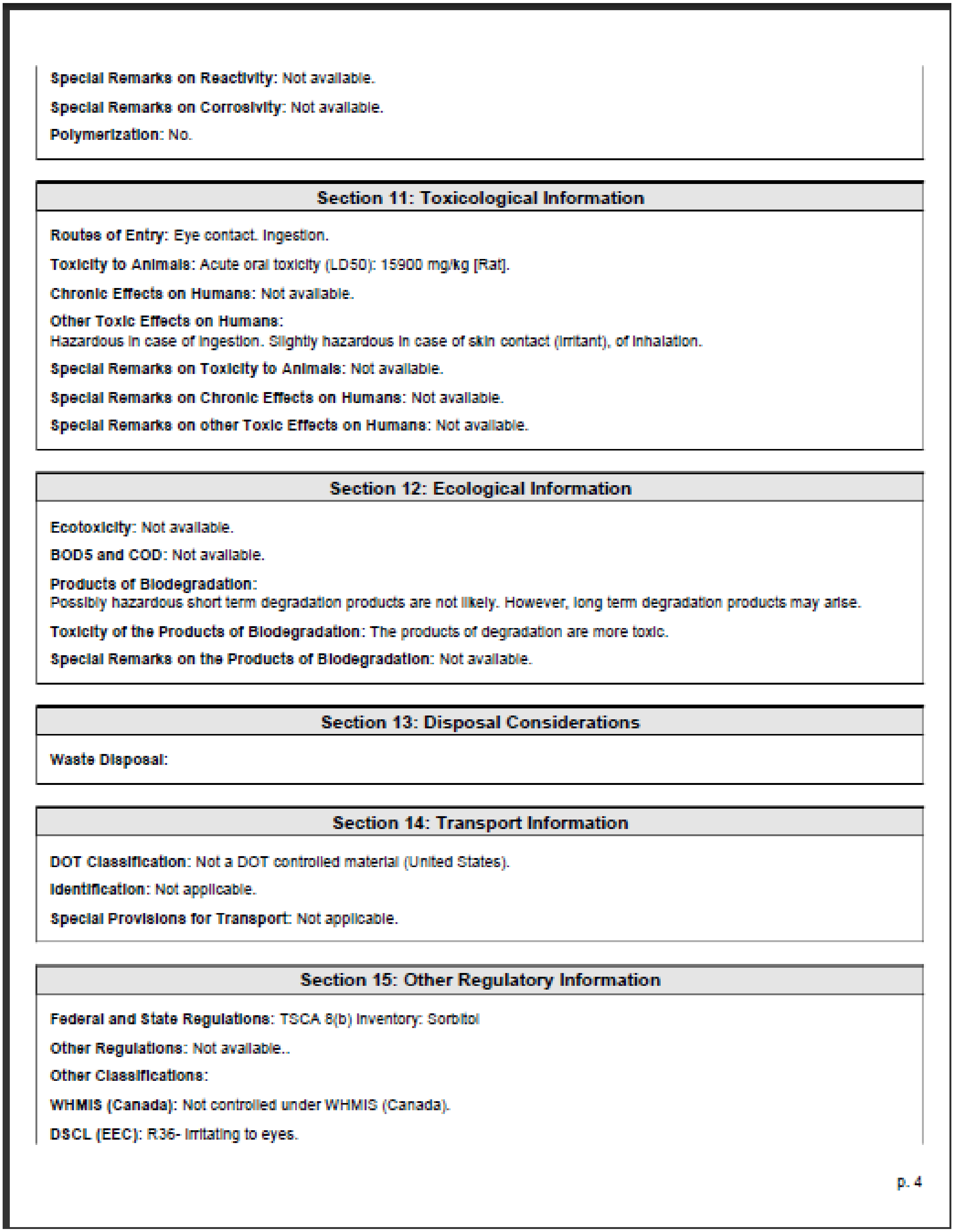
Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Non-corrosive in presence of glass.

p. 3



Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: No.

Section 11: Toxicological Information

Routes of Entry: Eye contact. Ingestion.

Toxicity to Animals: Acute oral toxicity (LD50): 15900 mg/kg [Rat].

Chronic Effects on Humans: Not available.

Other Toxic Effects on Humans:
Hazardous in case of ingestion. Slightly hazardous in case of skin contact (irritant), of inhalation.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are more toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: Not a DOT controlled material (United States).

Identification: Not applicable.

Special Provisions for Transport: Not applicable.

Section 15: Other Regulatory Information

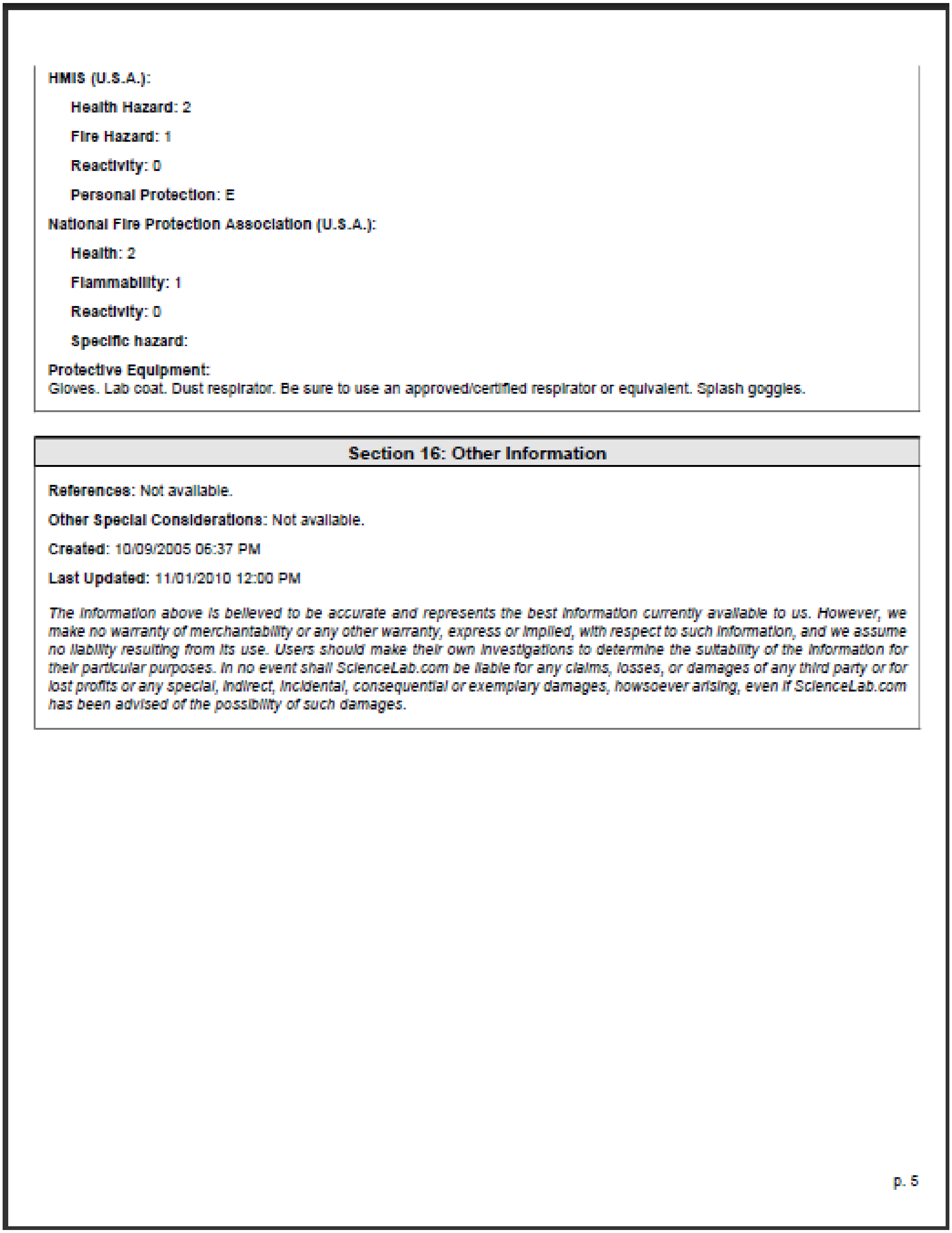
Federal and State Regulations: TSCA 8(b) inventory: Sorbitol

Other Regulations: Not available..

Other Classifications:

WHMIS (Canada): Not controlled under WHMIS (Canada).

DSCL (EEC): R36- Irritating to eyes.



HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 1

Reactivity: 0

Personal Protection: E

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 1

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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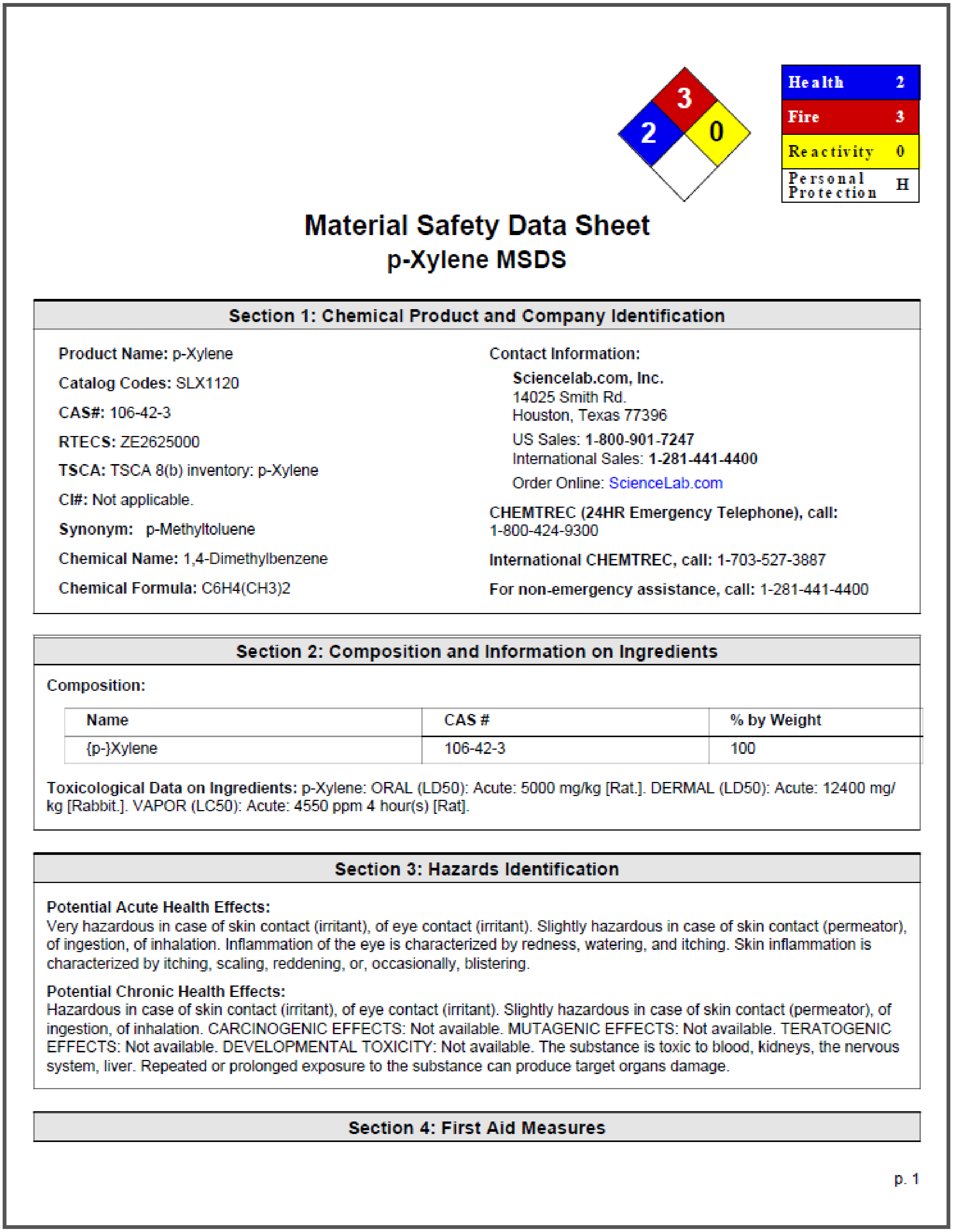


Health	2
Fire	3
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
p-Xylene MSDS

Section 1: Chemical Product and Company Identification

Product Name: p-Xylene

Catalog Codes: SLX1120

CAS#: 106-42-3

RTECS: ZE2625000

TSCA: TSCA 8(b) inventory: p-Xylene

CI#: Not applicable.

Synonym: p-Methyltoluene

Chemical Name: 1,4-Dimethylbenzene

Chemical Formula: C6H4(CH3)2

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
{p-}Xylene	106-42-3	100

Toxicological Data on Ingredients: p-Xylene: ORAL (LD50): Acute: 5000 mg/kg [Rat.]. DERMAL (LD50): Acute: 12400 mg/kg [Rabbit.]. VAPOR (LC50): Acute: 4550 ppm 4 hour(s) [Rat].

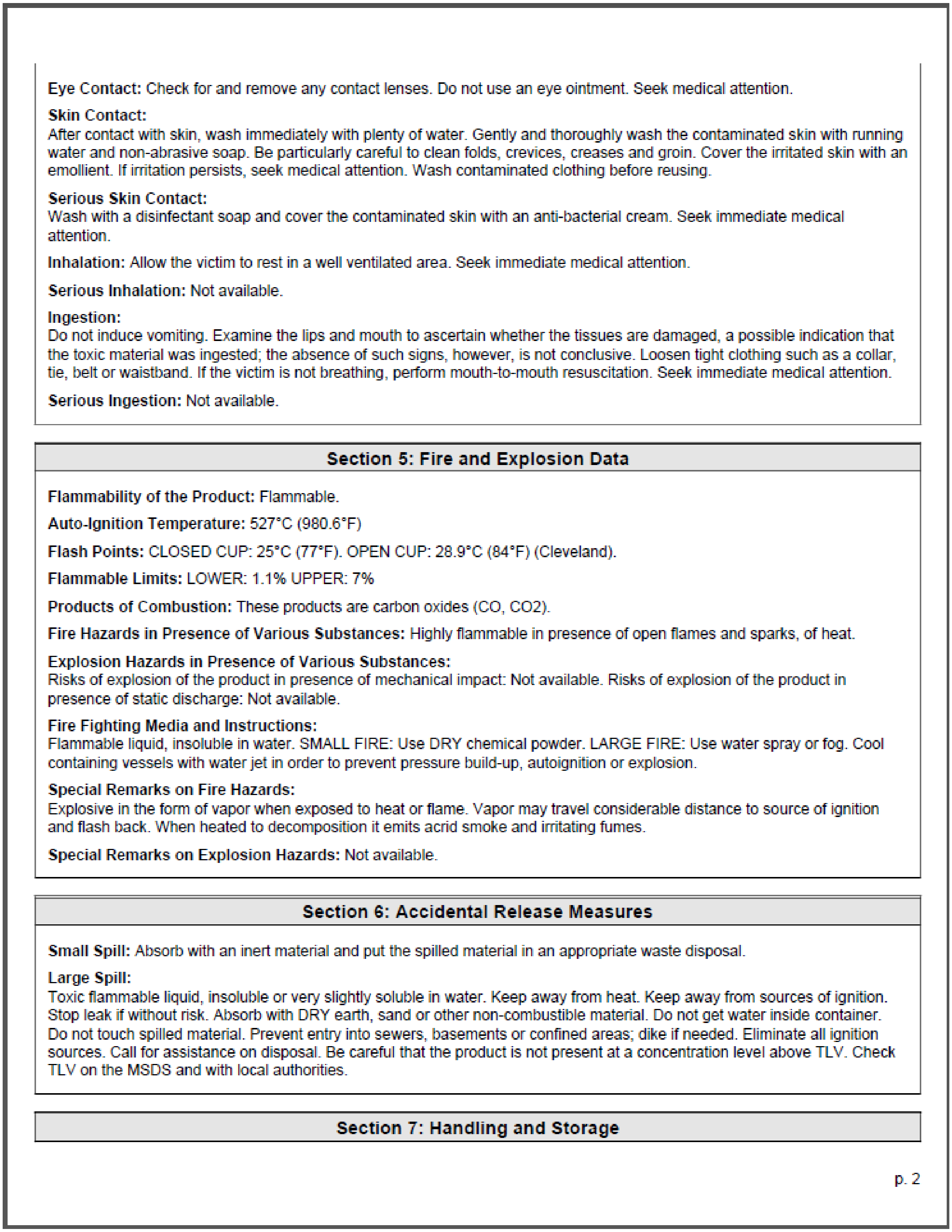
Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
Hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to blood, kidneys, the nervous system, liver. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

p. 1



Eye Contact: Check for and remove any contact lenses. Do not use an eye ointment. Seek medical attention.

Skin Contact:
After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate medical attention.

Serious Inhalation: Not available.

Ingestion:
Do not induce vomiting. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 527°C (980.6°F)

Flash Points: CLOSED CUP: 25°C (77°F). OPEN CUP: 28.9°C (84°F) (Cleveland).

Flammable Limits: LOWER: 1.1% UPPER: 7%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Highly flammable in presence of open flames and sparks, of heat.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
Flammable liquid, insoluble in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

Special Remarks on Fire Hazards:
Explosive in the form of vapor when exposed to heat or flame. Vapor may travel considerable distance to source of ignition and flash back. When heated to decomposition it emits acrid smoke and irritating fumes.

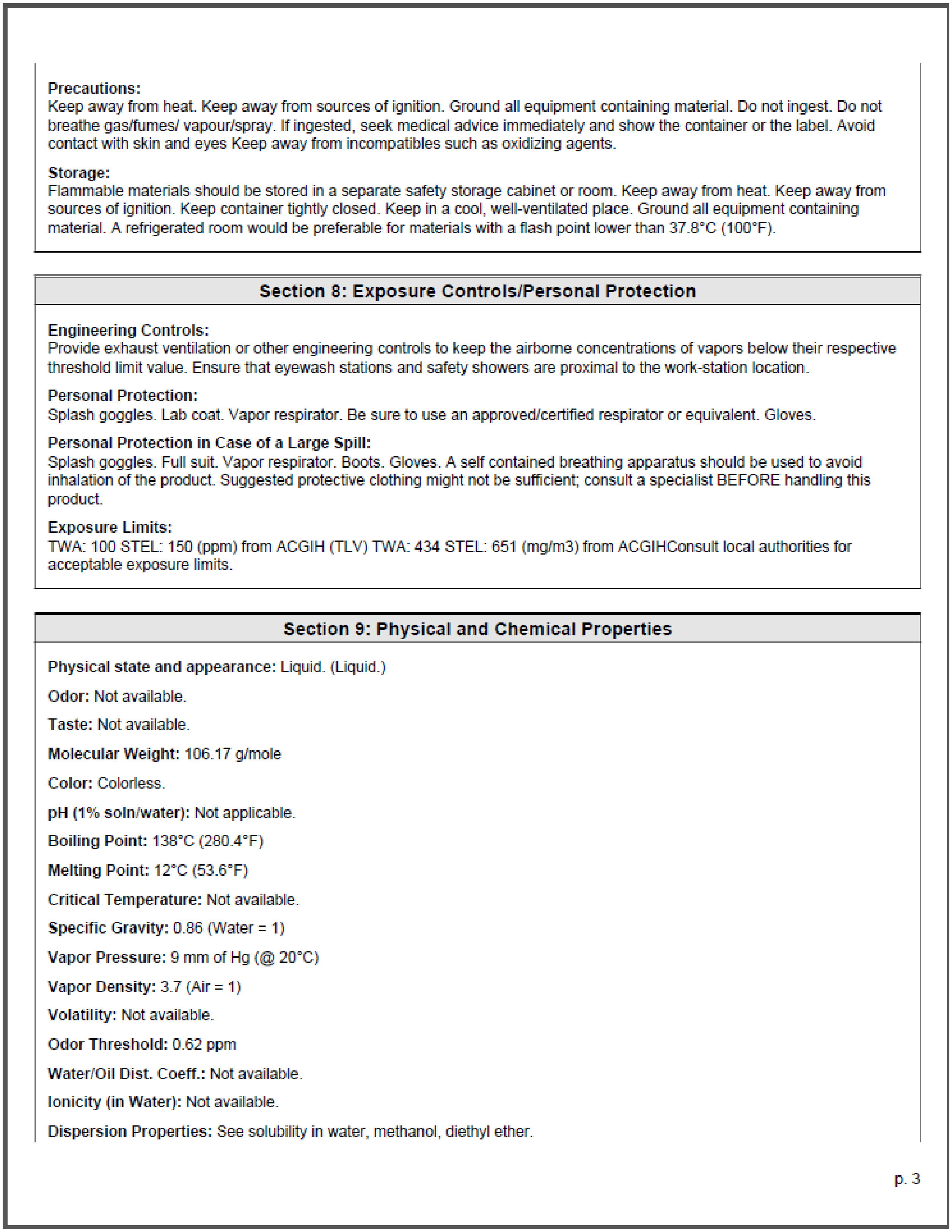
Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:
Toxic flammable liquid, insoluble or very slightly soluble in water. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage



Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapour/spray. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes Keep away from incompatibles such as oxidizing agents.

Storage:
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. A refrigerated room would be preferable for materials with a flash point lower than 37.8°C (100°F).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 100 STEL: 150 (ppm) from ACGIH (TLV) TWA: 434 STEL: 651 (mg/m3) from ACGIHConsult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Liquid.)

Odor: Not available.

Taste: Not available.

Molecular Weight: 106.17 g/mole

Color: Colorless.

pH (1% soln/water): Not applicable.

Boiling Point: 138°C (280.4°F)

Melting Point: 12°C (53.6°F)

Critical Temperature: Not available.

Specific Gravity: 0.86 (Water = 1)

Vapor Pressure: 9 mm of Hg (@ 20°C)

Vapor Density: 3.7 (Air = 1)

Volatility: Not available.

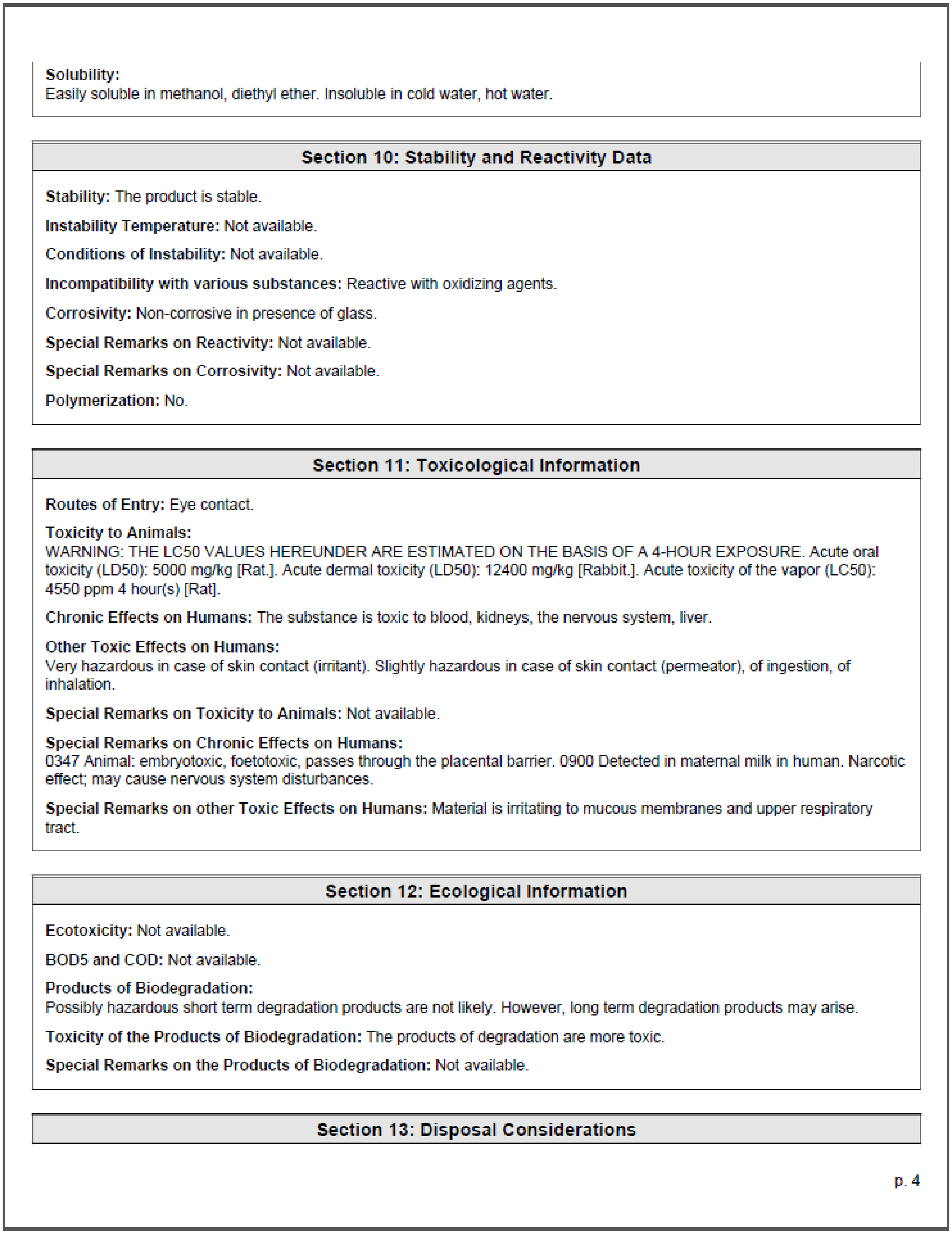
Odor Threshold: 0.62 ppm

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, methanol, diethyl ether.

p. 3



Solubility:
Easily soluble in methanol, diethyl ether. Insoluble in cold water, hot water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Reactive with oxidizing agents.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: No.

Section 11: Toxicological Information

Routes of Entry: Eye contact.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 5000 mg/kg [Rat.]. Acute dermal toxicity (LD50): 12400 mg/kg [Rabbit.]. Acute toxicity of the vapor (LC50): 4550 ppm 4 hour(s) [Rat].

Chronic Effects on Humans: The substance is toxic to blood, kidneys, the nervous system, liver.

Other Toxic Effects on Humans:
Very hazardous in case of skin contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
0347 Animal: embryotoxic, foetotoxic, passes through the placental barrier. 0900 Detected in maternal milk in human. Narcotic effect; may cause nervous system disturbances.

Special Remarks on other Toxic Effects on Humans: Material is irritating to mucous membranes and upper respiratory tract.

Section 12: Ecological Information

Ecotoxicity: Not available.

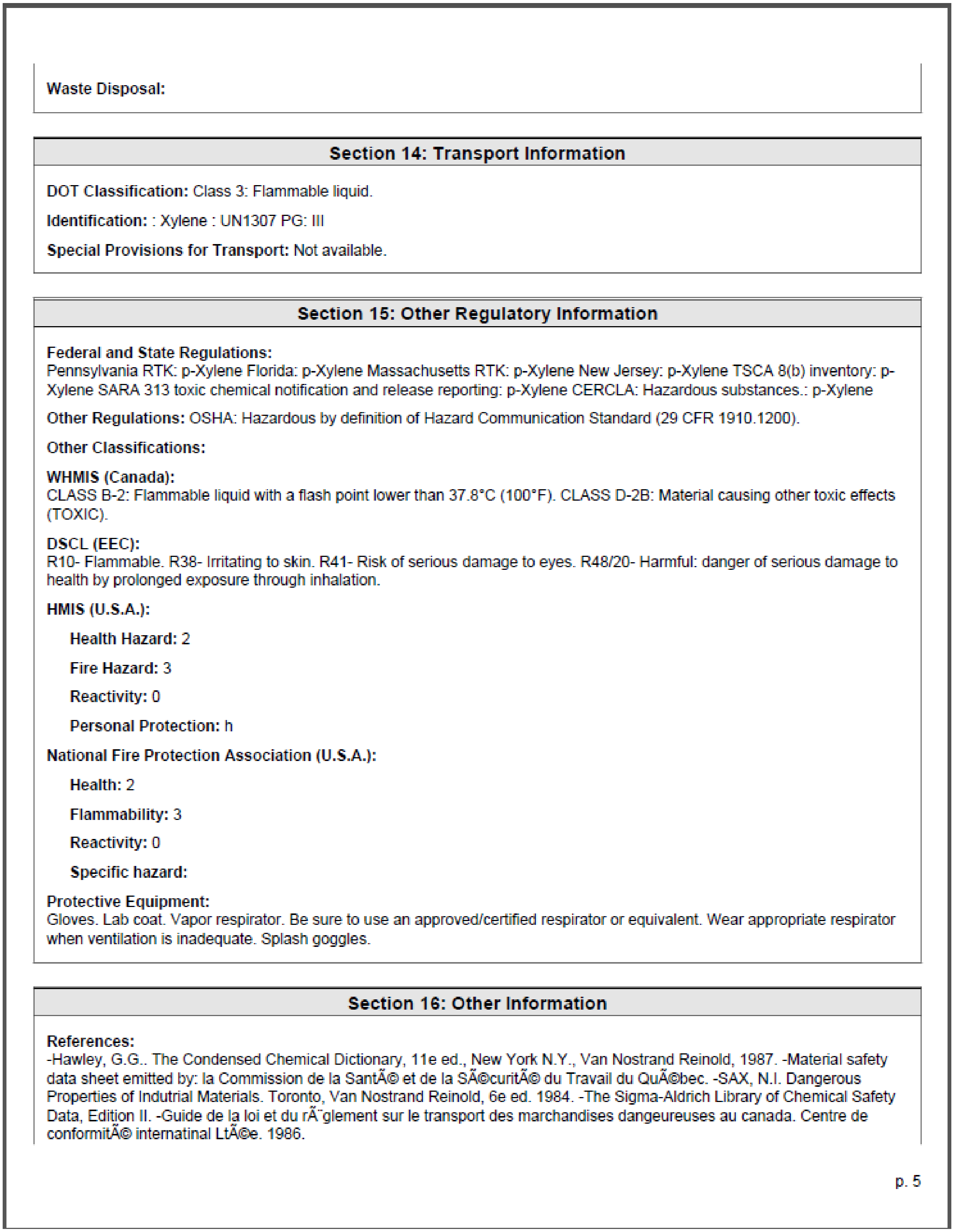
BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are more toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations



Waste Disposal:

Section 14: Transport Information

DOT Classification: Class 3: Flammable liquid.

Identification: : Xylene : UN1307 PG: III

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK: p-Xylene Florida: p-Xylene Massachusetts RTK: p-Xylene New Jersey: p-Xylene TSCA 8(b) inventory: p-Xylene SARA 313 toxic chemical notification and release reporting: p-Xylene CERCLA: Hazardous substances.: p-Xylene

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:

WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2B: Material causing other toxic effects (TOXIC).

DSCL (EEC):
R10- Flammable. R38- Irritating to skin. R41- Risk of serious damage to eyes. R48/20- Harmful: danger of serious damage to health by prolonged exposure through inhalation.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 3

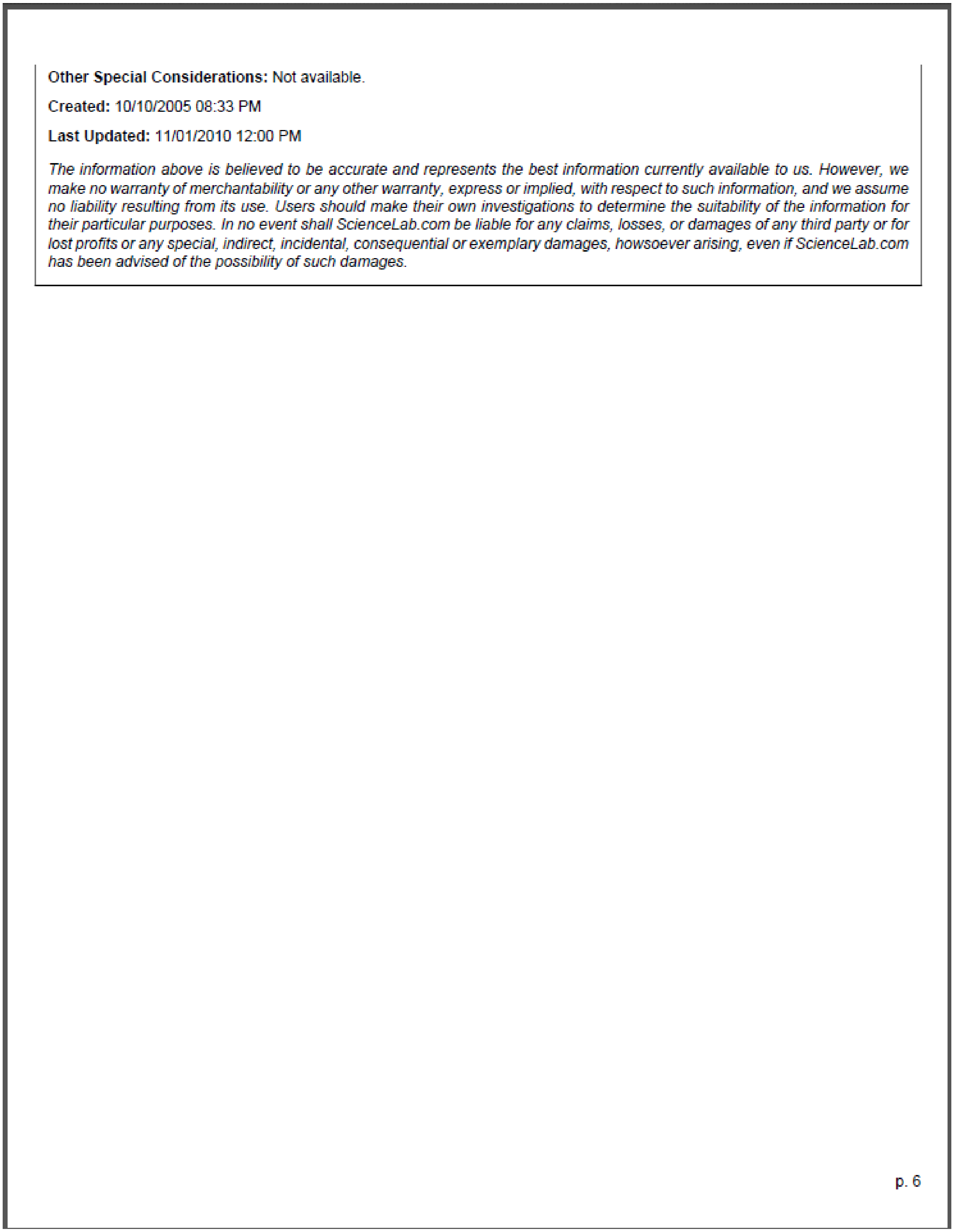
Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References:
-Hawley, G.G.. The Condensed Chemical Dictionary, 11e ed., New York N.Y., Van Nostrand Reinold, 1987. -Material safety data sheet emitted by: la Commission de la SantÃ© et de la SÃ©curitÃ© du Travail du QuÃ©bec. -SAX, N.I. Dangerous Properties of Indutrial Materials. Toronto, Van Nostrand Reinold, 6e ed. 1984. -The Sigma-Aldrich Library of Chemical Safety Data, Edition II. -Guide de la loi et du rÃ¨glement sur le transport des marchandises dangeureuses au canada. Centre de conformitÃ© internatinal LtÃ©e. 1986.



Other Special Considerations: Not available.

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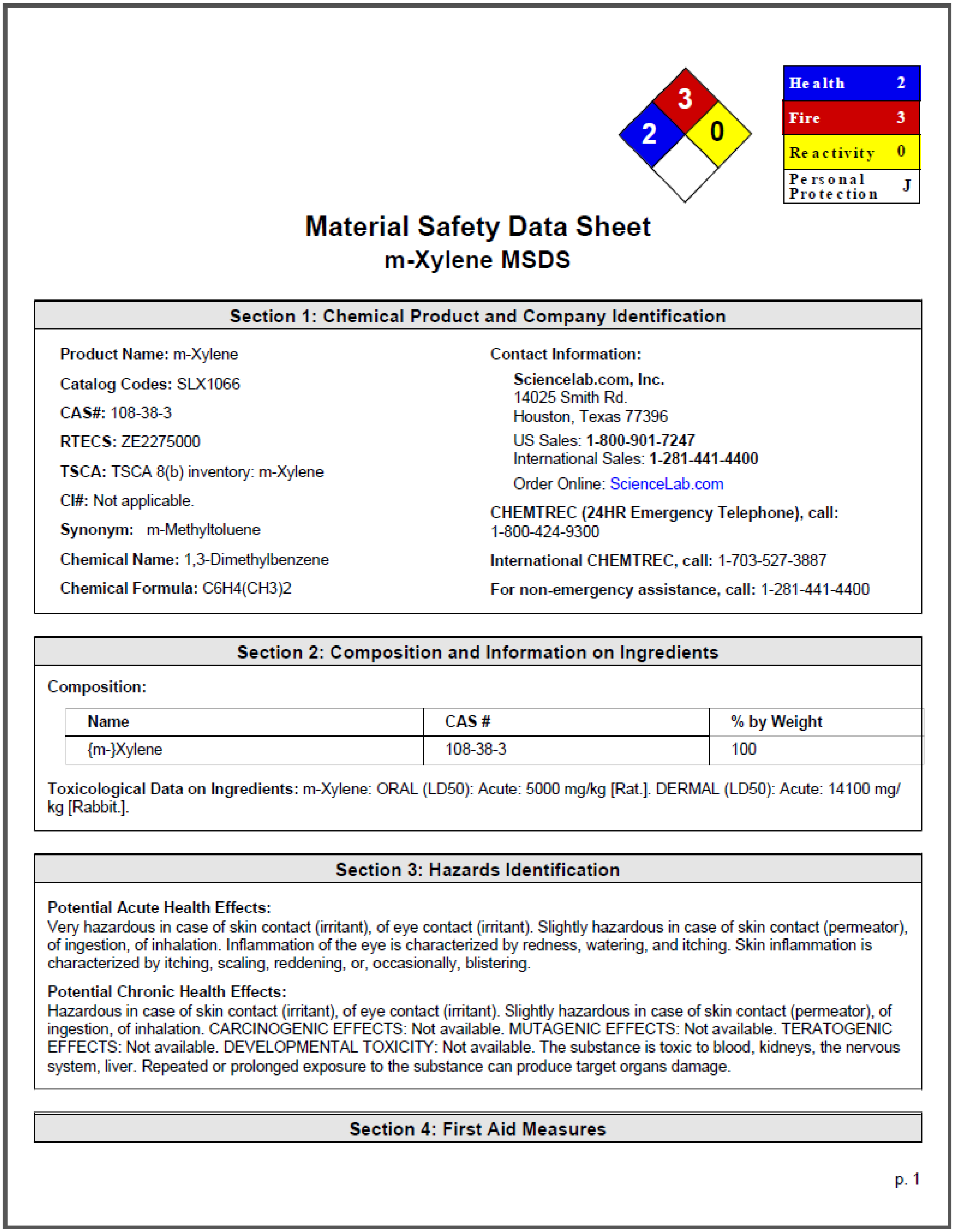


Health	2
Fire	3
Reactivity	0
Personal Protection	J

Material Safety Data Sheet
m-Xylene MSDS

Section 1: Chemical Product and Company Identification

Product Name: m-Xylene

Catalog Codes: SLX1066

CAS#: 108-38-3

RTECS: ZE2275000

TSCA: TSCA 8(b) inventory: m-Xylene

CI#: Not applicable.

Synonym: m-Methyltoluene

Chemical Name: 1,3-Dimethylbenzene

Chemical Formula: C6H4(CH3)2

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
{m-}Xylene	108-38-3	100

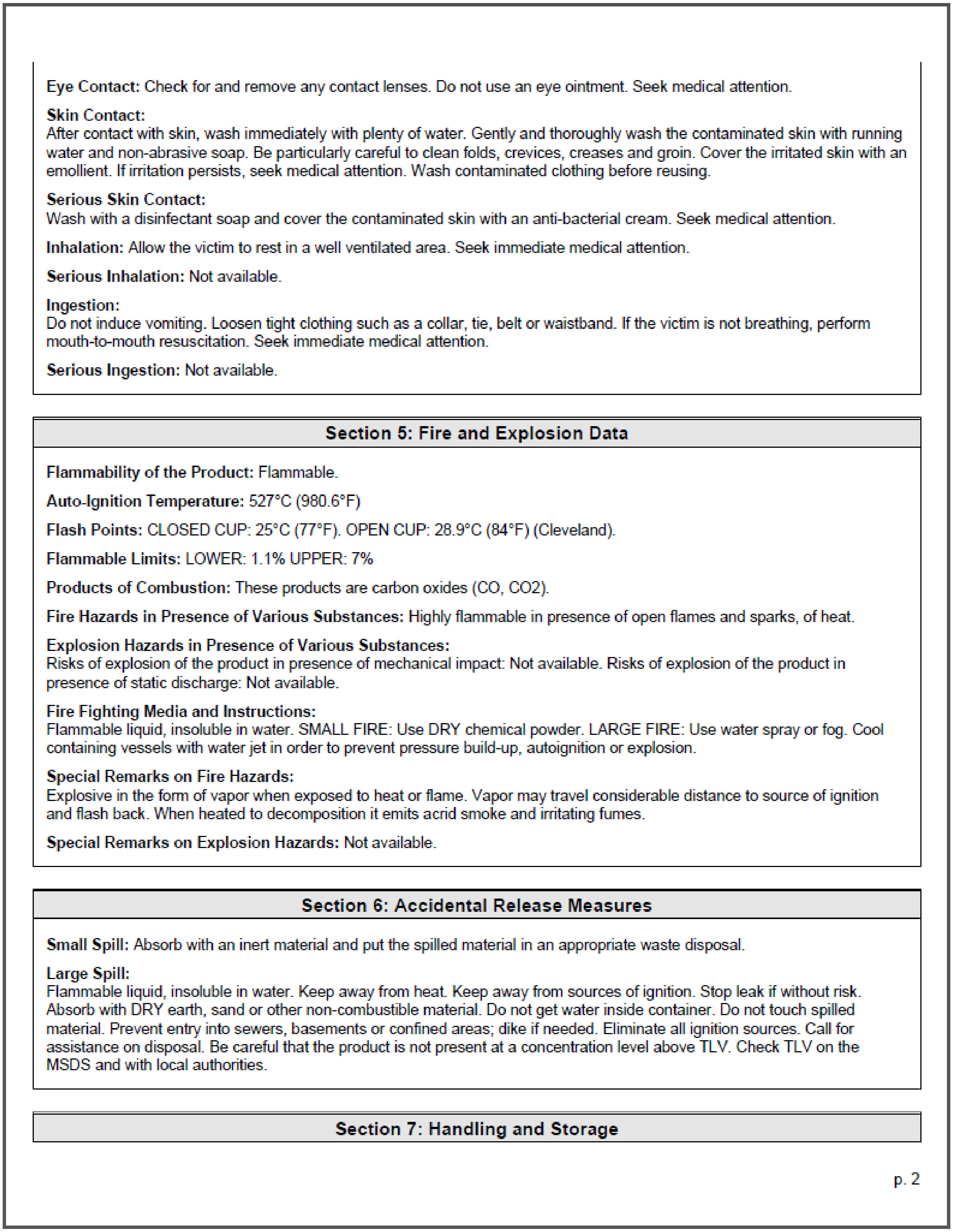
Toxicological Data on Ingredients: m-Xylene: ORAL (LD50): Acute: 5000 mg/kg [Rat.]. DERMAL (LD50): Acute: 14100 mg/kg [Rabbit.].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
Hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to blood, kidneys, the nervous system, liver. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures



Eye Contact: Check for and remove any contact lenses. Do not use an eye ointment. Seek medical attention.

Skin Contact:
After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek medical attention.

Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate medical attention.

Serious Inhalation: Not available.

Ingestion:
Do not induce vomiting. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 527°C (980.6°F)

Flash Points: CLOSED CUP: 25°C (77°F). OPEN CUP: 28.9°C (84°F) (Cleveland).

Flammable Limits: LOWER: 1.1% UPPER: 7%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Highly flammable in presence of open flames and sparks, of heat.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
Flammable liquid, insoluble in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

Special Remarks on Fire Hazards:
Explosive in the form of vapor when exposed to heat or flame. Vapor may travel considerable distance to source of ignition and flash back. When heated to decomposition it emits acrid smoke and irritating fumes.

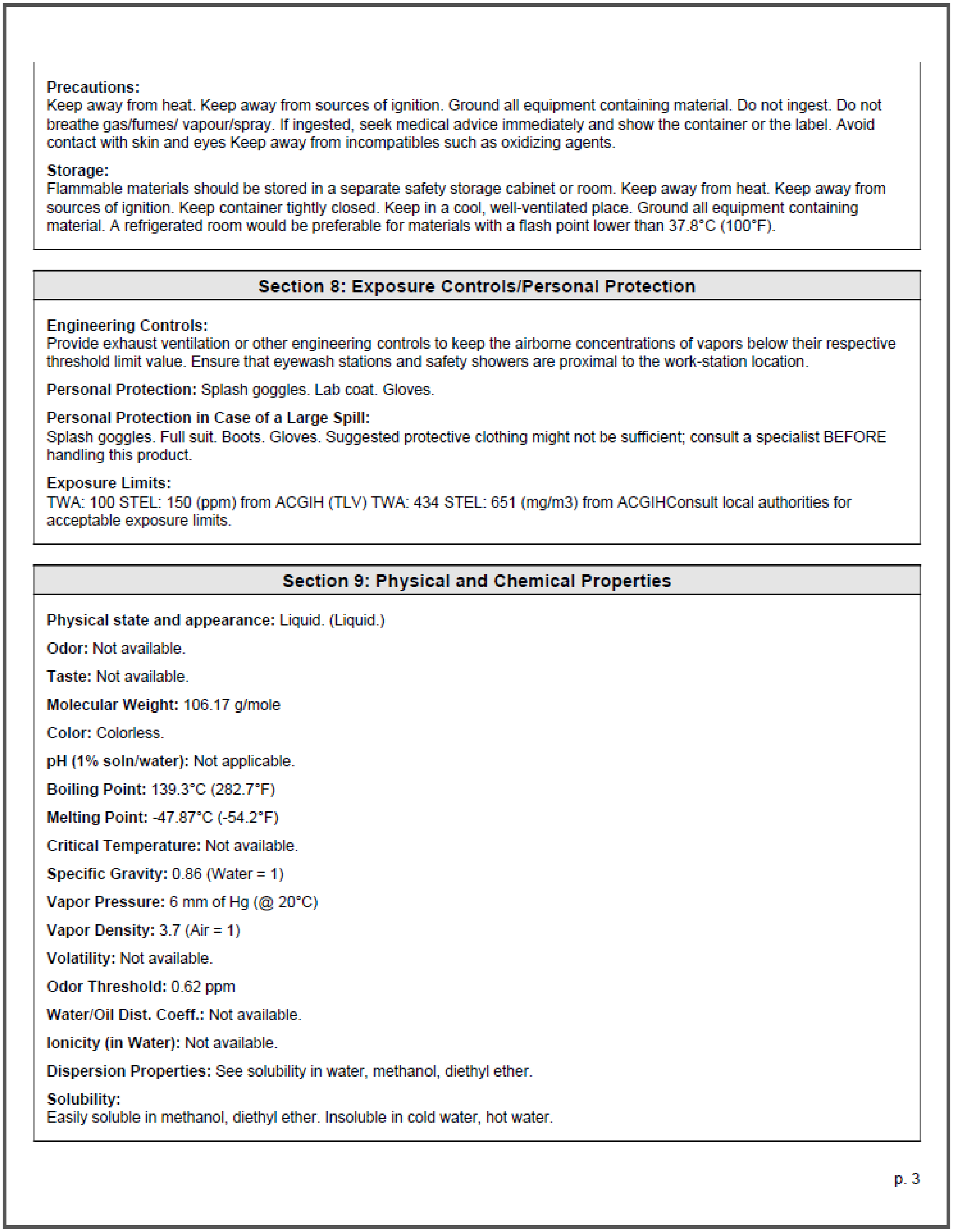
Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:
Flammable liquid, insoluble in water. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage



Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapour/spray. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes Keep away from incompatibles such as oxidizing agents.

Storage:
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. A refrigerated room would be preferable for materials with a flash point lower than 37.8°C (100°F).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection: Splash goggles. Lab coat. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Boots. Gloves. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 100 STEL: 150 (ppm) from ACGIH (TLV) TWA: 434 STEL: 651 (mg/m3) from ACGIHConsult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Liquid.)

Odor: Not available.

Taste: Not available.

Molecular Weight: 106.17 g/mole

Color: Colorless.

pH (1% soln/water): Not applicable.

Boiling Point: 139.3°C (282.7°F)

Melting Point: -47.87°C (-54.2°F)

Critical Temperature: Not available.

Specific Gravity: 0.86 (Water = 1)

Vapor Pressure: 6 mm of Hg (@ 20°C)

Vapor Density: 3.7 (Air = 1)

Volatility: Not available.

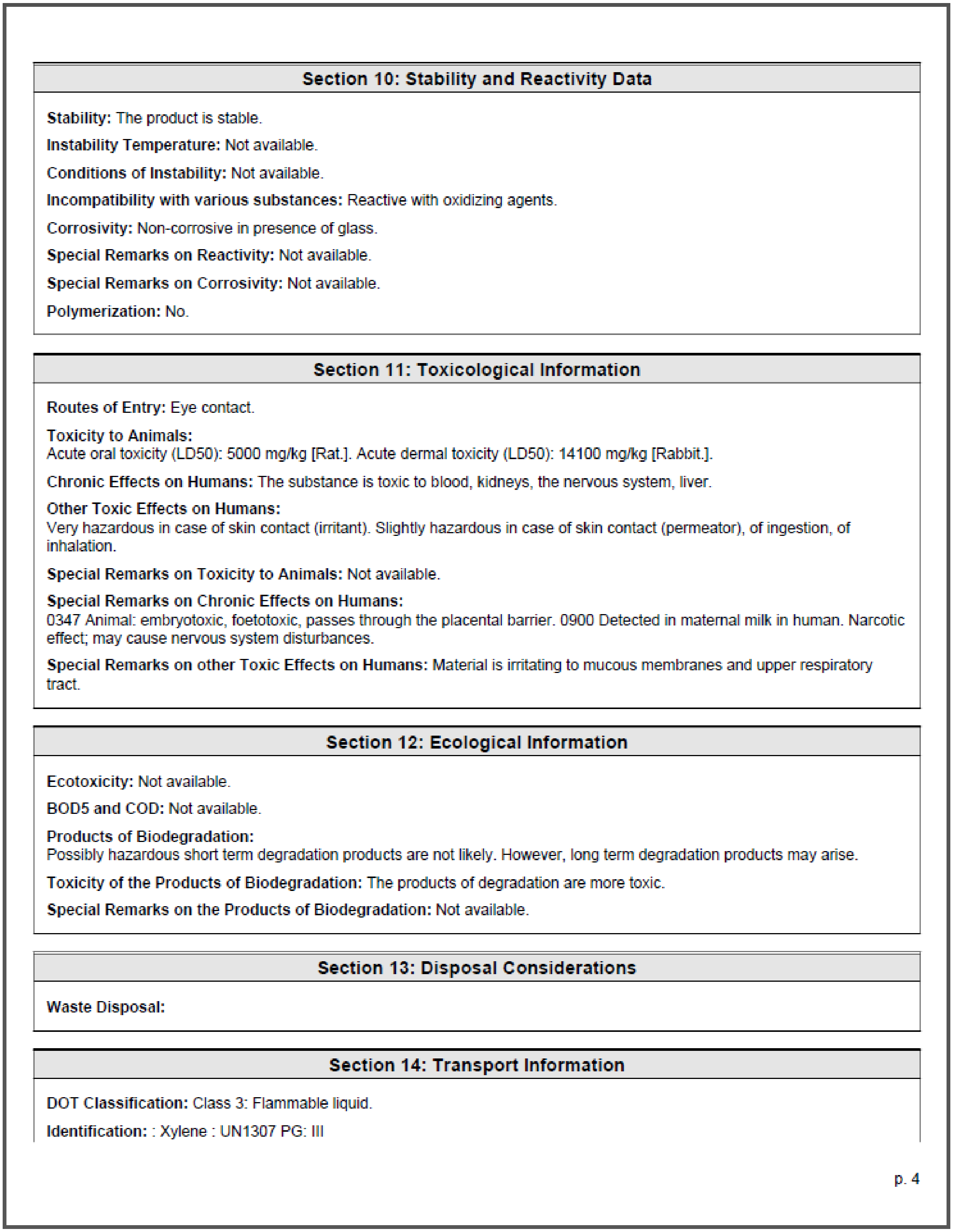
Odor Threshold: 0.62 ppm

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, methanol, diethyl ether.

Solubility:
Easily soluble in methanol, diethyl ether. Insoluble in cold water, hot water.



Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Reactive with oxidizing agents.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: No.

Section 11: Toxicological Information

Routes of Entry: Eye contact.

Toxicity to Animals:
Acute oral toxicity (LD50): 5000 mg/kg [Rat.]. Acute dermal toxicity (LD50): 14100 mg/kg [Rabbit.].

Chronic Effects on Humans: The substance is toxic to blood, kidneys, the nervous system, liver.

Other Toxic Effects on Humans:
Very hazardous in case of skin contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
0347 Animal: embryotoxic, foetotoxic, passes through the placental barrier. 0900 Detected in maternal milk in human. Narcotic effect; may cause nervous system disturbances.

Special Remarks on other Toxic Effects on Humans: Material is irritating to mucous membranes and upper respiratory tract.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are more toxic.

Special Remarks on the Products of Biodegradation: Not available.

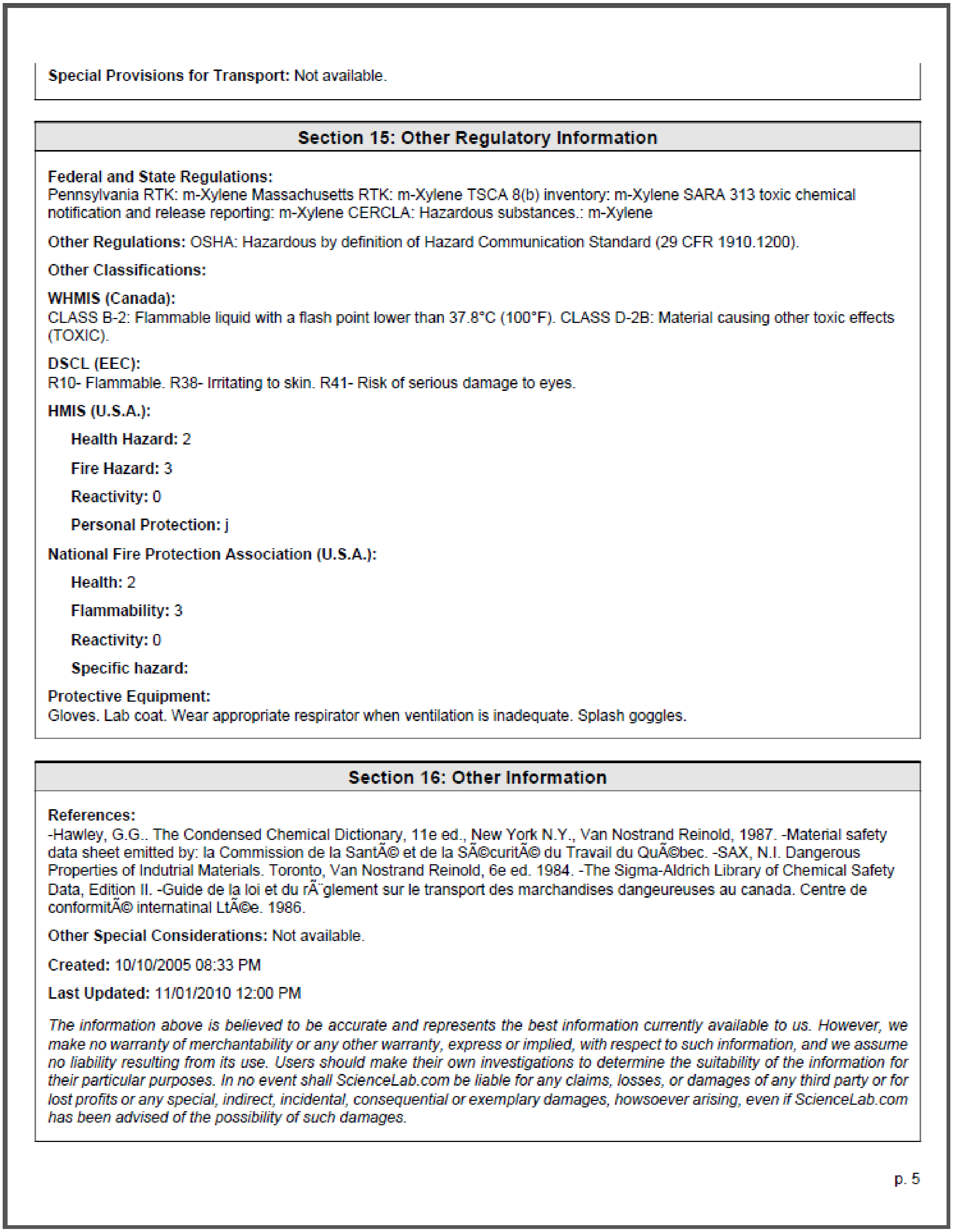
Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: Class 3: Flammable liquid.

Identification: : Xylene : UN1307 PG: III



Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK: m-Xylene Massachusetts RTK: m-Xylene TSCA 8(b) inventory: m-Xylene SARA 313 toxic chemical notification and release reporting: m-Xylene CERCLA: Hazardous substances.: m-Xylene

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:

WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2B: Material causing other toxic effects (TOXIC).

DSCL (EEC):
R10- Flammable. R38- Irritating to skin. R41- Risk of serious damage to eyes.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: j

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 3

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References:
-Hawley, G.G.. The Condensed Chemical Dictionary, 11e ed., New York N.Y., Van Nostrand Reinold, 1987. -Material safety data sheet emitted by: la Commission de la SantÃ© et de la SÃ©curitÃ© du Travail du QuÃ©bec. -SAX, N.I. Dangerous Properties of Indutrial Materials. Toronto, Van Nostrand Reinold, 6e ed. 1984. -The Sigma-Aldrich Library of Chemical Safety Data, Edition II. -Guide de la loi et du rÃ¨glement sur le transport des marchandises dangeureuses au canada. Centre de conformitÃ© internatinal LtÃ©e. 1986.

Other Special Considerations: Not available.

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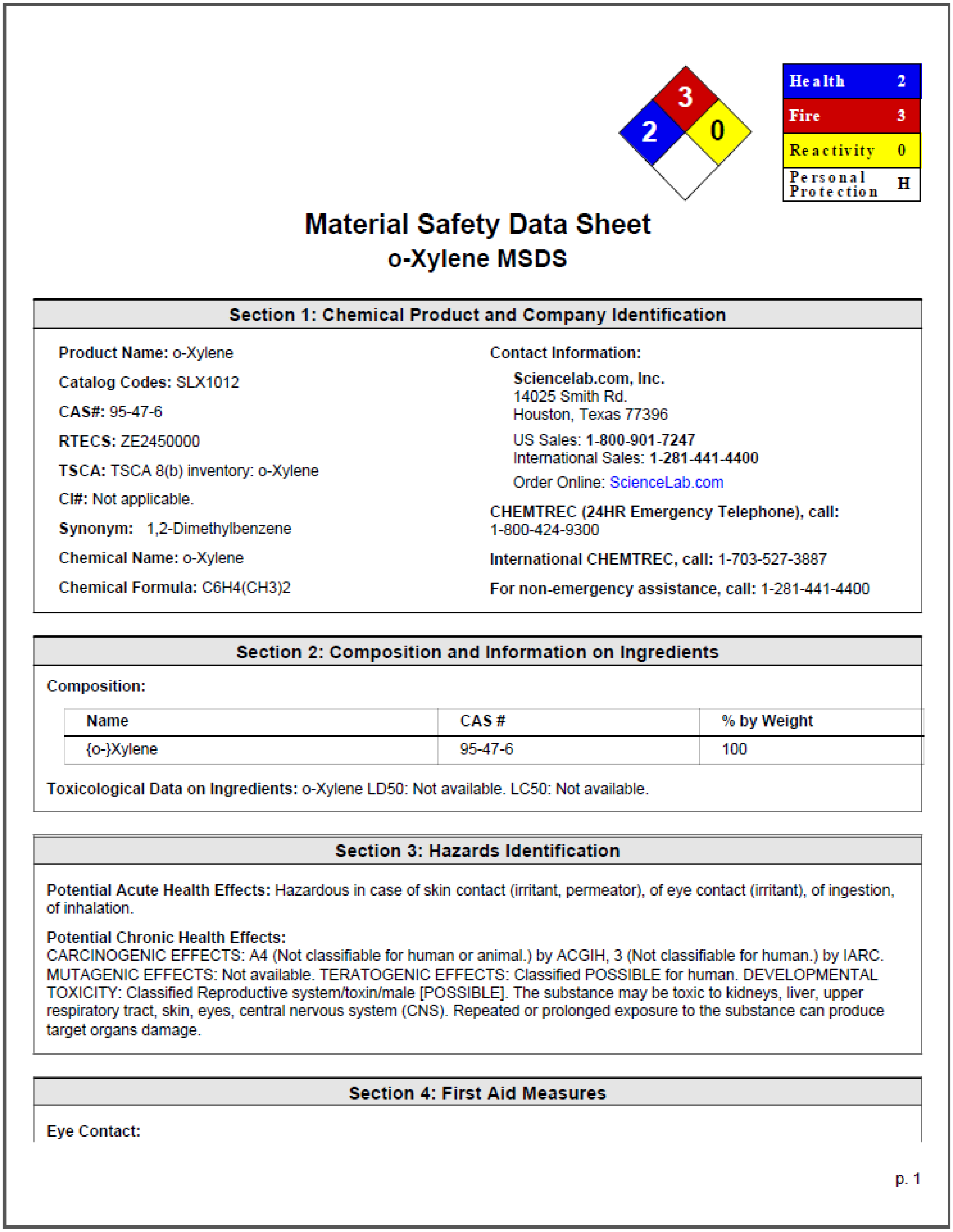


Health	2
Fire	3
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
o-Xylene MSDS

Section 1: Chemical Product and Company Identification

Product Name: o-Xylene

Catalog Codes: SLX1012

CAS#: 95-47-6

RTECS: ZE2450000

TSCA: TSCA 8(b) inventory: o-Xylene

CI#: Not applicable.

Synonym: 1,2-Dimethylbenzene

Chemical Name: o-Xylene

Chemical Formula: $C_6H_4(CH_3)_2$

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
{o-}Xylene	95-47-6	100

Toxicological Data on Ingredients: o-Xylene LD50: Not available. LC50: Not available.

Section 3: Hazards Identification

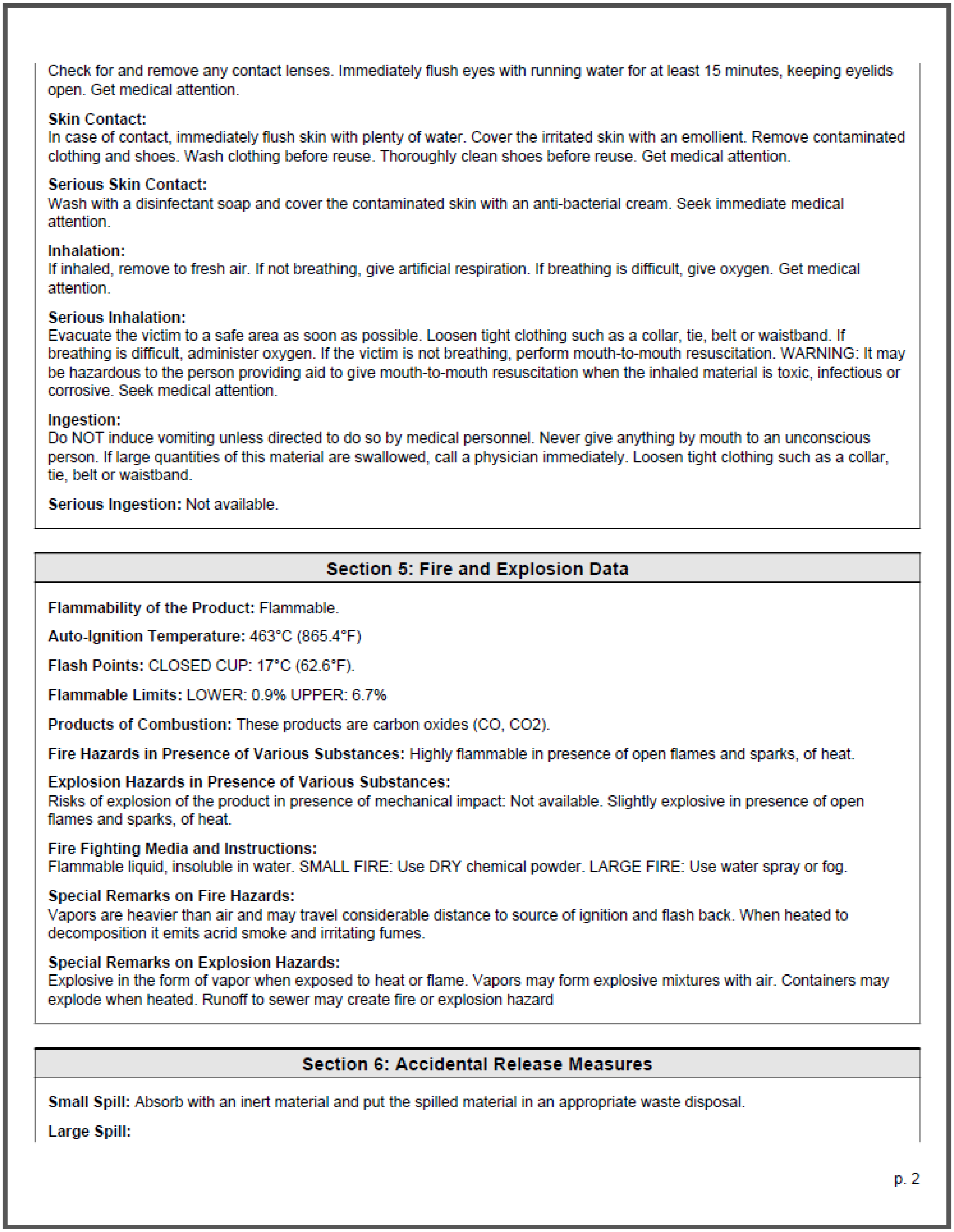
Potential Acute Health Effects: Hazardous in case of skin contact (irritant, permeator), of eye contact (irritant), of ingestion, of inhalation.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Classified POSSIBLE for human. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/male [POSSIBLE]. The substance may be toxic to kidneys, liver, upper respiratory tract, skin, eyes, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:

p. 1



Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Get medical attention.

Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 463°C (865.4°F)

Flash Points: CLOSED CUP: 17°C (62.6°F).

Flammable Limits: LOWER: 0.9% UPPER: 6.7%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Highly flammable in presence of open flames and sparks, of heat.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Slightly explosive in presence of open flames and sparks, of heat.

Fire Fighting Media and Instructions:
Flammable liquid, insoluble in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray or fog.

Special Remarks on Fire Hazards:
Vapors are heavier than air and may travel considerable distance to source of ignition and flash back. When heated to decomposition it emits acrid smoke and irritating fumes.

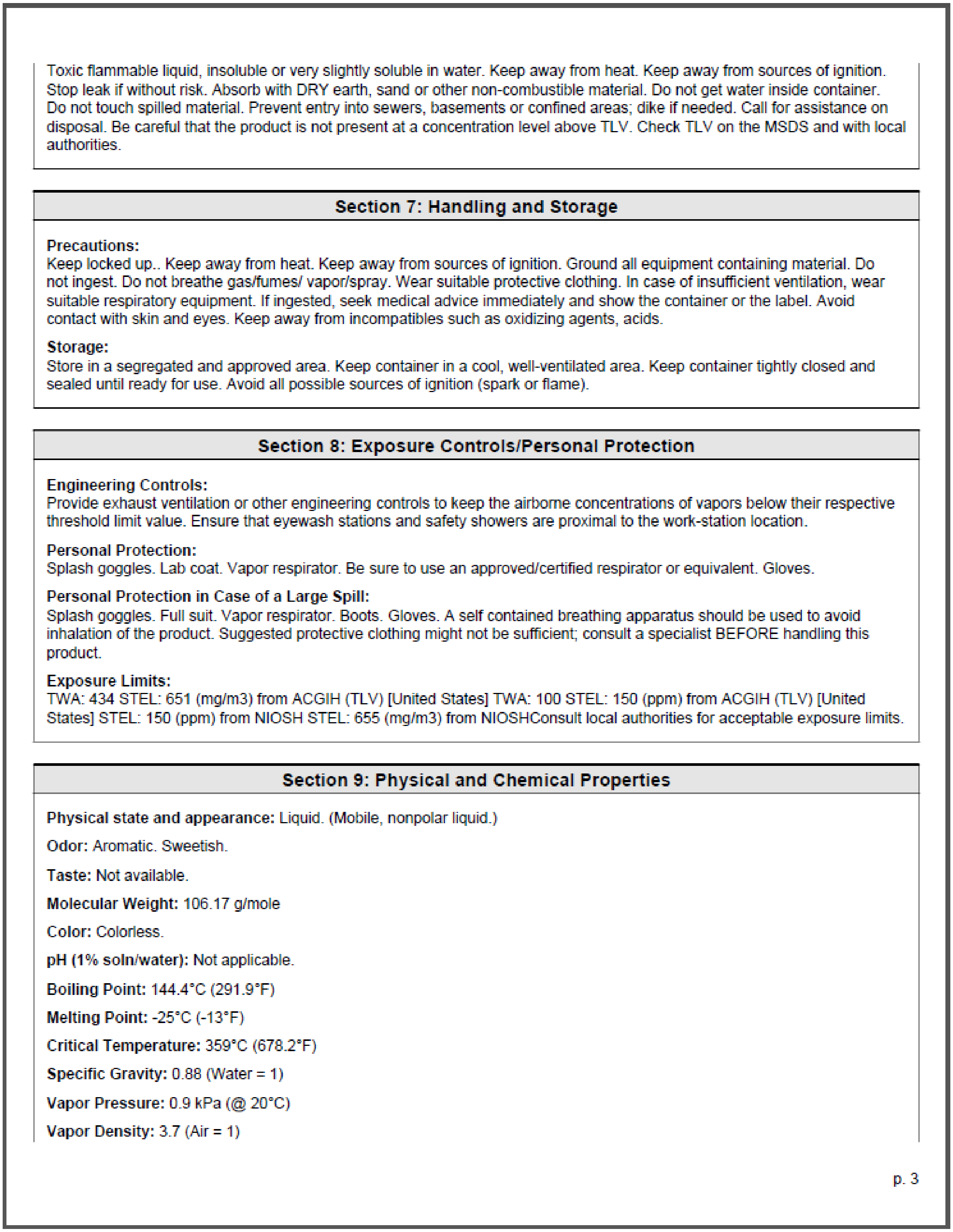
Special Remarks on Explosion Hazards:
Explosive in the form of vapor when exposed to heat or flame. Vapors may form explosive mixtures with air. Containers may explode when heated. Runoff to sewer may create fire or explosion hazard

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:

p. 2



Toxic flammable liquid, insoluble or very slightly soluble in water. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up.. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, acids.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 434 STEL: 651 (mg/m3) from ACGIH (TLV) [United States] TWA: 100 STEL: 150 (ppm) from ACGIH (TLV) [United States] STEL: 150 (ppm) from NIOSH STEL: 655 (mg/m3) from NIOSHConsult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Mobile, nonpolar liquid.)

Odor: Aromatic. Sweetish.

Taste: Not available.

Molecular Weight: 106.17 g/mole

Color: Colorless.

pH (1% soln/water): Not applicable.

Boiling Point: 144.4°C (291.9°F)

Melting Point: -25°C (-13°F)

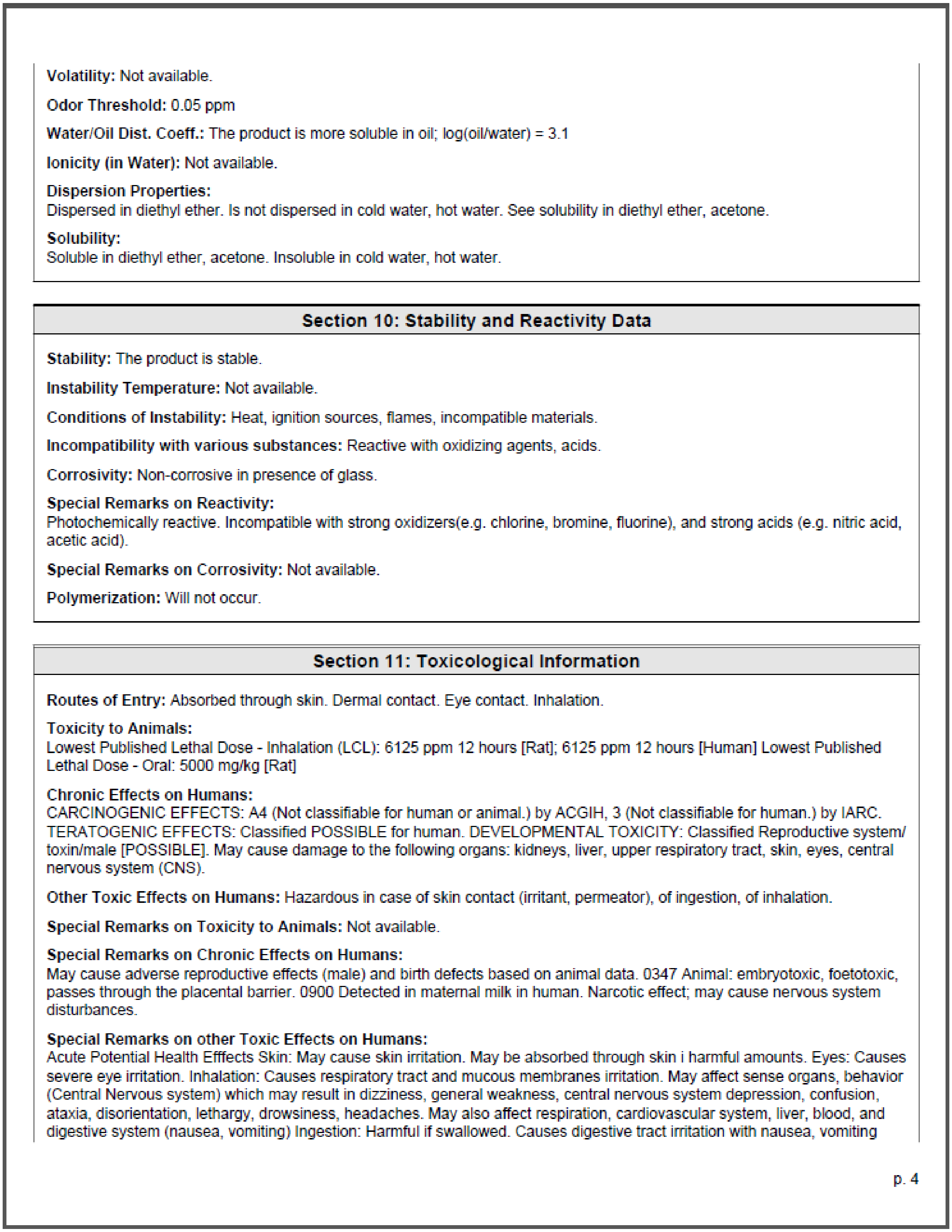
Critical Temperature: 359°C (678.2°F)

Specific Gravity: 0.88 (Water = 1)

Vapor Pressure: 0.9 kPa (@ 20°C)

Vapor Density: 3.7 (Air = 1)

p. 3



Volatility: Not available.

Odor Threshold: 0.05 ppm

Water/Oil Dist. Coeff.: The product is more soluble in oil; log(oil/water) = 3.1

Ionicity (in Water): Not available.

Dispersion Properties:
Dispersed in diethyl ether. Is not dispersed in cold water, hot water. See solubility in diethyl ether, acetone.

Solubility:
Soluble in diethyl ether, acetone. Insoluble in cold water, hot water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Heat, ignition sources, flames, incompatible materials.

Incompatibility with various substances: Reactive with oxidizing agents, acids.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Photochemically reactive. Incompatible with strong oxidizers(e.g. chlorine, bromine, fluorine), and strong acids (e.g. nitric acid, acetic acid).

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation.

Toxicity to Animals:
Lowest Published Lethal Dose - Inhalation (LCL): 6125 ppm 12 hours [Rat]; 6125 ppm 12 hours [Human] Lowest Published Lethal Dose - Oral: 5000 mg/kg [Rat]

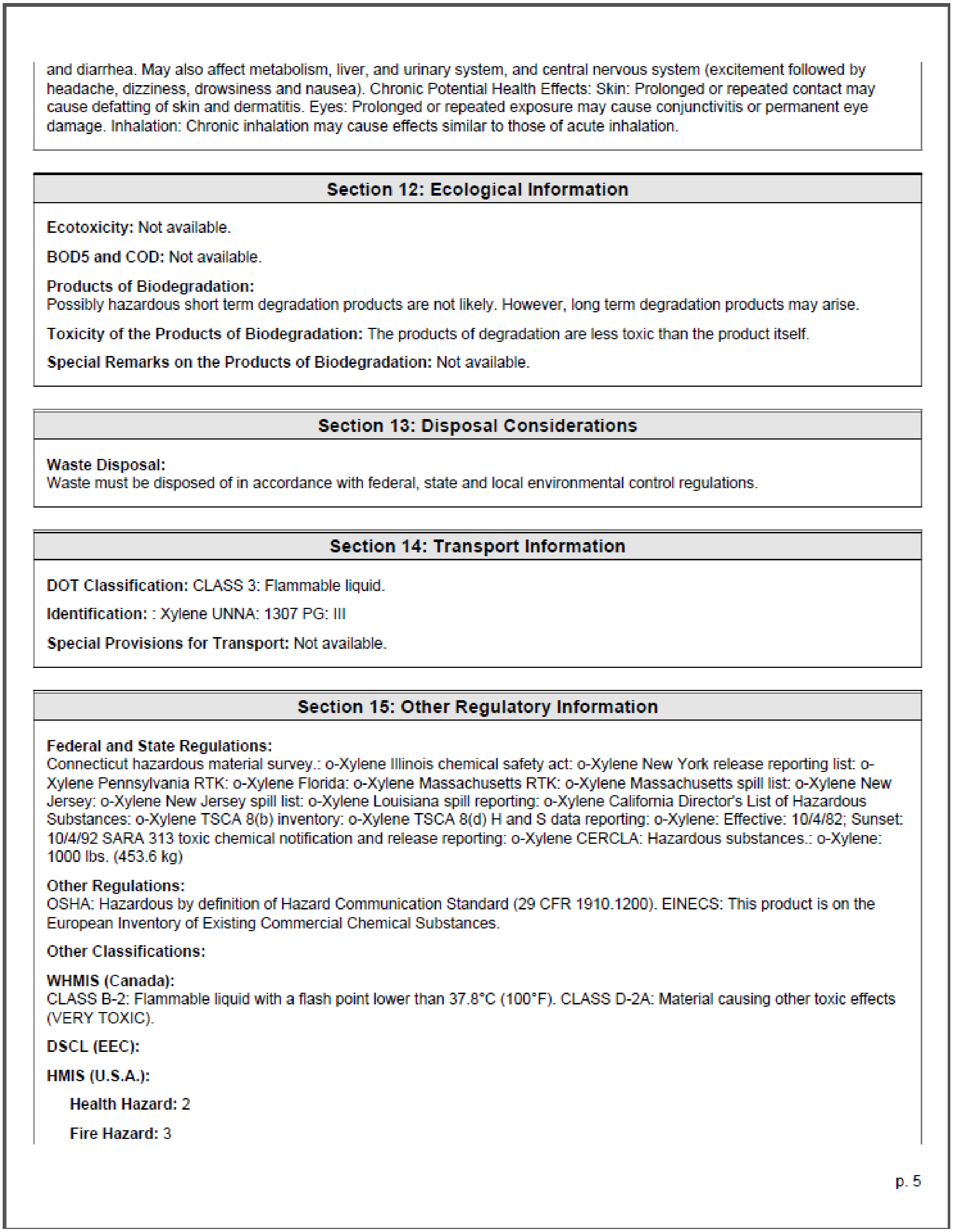
Chronic Effects on Humans:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. TERATOGENIC EFFECTS: Classified POSSIBLE for human. DEVELOPMENTAL TOXICITY: Classified Reproductive system/ toxin/male [POSSIBLE]. May cause damage to the following organs: kidneys, liver, upper respiratory tract, skin, eyes, central nervous system (CNS).

Other Toxic Effects on Humans: Hazardous in case of skin contact (irritant, permeator), of ingestion, of inhalation.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects (male) and birth defects based on animal data. 0347 Animal: embryotoxic, foetotoxic, passes through the placental barrier. 0900 Detected in maternal milk in human. Narcotic effect; may cause nervous system disturbances.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Efffects Skin: May cause skin irritation. May be absorbed through skin i harmful amounts. Eyes: Causes severe eye irritation. Inhalation: Causes respiratory tract and mucous membranes irritation. May affect sense organs, behavior (Central Nervous system) which may result in dizziness, general weakness, central nervous system depression, confusion, ataxia, disorientation, lethargy, drowsiness, headaches. May also affect respiration, cardiovascular system, liver, blood, and digestive system (nausea, vomiting) Ingestion: Harmful if swallowed. Causes digestive tract irritation with nausea, vomiting



and diarrhea. May also affect metabolism, liver, and urinary system, and central nervous system (excitement followed by headache, dizziness, drowsiness and nausea). Chronic Potential Health Effects: Skin: Prolonged or repeated contact may cause defatting of skin and dermatitis. Eyes: Prolonged or repeated exposure may cause conjunctivitis or permanent eye damage. Inhalation: Chronic inhalation may cause effects similar to those of acute inhalation.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 3: Flammable liquid.

Identification: : Xylene UNNA: 1307 PG: III

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Connecticut hazardous material survey.: o-Xylene Illinois chemical safety act: o-Xylene New York release reporting list: o-Xylene Pennsylvania RTK: o-Xylene Florida: o-Xylene Massachusetts RTK: o-Xylene Massachusetts spill list: o-Xylene New Jersey: o-Xylene New Jersey spill list: o-Xylene Louisiana spill reporting: o-Xylene California Director's List of Hazardous Substances: o-Xylene TSCA 8(b) inventory: o-Xylene TSCA 8(d) H and S data reporting: o-Xylene: Effective: 10/4/82; Sunset: 10/4/92 SARA 313 toxic chemical notification and release reporting: o-Xylene CERCLA: Hazardous substances.: o-Xylene: 1000 lbs. (453.6 kg)

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

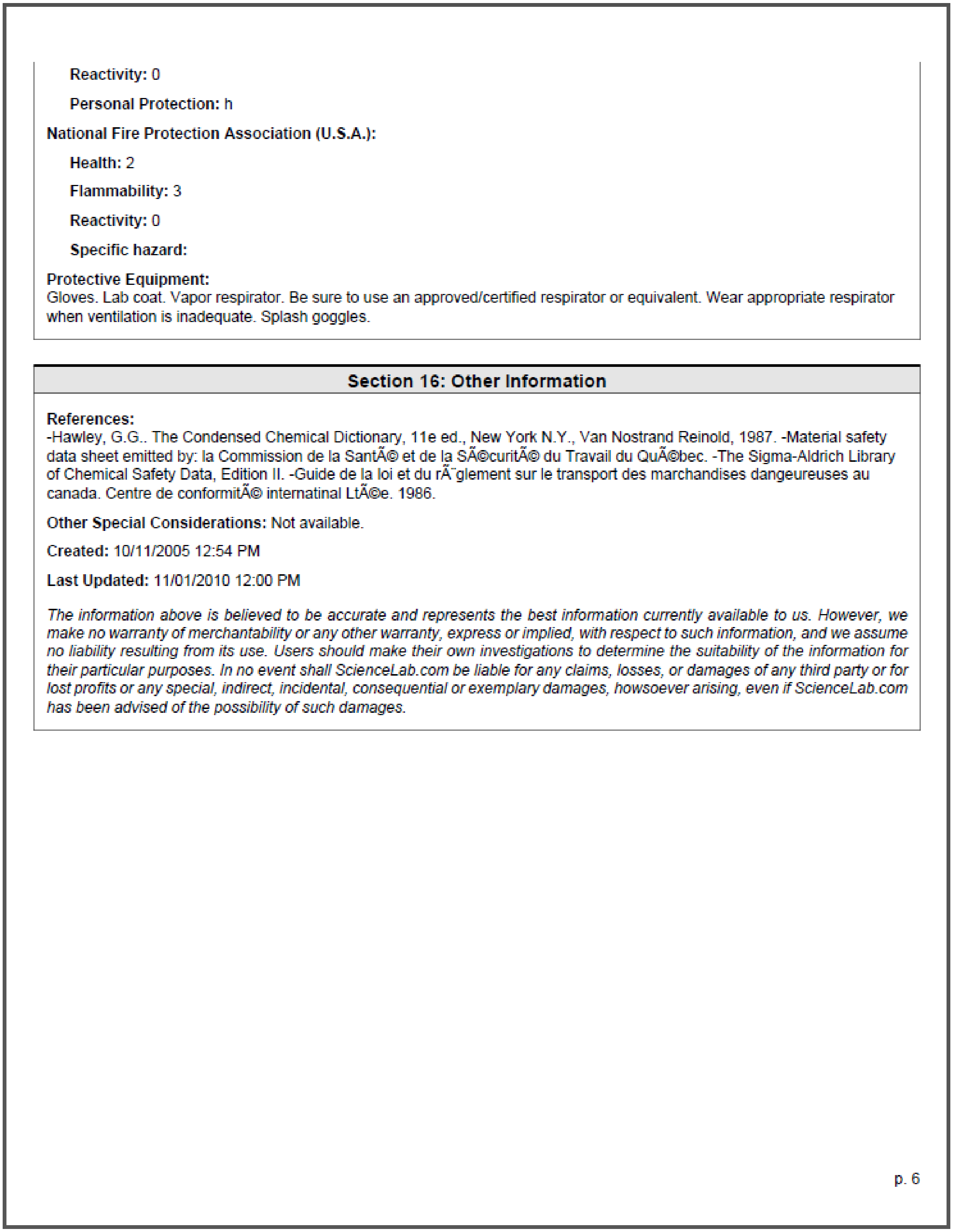
WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2A: Material causing other toxic effects (VERY TOXIC).

DSCL (EEC):

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3



Reactivity: 0

Personal Protection: h

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 3

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References:
-Hawley, G.G.. The Condensed Chemical Dictionary, 11e ed., New York N.Y., Van Nostrand Reinold, 1987. -Material safety data sheet emitted by: la Commission de la SantÃ© et de la SÃ©curitÃ© du Travail du QuÃ©bec. -The Sigma-Aldrich Library of Chemical Safety Data, Edition II. -Guide de la loi et du rÃ¨glement sur le transport des marchandises dangeureuses au canada. Centre de conformitÃ© internatinal LtÃ©e. 1986.

Other Special Considerations: Not available.

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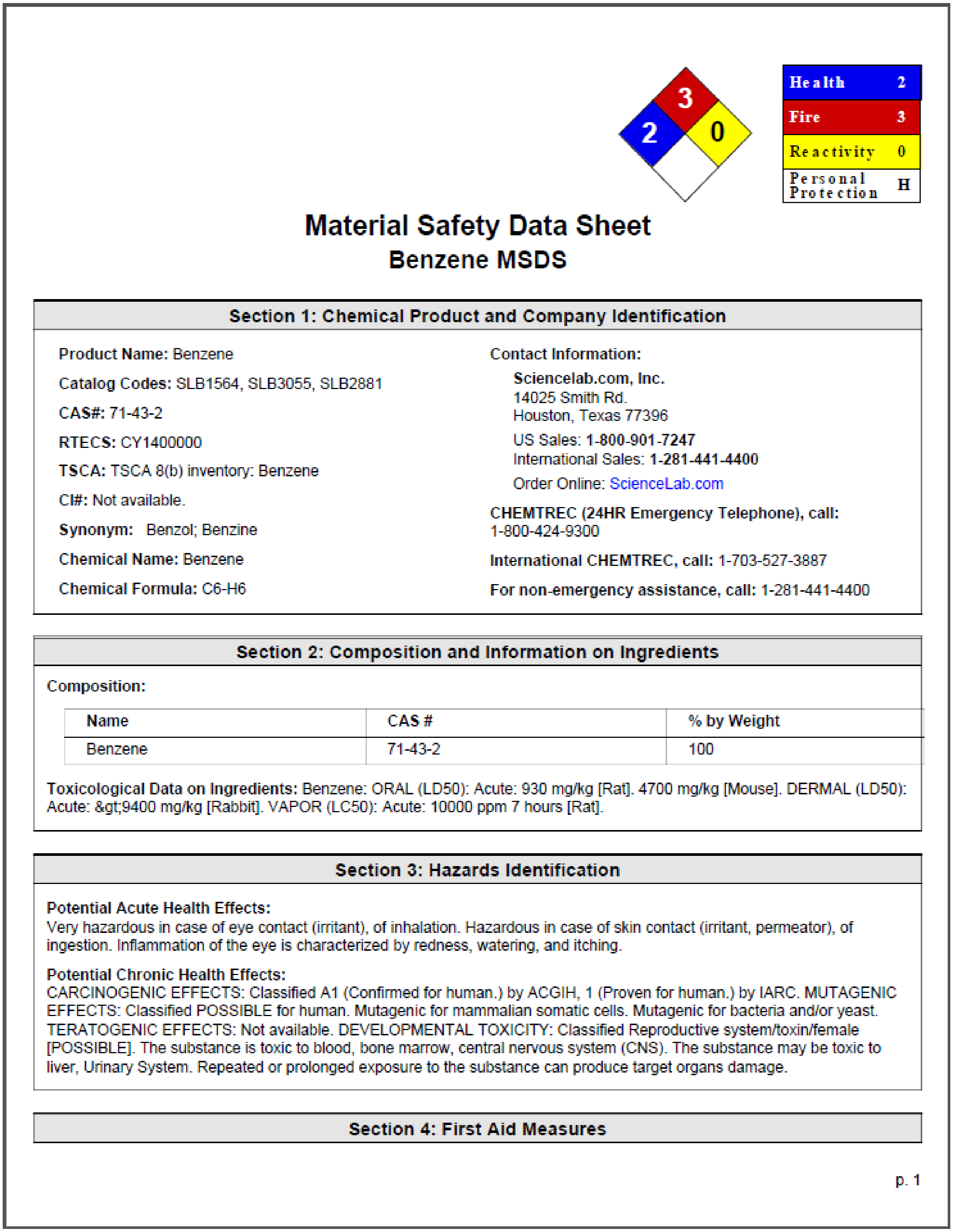

Health	2
Fire	3
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
Benzene MSDS

Section 1: Chemical Product and Company Identification

Product Name: Benzene

Catalog Codes: SLB1564, SLB3055, SLB2881

CAS#: 71-43-2

RTECS: CY1400000

TSCA: TSCA 8(b) inventory: Benzene

CI#: Not available.

Synonym: Benzol; Benzine

Chemical Name: Benzene

Chemical Formula: C6-H6

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Benzene	71-43-2	100

Toxicological Data on Ingredients: Benzene: ORAL (LD50): Acute: 930 mg/kg [Rat]. 4700 mg/kg [Mouse]. DERMAL (LD50): Acute: >9400 mg/kg [Rabbit]. VAPOR (LC50): Acute: 10000 ppm 7 hours [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of eye contact (irritant), of inhalation. Hazardous in case of skin contact (irritant, permeator), of ingestion. Inflammation of the eye is characterized by redness, watering, and itching.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Classified A1 (Confirmed for human.) by ACGIH, 1 (Proven for human.) by IARC. MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female [POSSIBLE]. The substance is toxic to blood, bone marrow, central nervous system (CNS). The substance may be toxic to liver, Urinary System. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

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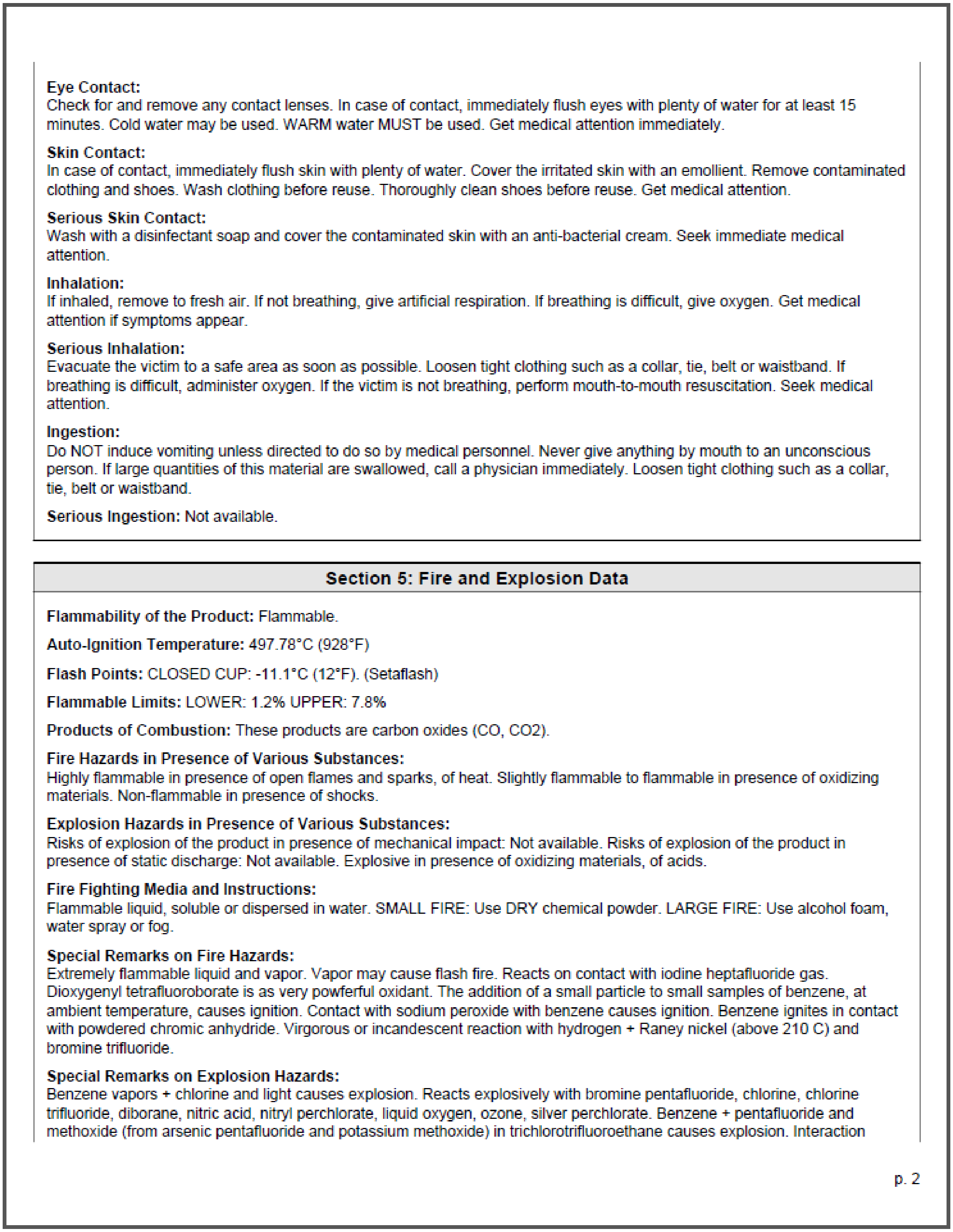


Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. WARM water MUST be used. Get medical attention immediately.

Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention if symptoms appear.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 497.78°C (928°F)

Flash Points: CLOSED CUP: -11.1°C (12°F). (Setaflash)

Flammable Limits: LOWER: 1.2% UPPER: 7.8%

Products of Combustion: These products are carbon oxides (CO, CO2).

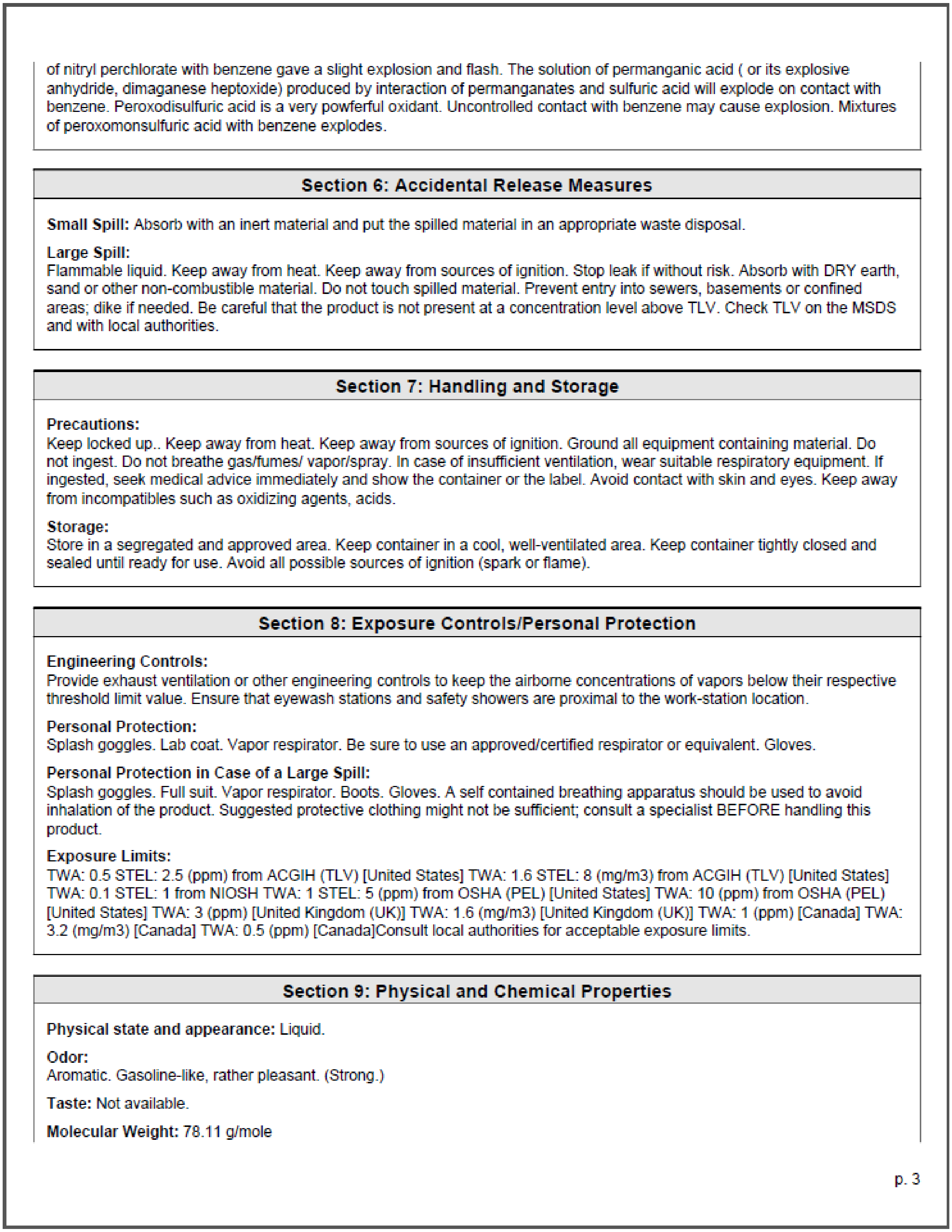
Fire Hazards in Presence of Various Substances:
Highly flammable in presence of open flames and sparks, of heat. Slightly flammable to flammable in presence of oxidizing materials. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available. Explosive in presence of oxidizing materials, of acids.

Fire Fighting Media and Instructions:
Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog.

Special Remarks on Fire Hazards:
Extremely flammable liquid and vapor. Vapor may cause flash fire. Reacts on contact with iodine heptafluoride gas. Dioxygenyl tetrafluoroborate is as very powferful oxidant. The addition of a small particle to small samples of benzene, at ambient temperature, causes ignition. Contact with sodium peroxide with benzene causes ignition. Benzene ignites in contact with powdered chromic anhydride. Virgorous or incandescent reaction with hydrogen + Raney nickel (above 210 C) and bromine trifluoride.

Special Remarks on Explosion Hazards:
Benzene vapors + chlorine and light causes explosion. Reacts explosively with bromine pentafluoride, chlorine, chlorine trifluoride, diborane, nitric acid, nitryl perchlorate, liquid oxygen, ozone, silver perchlorate. Benzene + pentafluoride and methoxide (from arsenic pentafluoride and potassium methoxide) in trichlorotrifluoroethane causes explosion. Interaction



of nitryl perchlorate with benzene gave a slight explosion and flash. The solution of permanganic acid (or its explosive anhydride, dimaganese heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene. Peroxodisulfuric acid is a very powfeful oxidant. Uncontrolled contact with benzene may cause explosion. Mixtures of peroxomonsulfuric acid with benzene explodes.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:
Flammable liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up.. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, acids.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 0.5 STEL: 2.5 (ppm) from ACGIH (TLV) [United States] TWA: 1.6 STEL: 8 (mg/m3) from ACGIH (TLV) [United States] TWA: 0.1 STEL: 1 from NIOSH TWA: 1 STEL: 5 (ppm) from OSHA (PEL) [United States] TWA: 10 (ppm) from OSHA (PEL) [United States] TWA: 3 (ppm) [United Kingdom (UK)] TWA: 1.6 (mg/m3) [United Kingdom (UK)] TWA: 1 (ppm) [Canada] TWA: 3.2 (mg/m3) [Canada] TWA: 0.5 (ppm) [Canada]Consult local authorities for acceptable exposure limits.

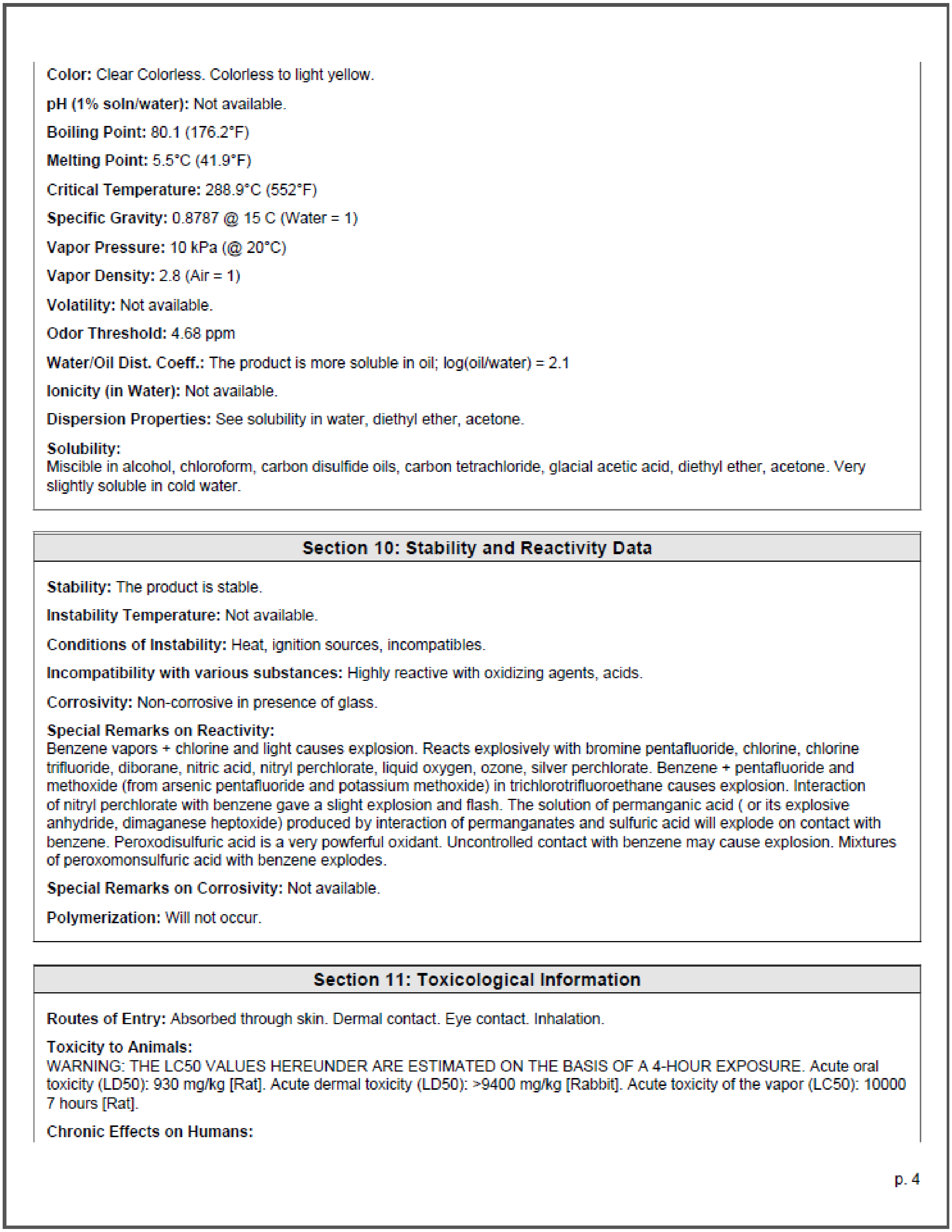
Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor:
Aromatic. Gasoline-like, rather pleasant. (Strong.)

Taste: Not available.

Molecular Weight: 78.11 g/mole



Color: Clear Colorless. Colorless to light yellow.

pH (1% soln/water): Not available.

Boiling Point: 80.1 (176.2°F)

Melting Point: 5.5°C (41.9°F)

Critical Temperature: 288.9°C (552°F)

Specific Gravity: 0.8787 @ 15 C (Water = 1)

Vapor Pressure: 10 kPa (@ 20°C)

Vapor Density: 2.8 (Air = 1)

Volatility: Not available.

Odor Threshold: 4.68 ppm

Water/Oil Dist. Coeff.: The product is more soluble in oil; log(oil/water) = 2.1

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, diethyl ether, acetone.

Solubility:
Miscible in alcohol, chloroform, carbon disulfide oils, carbon tetrachloride, glacial acetic acid, diethyl ether, acetone. Very slightly soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Heat, ignition sources, incompatibles.

Incompatibility with various substances: Highly reactive with oxidizing agents, acids.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Benzene vapors + chlorine and light causes explosion. Reacts explosively with bromine pentafluoride, chlorine, chlorine trifluoride, diborane, nitric acid, nitryl perchlorate, liquid oxygen, ozone, silver perchlorate. Benzene + pentafluoride and methoxide (from arsenic pentafluoride and potassium methoxide) in trichlorotrifluoroethane causes explosion. Interaction of nitryl perchlorate with benzene gave a slight explosion and flash. The solution of permanganic acid (or its explosive anhydride, dimaganese heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene. Peroxodisulfuric acid is a very powferful oxidant. Uncontrolled contact with benzene may cause explosion. Mixtures of peroxomonsulfuric acid with benzene explodes.

Special Remarks on Corrosivity: Not available.

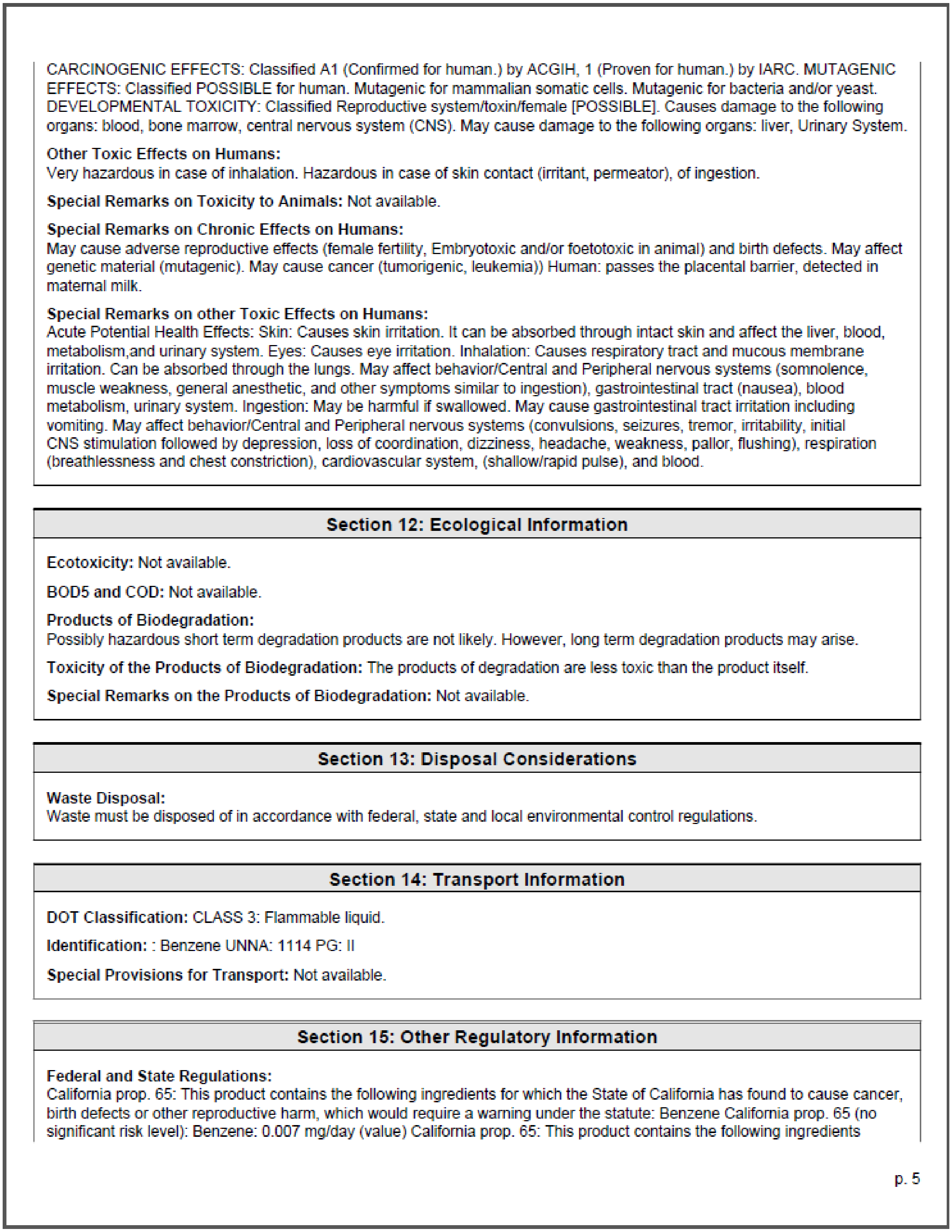
Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 930 mg/kg [Rat]. Acute dermal toxicity (LD50): >9400 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 10000 7 hours [Rat].

Chronic Effects on Humans:



CARCINOGENIC EFFECTS: Classified A1 (Confirmed for human.) by ACGIH, 1 (Proven for human.) by IARC. MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female [POSSIBLE]. Causes damage to the following organs: blood, bone marrow, central nervous system (CNS). May cause damage to the following organs: liver, Urinary System.

Other Toxic Effects on Humans:
Very hazardous in case of inhalation. Hazardous in case of skin contact (irritant, permeator), of ingestion.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects (female fertility, Embryotoxic and/or foetotoxic in animal) and birth defects. May affect genetic material (mutagenic). May cause cancer (tumorigenic, leukemia)) Human: passes the placental barrier, detected in maternal milk.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes skin irritation. It can be absorbed through intact skin and affect the liver, blood, metabolism,and urinary system. Eyes: Causes eye irritation. Inhalation: Causes respiratory tract and mucous membrane irritation. Can be absorbed through the lungs. May affect behavior/Central and Peripheral nervous systems (somnolence, muscle weakness, general anesthetic, and other symptoms similar to ingestion), gastrointestinal tract (nausea), blood metabolism, urinary system. Ingestion: May be harmful if swallowed. May cause gastrointestinal tract irritation including vomiting. May affect behavior/Central and Peripheral nervous systems (convulsions, seizures, tremor, irritability, initial CNS stimulation followed by depression, loss of coordination, dizziness, headache, weakness, pallor, flushing), respiration (breathlessness and chest constriction), cardiovascular system, (shallow/rapid pulse), and blood.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 3: Flammable liquid.

Identification: : Benzene UNNA: 1114 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer, birth defects or other reproductive harm, which would require a warning under the statute: Benzene California prop. 65 (no significant risk level): Benzene: 0.007 mg/day (value) California prop. 65: This product contains the following ingredients

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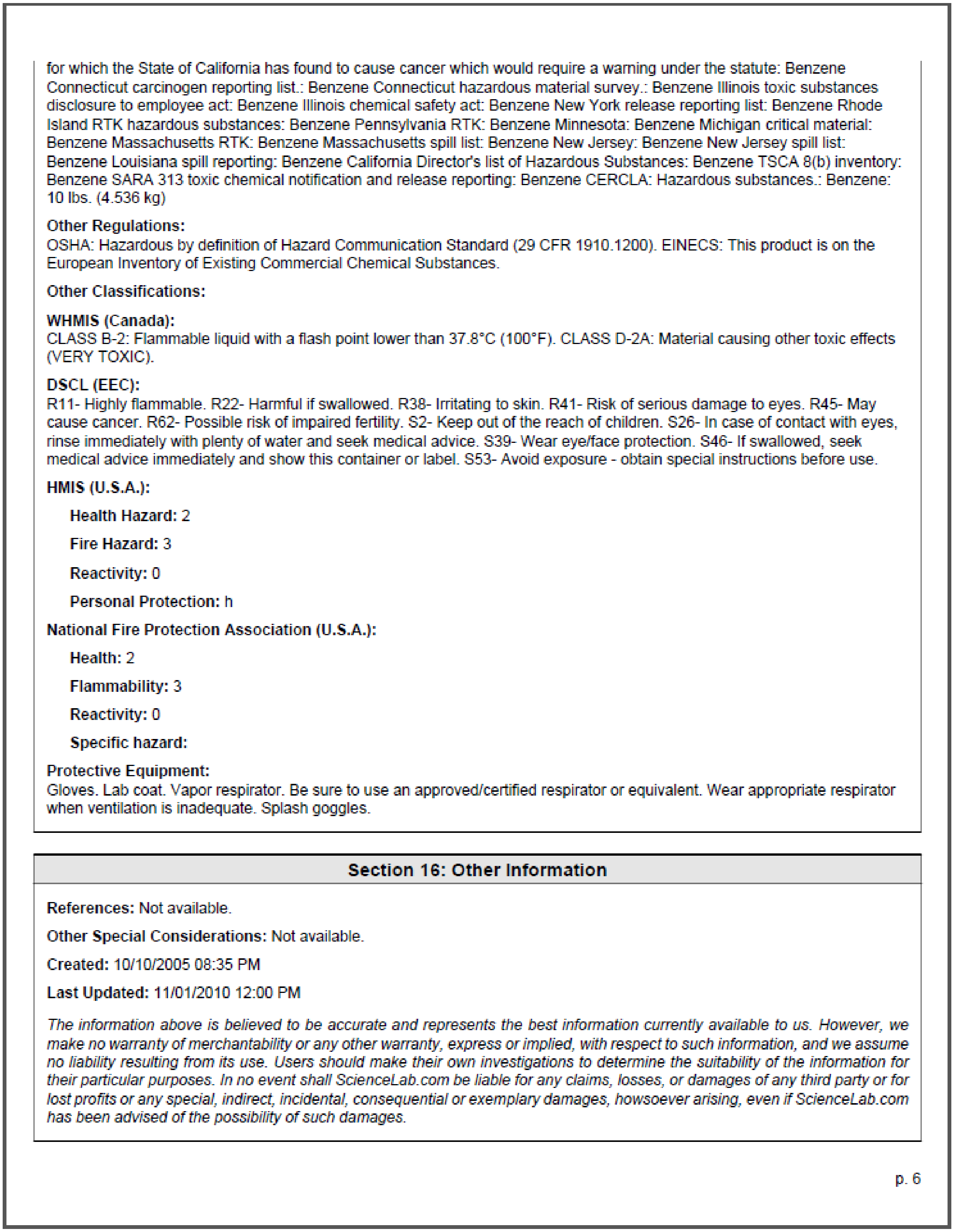

for which the State of California has found to cause cancer which would require a warning under the statute: Benzene Connecticut carcinogen reporting list.: Benzene Connecticut hazardous material survey.: Benzene Illinois toxic substances disclosure to employee act: Benzene Illinois chemical safety act: Benzene New York release reporting list: Benzene Rhode Island RTK hazardous substances: Benzene Pennsylvania RTK: Benzene Minnesota: Benzene Michigan critical material: Benzene Massachusetts RTK: Benzene Massachusetts spill list: Benzene New Jersey: Benzene New Jersey spill list: Benzene Louisiana spill reporting: Benzene California Director's list of Hazardous Substances: Benzene TSCA 8(b) inventory: Benzene SARA 313 toxic chemical notification and release reporting: Benzene CERCLA: Hazardous substances.: Benzene: 10 lbs. (4.536 kg)

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2A: Material causing other toxic effects (VERY TOXIC).

DSCL (EEC):
R11- Highly flammable. R22- Harmful if swallowed. R38- Irritating to skin. R41- Risk of serious damage to eyes. R45- May cause cancer. R62- Possible risk of impaired fertility. S2- Keep out of the reach of children. S26- In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. S39- Wear eye/face protection. S46- If swallowed, seek medical advice immediately and show this container or label. S53- Avoid exposure - obtain special instructions before use.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 3

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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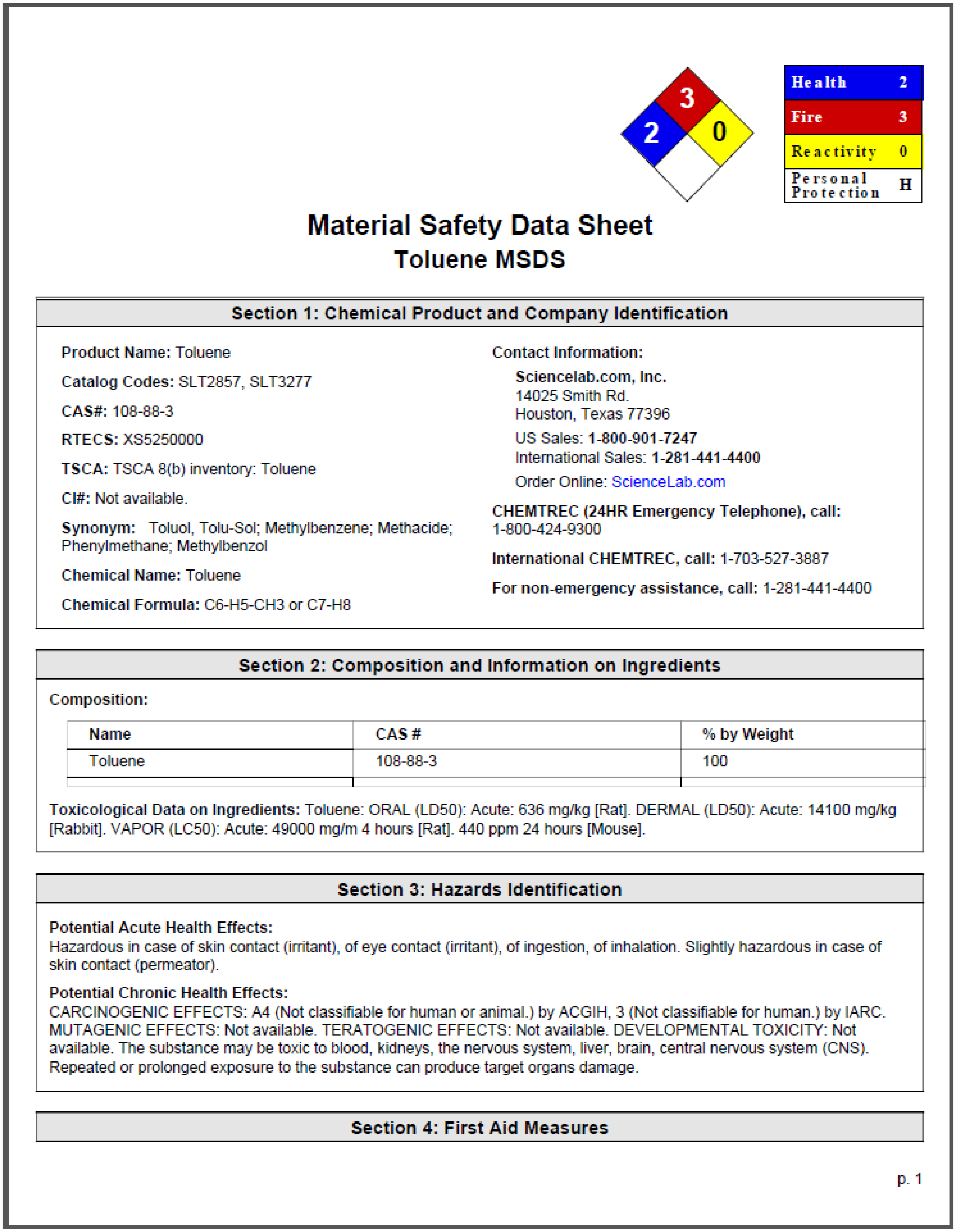

Health	2
Fire	3
Reactivity	0
Personal Protection	H

Material Safety Data Sheet

Toluene MSDS

Section 1: Chemical Product and Company Identification

Product Name: Toluene

Catalog Codes: SLT2857, SLT3277

CAS#: 108-88-3

RTECS: XS5250000

TSCA: TSCA 8(b) inventory: Toluene

CI#: Not available.

Synonym: Toluol, Tolu-Sol; Methylbenzene; Methacide; Phenylmethane; Methylbenzol

Chemical Name: Toluene

Chemical Formula: C6-H5-CH3 or C7-H8

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Toluene	108-88-3	100

Toxicological Data on Ingredients: Toluene: ORAL (LD50): Acute: 636 mg/kg [Rat]. DERMAL (LD50): Acute: 14100 mg/kg [Rabbit]. VAPOR (LC50): Acute: 49000 mg/m 4 hours [Rat]. 440 ppm 24 hours [Mouse].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (permeator).

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to blood, kidneys, the nervous system, liver, brain, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

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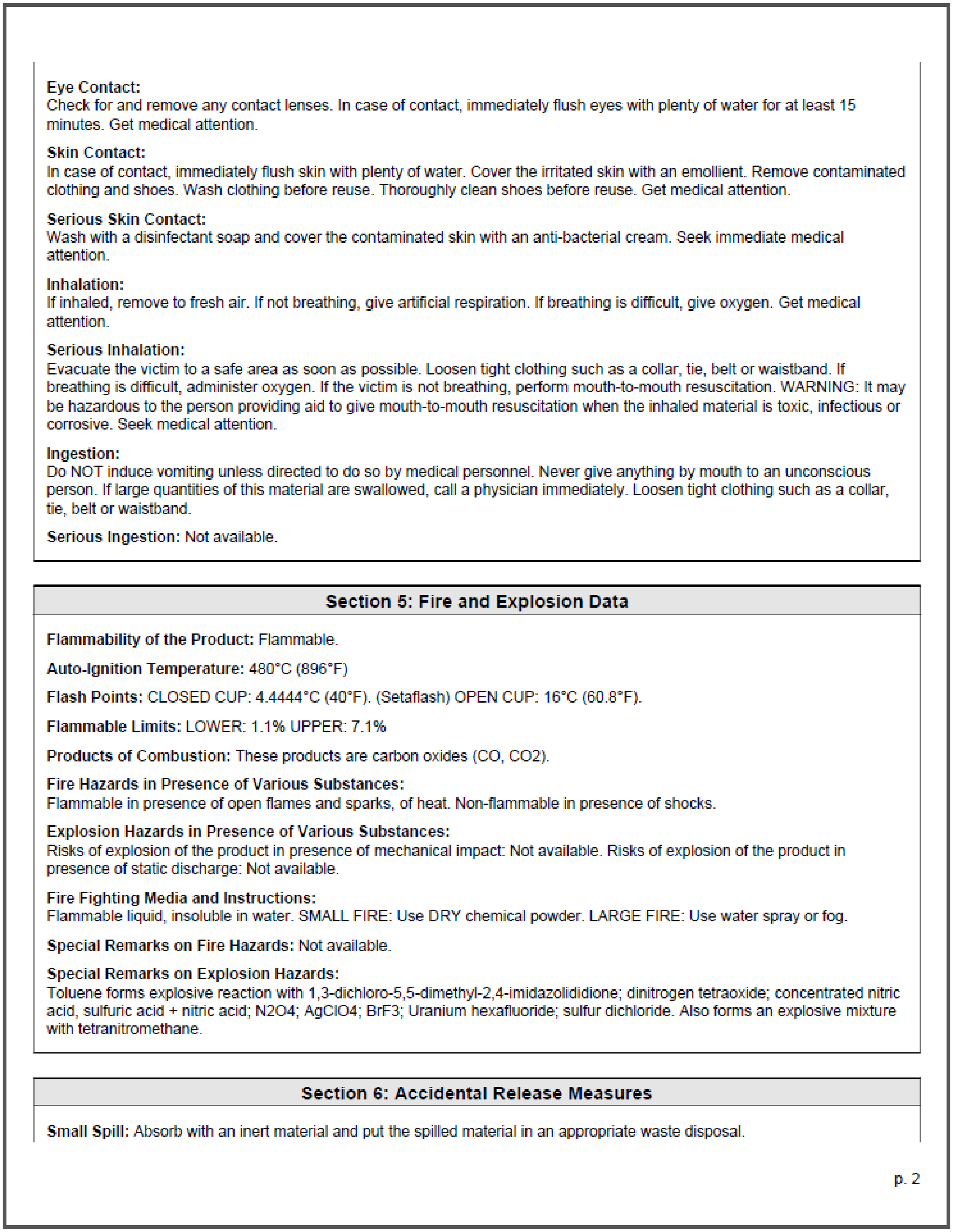


Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Get medical attention.

Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 480°C (896°F)

Flash Points: CLOSED CUP: 4.4444°C (40°F). (Setaflash) OPEN CUP: 16°C (60.8°F).

Flammable Limits: LOWER: 1.1% UPPER: 7.1%

Products of Combustion: These products are carbon oxides (CO, CO_2).

Fire Hazards in Presence of Various Substances:
Flammable in presence of open flames and sparks, of heat. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

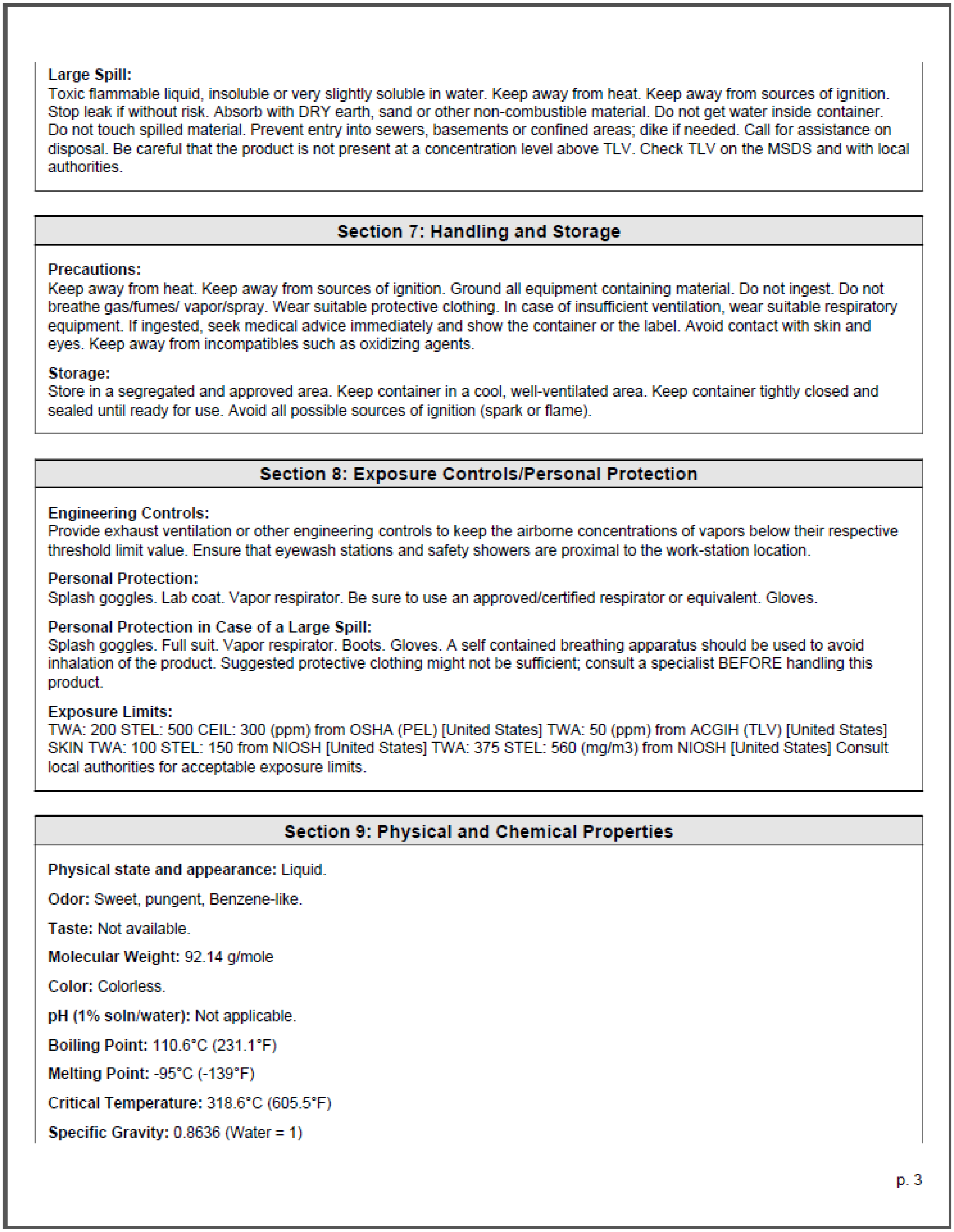
Fire Fighting Media and Instructions:
Flammable liquid, insoluble in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray or fog.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards:
Toluene forms explosive reaction with 1,3-dichloro-5,5-dimethyl-2,4-imidazolididione; dinitrogen tetraoxide; concentrated nitric acid, sulfuric acid + nitric acid; N_2O_4; $AgClO_4$; BrF_3; Uranium hexafluoride; sulfur dichloride. Also forms an explosive mixture with tetranitromethane.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.



Large Spill:
Toxic flammable liquid, insoluble or very slightly soluble in water. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 200 STEL: 500 CEIL: 300 (ppm) from OSHA (PEL) [United States] TWA: 50 (ppm) from ACGIH (TLV) [United States] SKIN TWA: 100 STEL: 150 from NIOSH [United States] TWA: 375 STEL: 560 (mg/m3) from NIOSH [United States] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Sweet, pungent, Benzene-like.

Taste: Not available.

Molecular Weight: 92.14 g/mole

Color: Colorless.

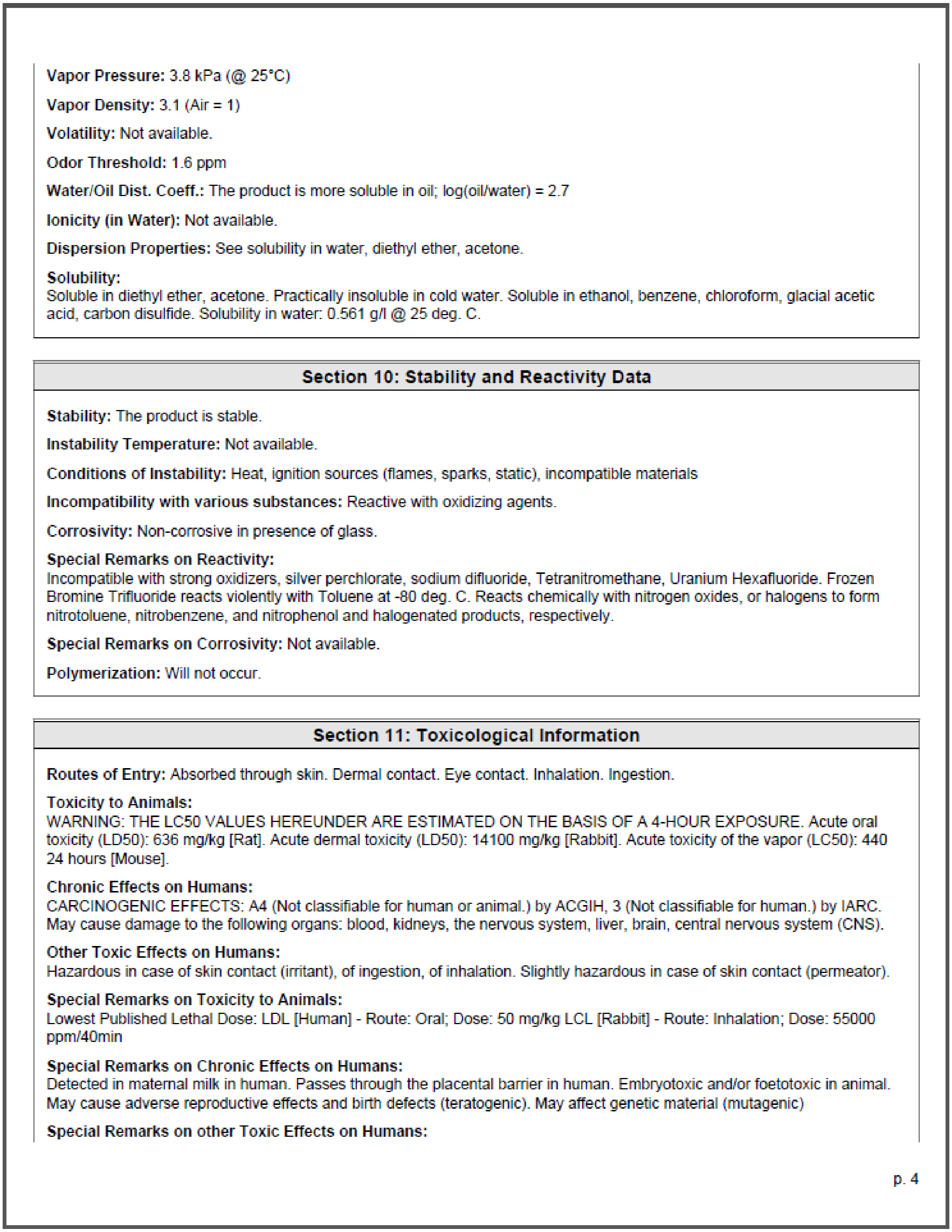
pH (1% soln/water): Not applicable.

Boiling Point: 110.6°C (231.1°F)

Melting Point: -95°C (-139°F)

Critical Temperature: 318.6°C (605.5°F)

Specific Gravity: 0.8636 (Water = 1)



Vapor Pressure: 3.8 kPa (@ 25°C)

Vapor Density: 3.1 (Air = 1)

Volatility: Not available.

Odor Threshold: 1.6 ppm

Water/Oil Dist. Coeff.: The product is more soluble in oil; log(oil/water) = 2.7

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, diethyl ether, acetone.

Solubility:
Soluble in diethyl ether, acetone. Practically insoluble in cold water. Soluble in ethanol, benzene, chloroform, glacial acetic acid, carbon disulfide. Solubility in water: 0.561 g/l @ 25 deg. C.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Heat, ignition sources (flames, sparks, static), incompatible materials

Incompatibility with various substances: Reactive with oxidizing agents.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Incompatible with strong oxidizers, silver perchlorate, sodium difluoride, Tetranitromethane, Uranium Hexafluoride. Frozen Bromine Trifluoride reacts violently with Toluene at -80 deg. C. Reacts chemically with nitrogen oxides, or halogens to form nitrotoluene, nitrobenzene, and nitrophenol and halogenated products, respectively.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 636 mg/kg [Rat]. Acute dermal toxicity (LD50): 14100 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 440 24 hours [Mouse].

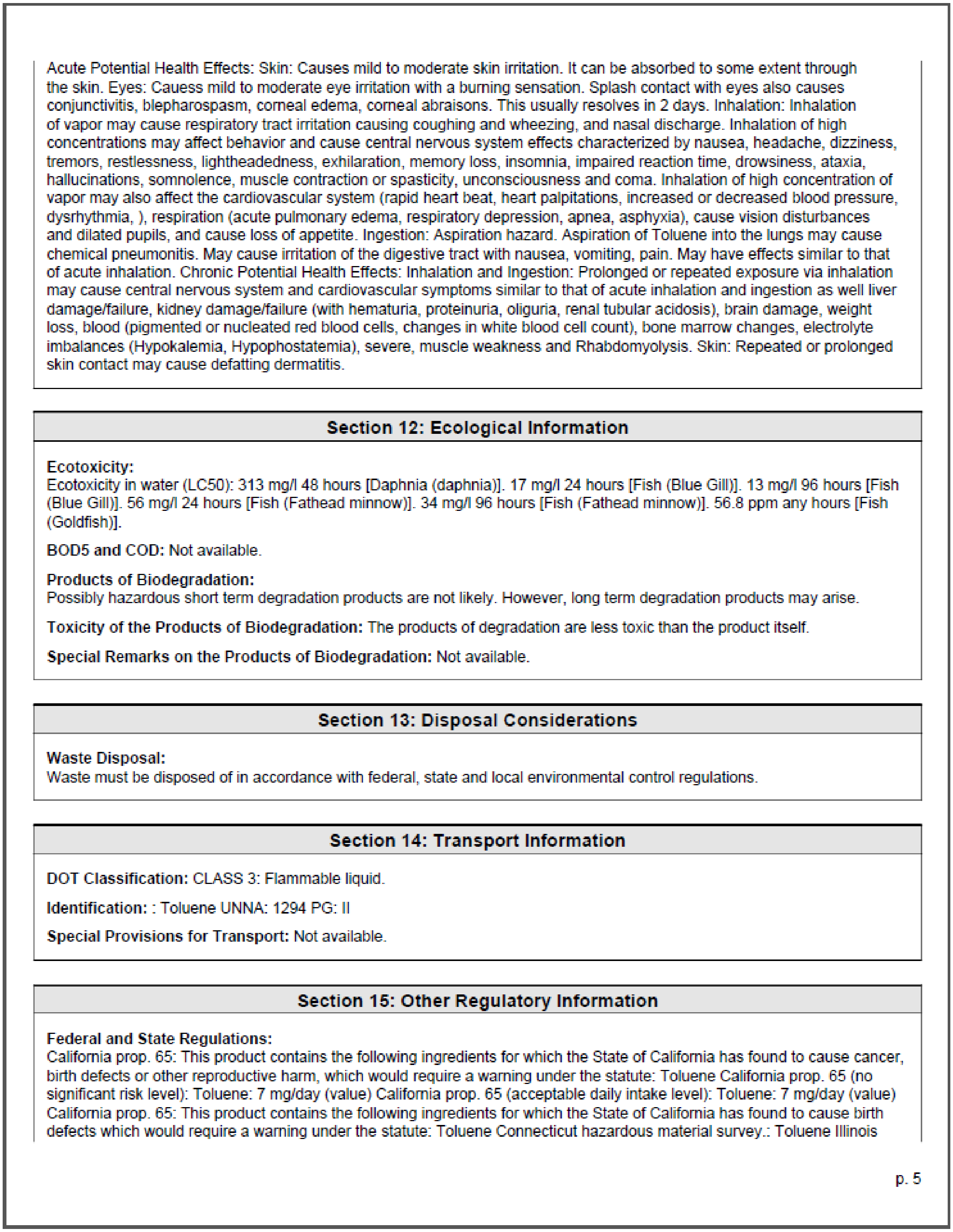
Chronic Effects on Humans:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. May cause damage to the following organs: blood, kidneys, the nervous system, liver, brain, central nervous system (CNS).

Other Toxic Effects on Humans:
Hazardous in case of skin contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (permeator).

Special Remarks on Toxicity to Animals:
Lowest Published Lethal Dose: LDL [Human] - Route: Oral; Dose: 50 mg/kg LCL [Rabbit] - Route: Inhalation; Dose: 55000 ppm/40min

Special Remarks on Chronic Effects on Humans:
Detected in maternal milk in human. Passes through the placental barrier in human. Embryotoxic and/or foetotoxic in animal. May cause adverse reproductive effects and birth defects (teratogenic). May affect genetic material (mutagenic)

Special Remarks on other Toxic Effects on Humans:



Acute Potential Health Effects: Skin: Causes mild to moderate skin irritation. It can be absorbed to some extent through the skin. Eyes: Cauess mild to moderate eye irritation with a burning sensation. Splash contact with eyes also causes conjunctivitis, blepharospasm, corneal edema, corneal abraisons. This usually resolves in 2 days. Inhalation: Inhalation of vapor may cause respiratory tract irritation causing coughing and wheezing, and nasal discharge. Inhalation of high concentrations may affect behavior and cause central nervous system effects characterized by nausea, headache, dizziness, tremors, restlessness, lightheadedness, exhilaration, memory loss, insomnia, impaired reaction time, drowsiness, ataxia, hallucinations, somnolence, muscle contraction or spasticity, unconsciousness and coma. Inhalation of high concentration of vapor may also affect the cardiovascular system (rapid heart beat, heart palpitations, increased or decreased blood pressure, dysrhythmia,), respiration (acute pulmonary edema, respiratory depression, apnea, asphyxia), cause vision disturbances and dilated pupils, and cause loss of appetite. Ingestion: Aspiration hazard. Aspiration of Toluene into the lungs may cause chemical pneumonitis. May cause irritation of the digestive tract with nausea, vomiting, pain. May have effects similar to that of acute inhalation. Chronic Potential Health Effects: Inhalation and Ingestion: Prolonged or repeated exposure via inhalation may cause central nervous system and cardiovascular symptoms similar to that of acute inhalation and ingestion as well liver damage/failure, kidney damage/failure (with hematuria, proteinuria, oliguria, renal tubular acidosis), brain damage, weight loss, blood (pigmented or nucleated red blood cells, changes in white blood cell count), bone marrow changes, electrolyte imbalances (Hypokalemia, Hypophostatemia), severe, muscle weakness and Rhabdomyolysis. Skin: Repeated or prolonged skin contact may cause defatting dermatitis.

Section 12: Ecological Information

Ecotoxicity:
Ecotoxicity in water (LC50): 313 mg/l 48 hours [Daphnia (daphnia)]. 17 mg/l 24 hours [Fish (Blue Gill)]. 13 mg/l 96 hours [Fish (Blue Gill)]. 56 mg/l 24 hours [Fish (Fathead minnow)]. 34 mg/l 96 hours [Fish (Fathead minnow)]. 56.8 ppm any hours [Fish (Goldfish)].

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

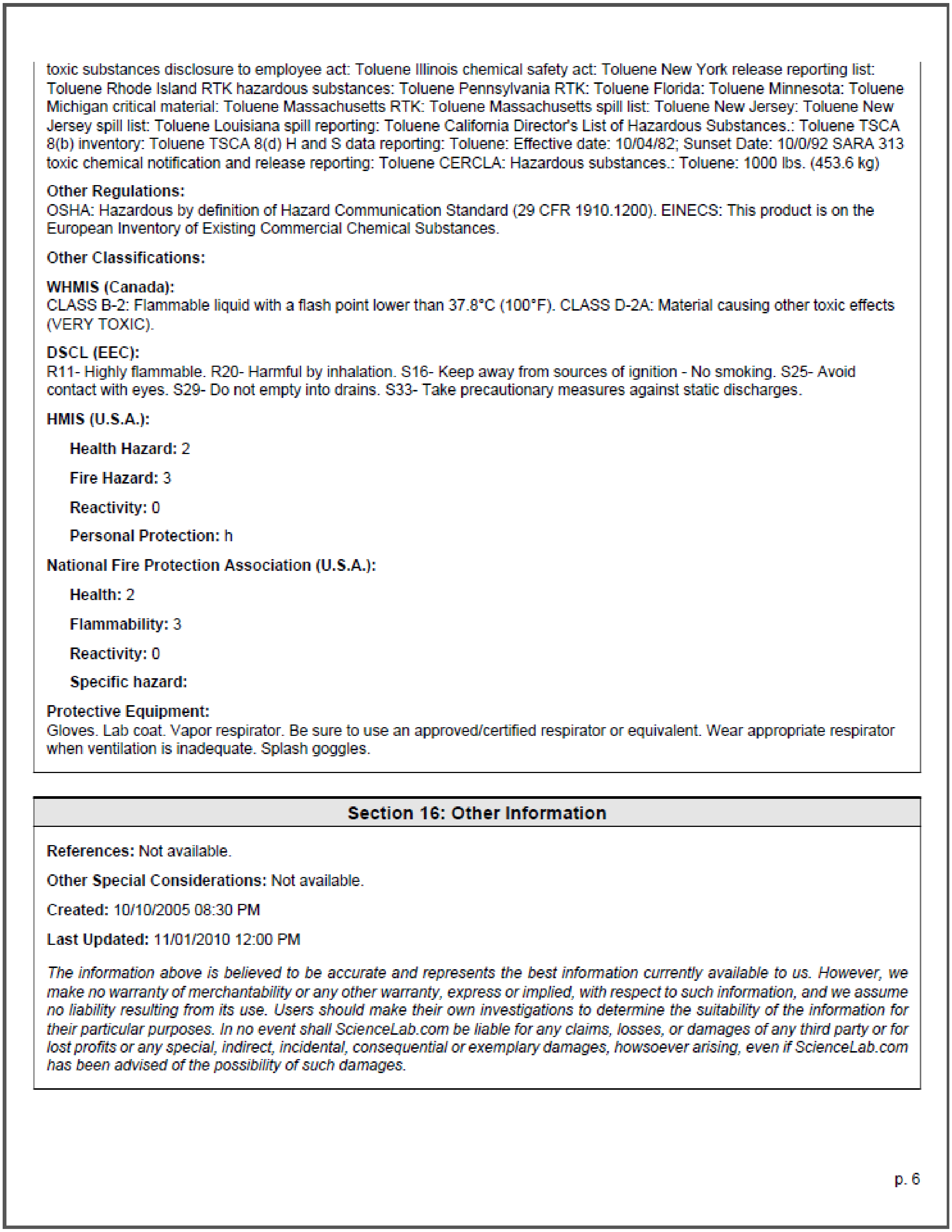
DOT Classification: CLASS 3: Flammable liquid.

Identification: : Toluene UNNA: 1294 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer, birth defects or other reproductive harm, which would require a warning under the statute: Toluene California prop. 65 (no significant risk level): Toluene: 7 mg/day (value) California prop. 65 (acceptable daily intake level): Toluene: 7 mg/day (value) California prop. 65: This product contains the following ingredients for which the State of California has found to cause birth defects which would require a warning under the statute: Toluene Connecticut hazardous material survey.: Toluene Illinois



toxic substances disclosure to employee act: Toluene Illinois chemical safety act: Toluene New York release reporting list: Toluene Rhode Island RTK hazardous substances: Toluene Pennsylvania RTK: Toluene Florida: Toluene Minnesota: Toluene Michigan critical material: Toluene Massachusetts RTK: Toluene Massachusetts spill list: Toluene New Jersey: Toluene New Jersey spill list: Toluene Louisiana spill reporting: Toluene California Director's List of Hazardous Substances.: Toluene TSCA 8(b) inventory: Toluene TSCA 8(d) H and S data reporting: Toluene: Effective date: 10/04/82; Sunset Date: 10/0/92 SARA 313 toxic chemical notification and release reporting: Toluene CERCLA: Hazardous substances.: Toluene: 1000 lbs. (453.6 kg)

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2A: Material causing other toxic effects (VERY TOXIC).

DSCL (EEC):
R11- Highly flammable. R20- Harmful by inhalation. S16- Keep away from sources of ignition - No smoking. S25- Avoid contact with eyes. S29- Do not empty into drains. S33- Take precautionary measures against static discharges.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 3

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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Last Updated: 11/01/2010 12:00 PM

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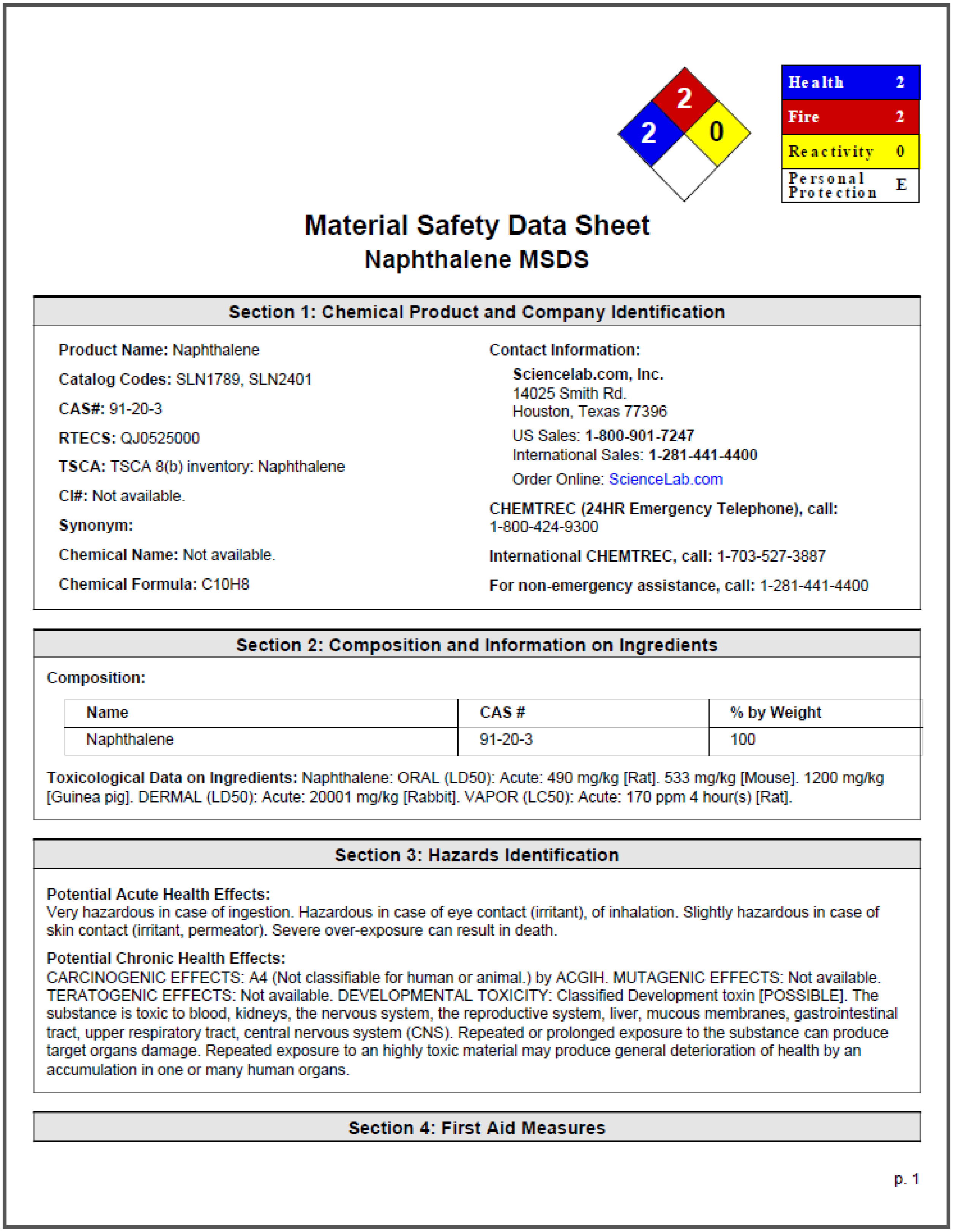

Health	2
Fire	2
Reactivity	0
Personal Protection	E

Material Safety Data Sheet
Naphthalene MSDS

Section 1: Chemical Product and Company Identification

Product Name: Naphthalene

Catalog Codes: SLN1789, SLN2401

CAS#: 91-20-3

RTECS: QJ0525000

TSCA: TSCA 8(b) inventory: Naphthalene

CI#: Not available.

Synonym:

Chemical Name: Not available.

Chemical Formula: C10H8

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Naphthalene	91-20-3	100

Toxicological Data on Ingredients: Naphthalene: ORAL (LD50): Acute: 490 mg/kg [Rat]. 533 mg/kg [Mouse]. 1200 mg/kg [Guinea pig]. DERMAL (LD50): Acute: 20001 mg/kg [Rabbit]. VAPOR (LC50): Acute: 170 ppm 4 hour(s) [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of ingestion. Hazardous in case of eye contact (irritant), of inhalation. Slightly hazardous in case of skin contact (irritant, permeator). Severe over-exposure can result in death.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Classified Development toxin [POSSIBLE]. The substance is toxic to blood, kidneys, the nervous system, the reproductive system, liver, mucous membranes, gastrointestinal tract, upper respiratory tract, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage. Repeated exposure to an highly toxic material may produce general deterioration of health by an accumulation in one or many human organs.

Section 4: First Aid Measures

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Eye Contact:
Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Do not use an eye ointment. Seek medical attention.

Skin Contact:
After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

Serious Skin Contact: Not available.

Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

Ingestion:
Do not induce vomiting. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 567°C (1052.6°F)

Flash Points: CLOSED CUP: 88°C (190.4°F). OPEN CUP: 79°C (174.2°F).

Flammable Limits: LOWER: 0.9% UPPER: 5.9%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Not available.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
Flammable solid. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

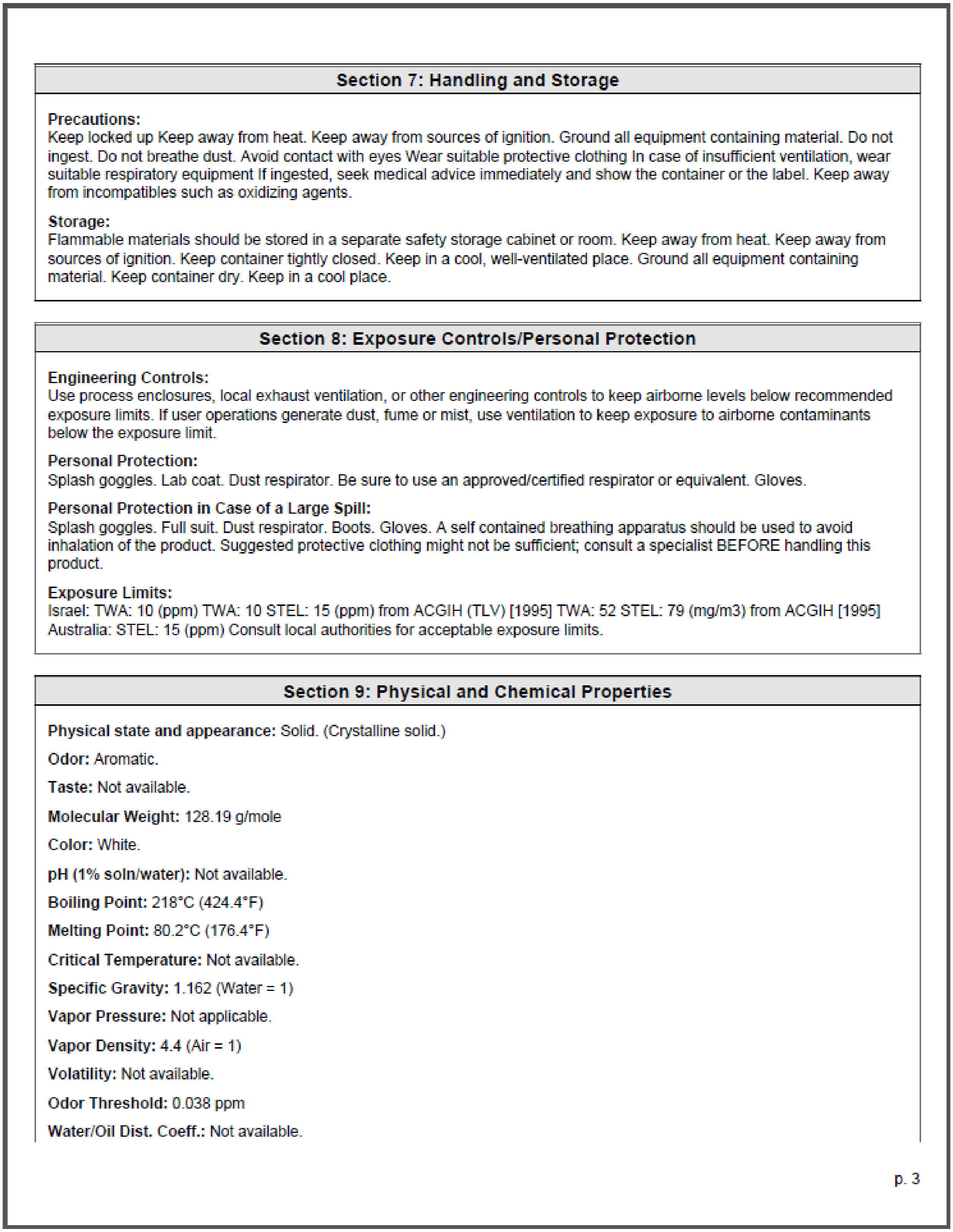
Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Use appropriate tools to put the spilled solid in a convenient waste disposal container.

Large Spill:
Flammable solid. Stop leak if without risk. Do not touch spilled material. Use water spray curtain to divert vapor drift. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.



Section 7: Handling and Storage

Precautions:
Keep locked up Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe dust. Avoid contact with eyes Wear suitable protective clothing In case of insufficient ventilation, wear suitable respiratory equipment If ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibles such as oxidizing agents.

Storage:
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. Keep container dry. Keep in a cool place.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
Israel: TWA: 10 (ppm) TWA: 10 STEL: 15 (ppm) from ACGIH (TLV) [1995] TWA: 52 STEL: 79 (mg/m3) from ACGIH [1995] Australia: STEL: 15 (ppm) Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid. (Crystalline solid.)

Odor: Aromatic.

Taste: Not available.

Molecular Weight: 128.19 g/mole

Color: White.

pH (1% soln/water): Not available.

Boiling Point: 218°C (424.4°F)

Melting Point: 80.2°C (176.4°F)

Critical Temperature: Not available.

Specific Gravity: 1.162 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: 4.4 (Air = 1)

Volatility: Not available.

Odor Threshold: 0.038 ppm

Water/Oil Dist. Coeff.: Not available.

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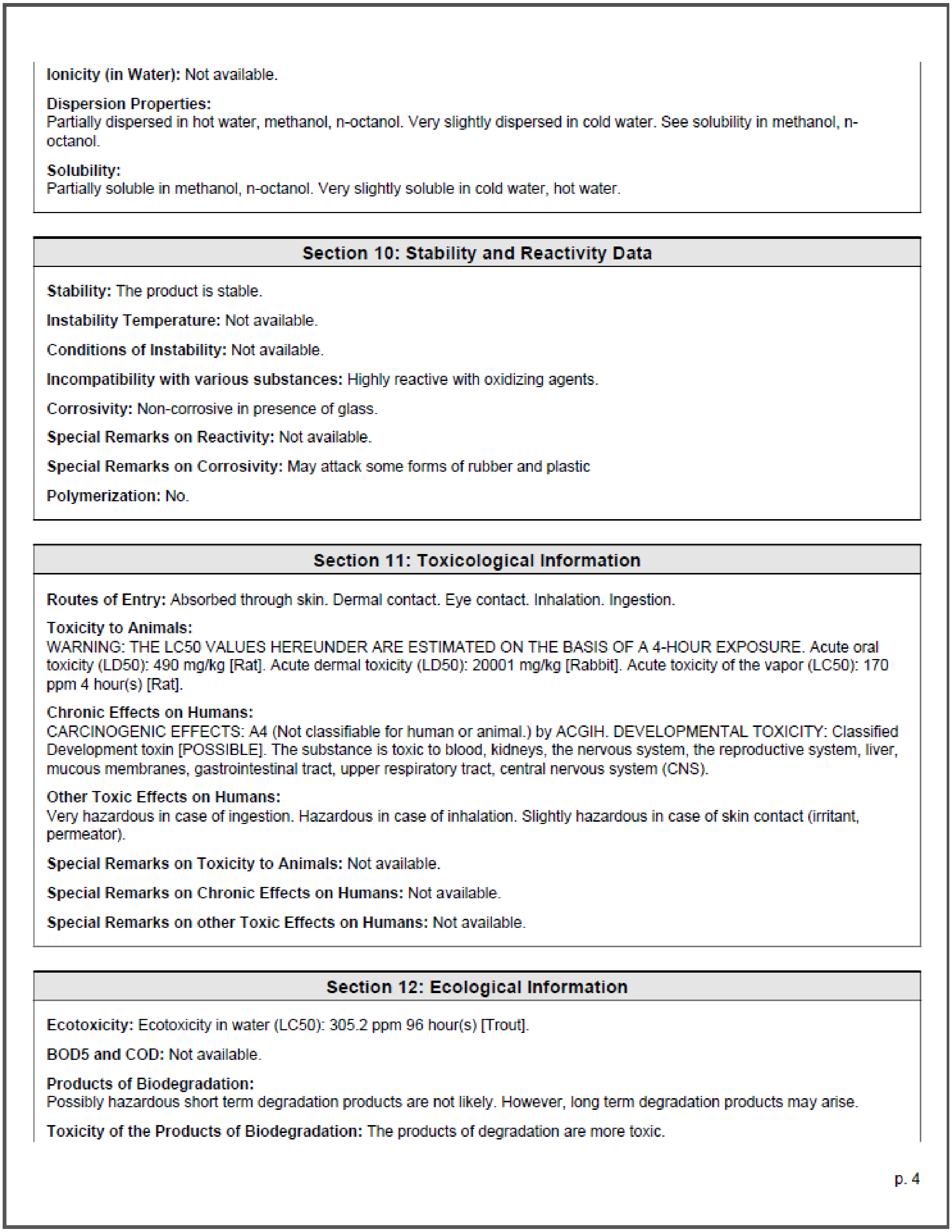


Ionicity (in Water): Not available.

Dispersion Properties:
Partially dispersed in hot water, methanol, n-octanol. Very slightly dispersed in cold water. See solubility in methanol, n-octanol.

Solubility:
Partially soluble in methanol, n-octanol. Very slightly soluble in cold water, hot water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Highly reactive with oxidizing agents.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: May attack some forms of rubber and plastic

Polymerization: No.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 490 mg/kg [Rat]. Acute dermal toxicity (LD50): 20001 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 170 ppm 4 hour(s) [Rat].

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH. DEVELOPMENTAL TOXICITY: Classified Development toxin [POSSIBLE]. The substance is toxic to blood, kidneys, the nervous system, the reproductive system, liver, mucous membranes, gastrointestinal tract, upper respiratory tract, central nervous system (CNS).

Other Toxic Effects on Humans:
Very hazardous in case of ingestion. Hazardous in case of inhalation. Slightly hazardous in case of skin contact (irritant, permeator).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

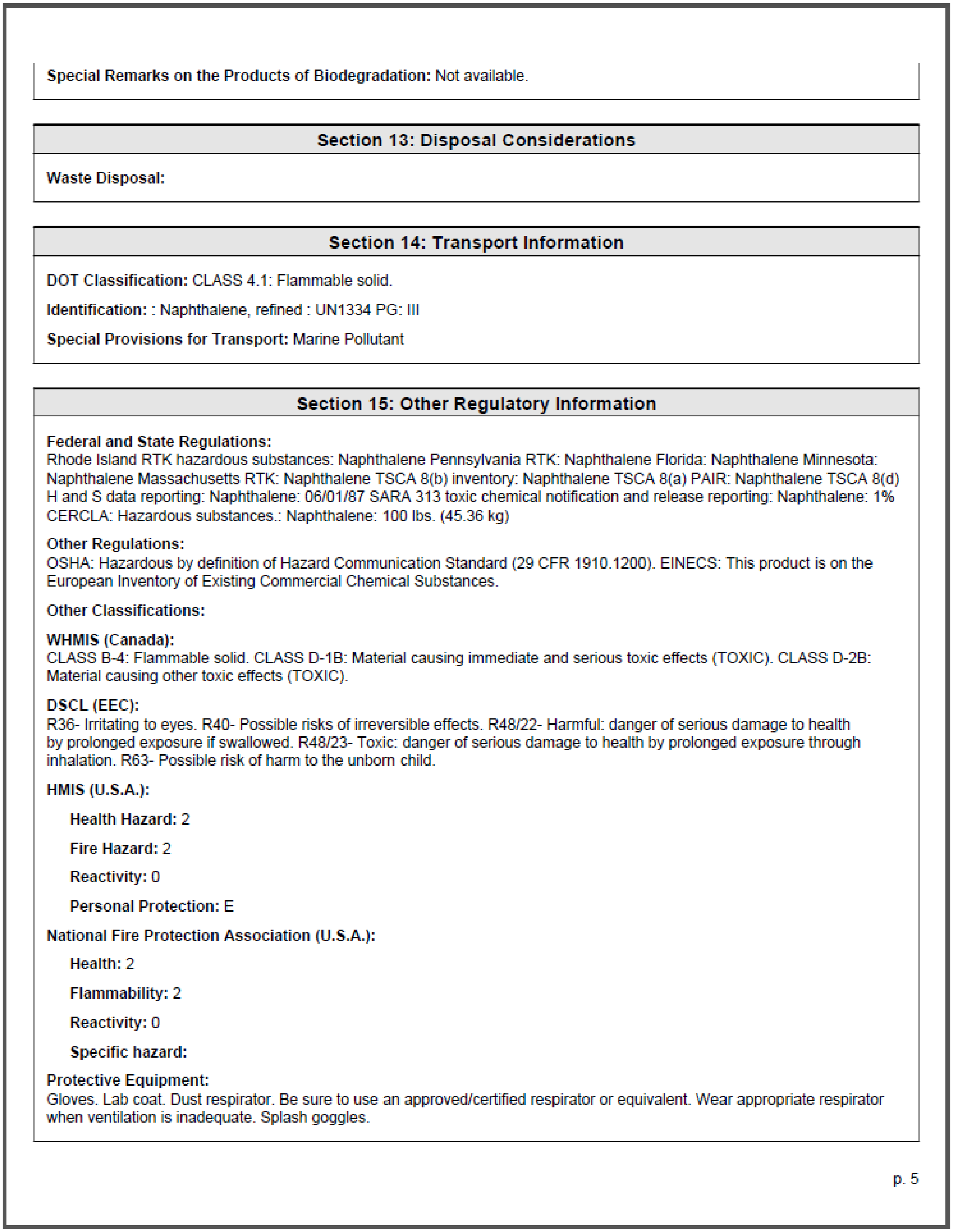
Section 12: Ecological Information

Ecotoxicity: Ecotoxicity in water (LC50): 305.2 ppm 96 hour(s) [Trout].

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are more toxic.



Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: CLASS 4.1: Flammable solid.

Identification: : Naphthalene, refined : UN1334 PG: III

Special Provisions for Transport: Marine Pollutant

Section 15: Other Regulatory Information

Federal and State Regulations:
Rhode Island RTK hazardous substances: Naphthalene Pennsylvania RTK: Naphthalene Florida: Naphthalene Minnesota: Naphthalene Massachusetts RTK: Naphthalene TSCA 8(b) inventory: Naphthalene TSCA 8(a) PAIR: Naphthalene TSCA 8(d) H and S data reporting: Naphthalene: 06/01/87 SARA 313 toxic chemical notification and release reporting: Naphthalene: 1% CERCLA: Hazardous substances.: Naphthalene: 100 lbs. (45.36 kg)

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS B-4: Flammable solid. CLASS D-1B: Material causing immediate and serious toxic effects (TOXIC). CLASS D-2B: Material causing other toxic effects (TOXIC).

DSCL (EEC):
R36- Irritating to eyes. R40- Possible risks of irreversible effects. R48/22- Harmful: danger of serious damage to health by prolonged exposure if swallowed. R48/23- Toxic: danger of serious damage to health by prolonged exposure through inhalation. R63- Possible risk of harm to the unborn child.

HMIS (U.S.A.):

- **Health Hazard:** 2
- **Fire Hazard:** 2
- **Reactivity:** 0
- **Personal Protection:** E

National Fire Protection Association (U.S.A.):

- **Health:** 2
- **Flammability:** 2
- **Reactivity:** 0
- **Specific hazard:**

Protective Equipment:
Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

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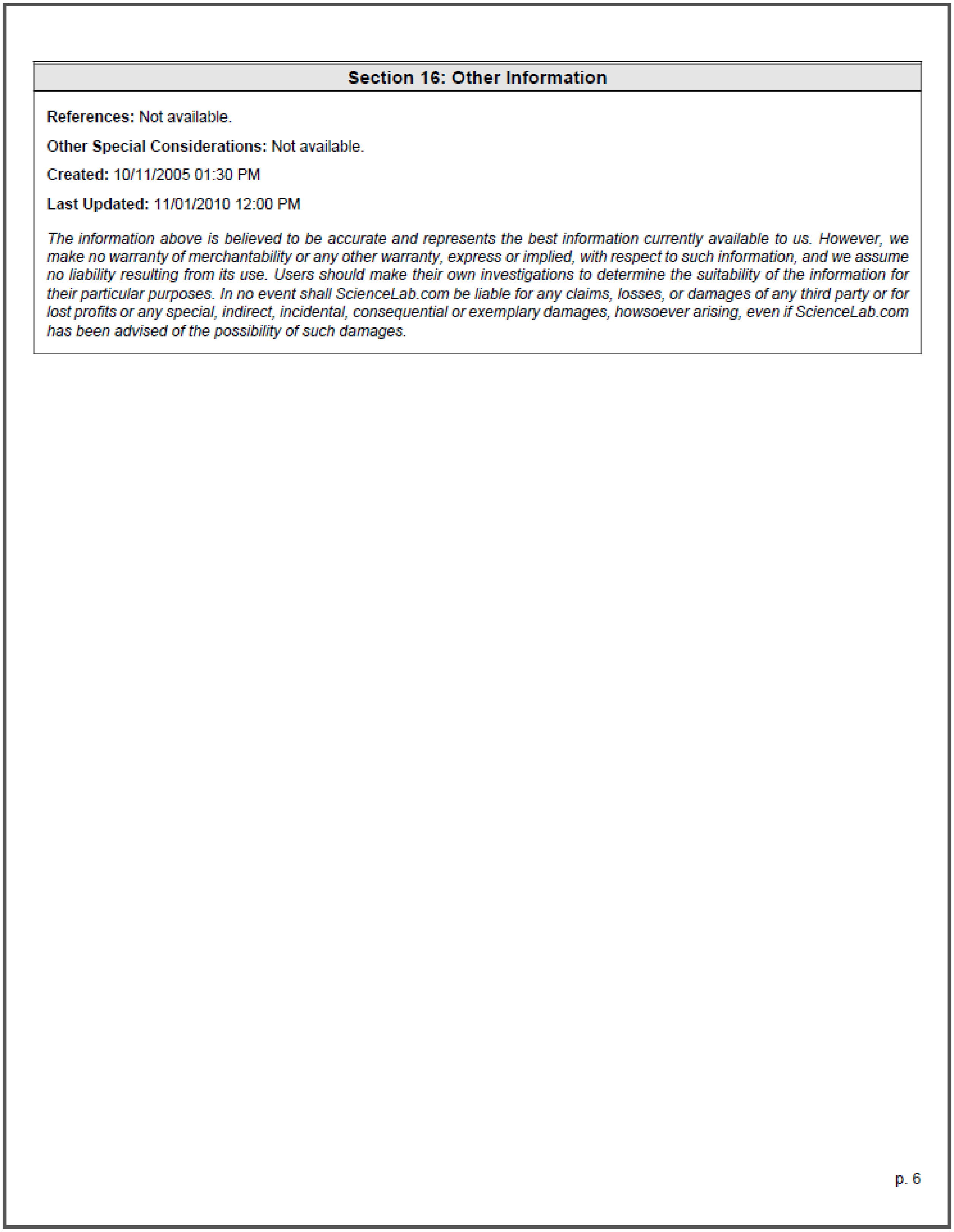

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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Last Updated: 11/01/2010 12:00 PM

Health	**2**
Fire	**3**
Reactivity	**0**
Personal Protection	**H**

Material Safety Data Sheet
Ethylbenzene MSDS

Section 1: Chemical Product and Company Identification

Product Name: Ethylbenzene

Catalog Codes: SLE2044

CAS#: 100-41-4

RTECS: DA0700000

TSCA: TSCA 8(b) inventory: Ethylbenzene

CI#: Not available.

Synonym: Ethyl Benzene; Ethylbenzol; Phenylethane

Chemical Name: Ethylbenzene

Chemical Formula: C8H10

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Ethylbenzene	100-41-4	100

Toxicological Data on Ingredients: Ethylbenzene: ORAL (LD50): Acute: 3500 mg/kg [Rat].

Section 3: Hazards Identification

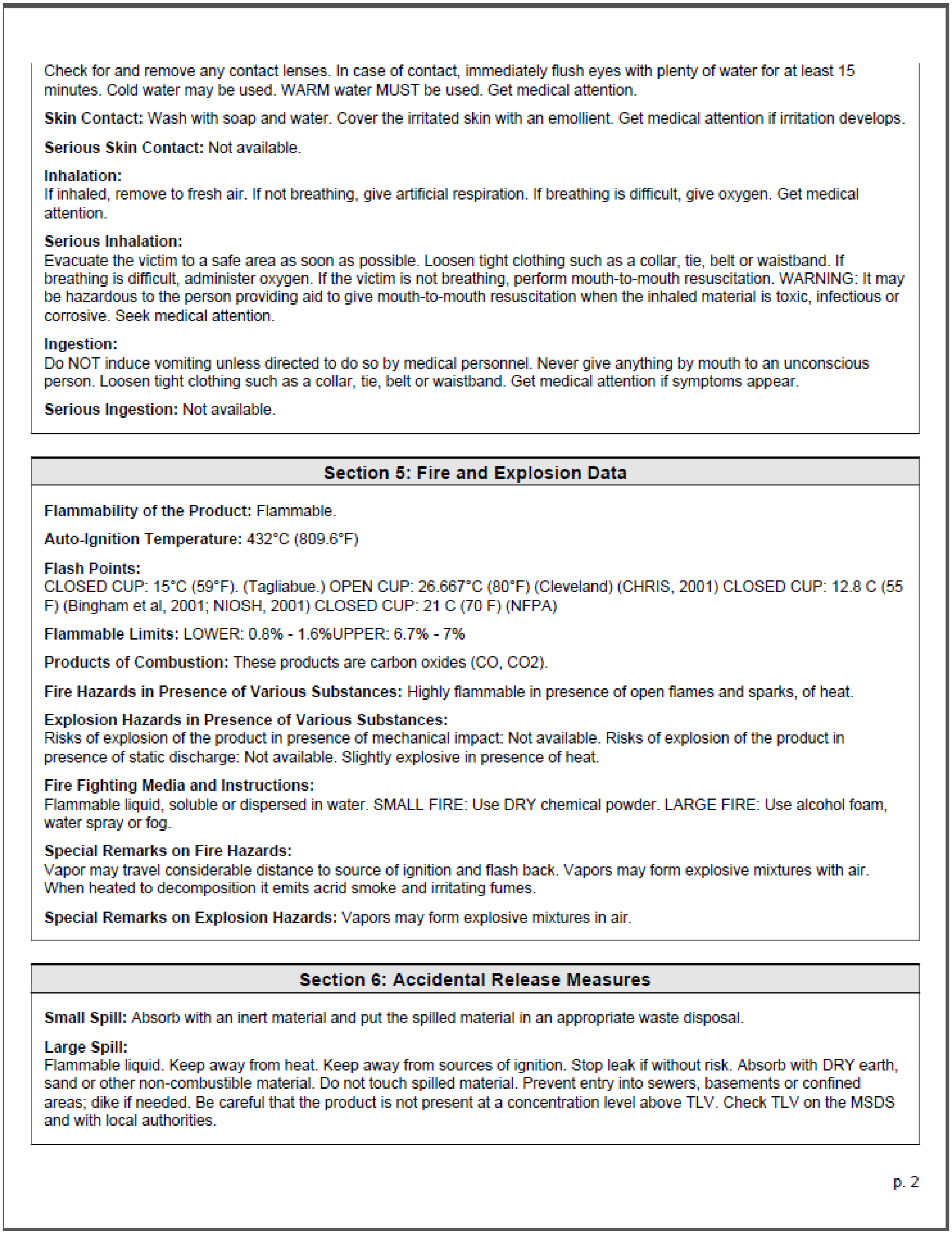
Potential Acute Health Effects:
Hazardous in case of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant, permeator).

Potential Chronic Health Effects:
Slightly hazardous in case of skin contact (irritant, sensitizer). CARCINOGENIC EFFECTS: Classified 2B (Possible for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:

p. 1



Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. WARM water MUST be used. Get medical attention.

Skin Contact: Wash with soap and water. Cover the irritated skin with an emollient. Get medical attention if irritation develops.

Serious Skin Contact: Not available.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention if symptoms appear.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 432°C (809.6°F)

Flash Points:
CLOSED CUP: 15°C (59°F). (Tagliabue.) OPEN CUP: 26.667°C (80°F) (Cleveland) (CHRIS, 2001) CLOSED CUP: 12.8 C (55 F) (Bingham et al, 2001; NIOSH, 2001) CLOSED CUP: 21 C (70 F) (NFPA)

Flammable Limits: LOWER: 0.8% - 1.6%UPPER: 6.7% - 7%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Highly flammable in presence of open flames and sparks, of heat.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available. Slightly explosive in presence of heat.

Fire Fighting Media and Instructions:
Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog.

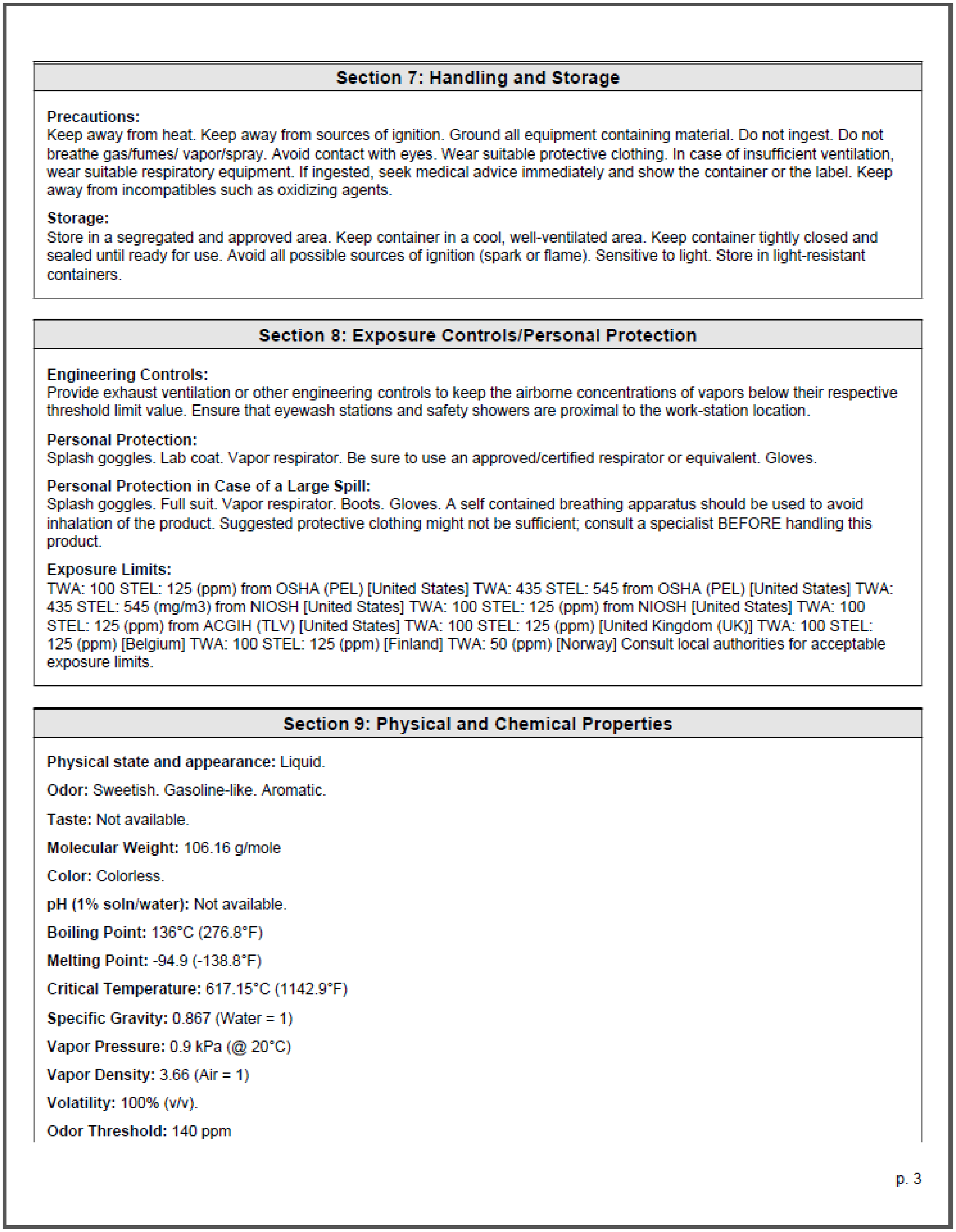
Special Remarks on Fire Hazards:
Vapor may travel considerable distance to source of ignition and flash back. Vapors may form explosive mixtures with air. When heated to decomposition it emits acrid smoke and irritating fumes.

Special Remarks on Explosion Hazards: Vapors may form explosive mixtures in air.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:
Flammable liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.



Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Avoid contact with eyes. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibles such as oxidizing agents.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Sensitive to light. Store in light-resistant containers.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 100 STEL: 125 (ppm) from OSHA (PEL) [United States] TWA: 435 STEL: 545 from OSHA (PEL) [United States] TWA: 435 STEL: 545 (mg/m3) from NIOSH [United States] TWA: 100 STEL: 125 (ppm) from NIOSH [United States] TWA: 100 STEL: 125 (ppm) from ACGIH (TLV) [United States] TWA: 100 STEL: 125 (ppm) [United Kingdom (UK)] TWA: 100 STEL: 125 (ppm) [Belgium] TWA: 100 STEL: 125 (ppm) [Finland] TWA: 50 (ppm) [Norway] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Sweetish. Gasoline-like. Aromatic.

Taste: Not available.

Molecular Weight: 106.16 g/mole

Color: Colorless.

pH (1% soln/water): Not available.

Boiling Point: 136°C (276.8°F)

Melting Point: -94.9 (-138.8°F)

Critical Temperature: 617.15°C (1142.9°F)

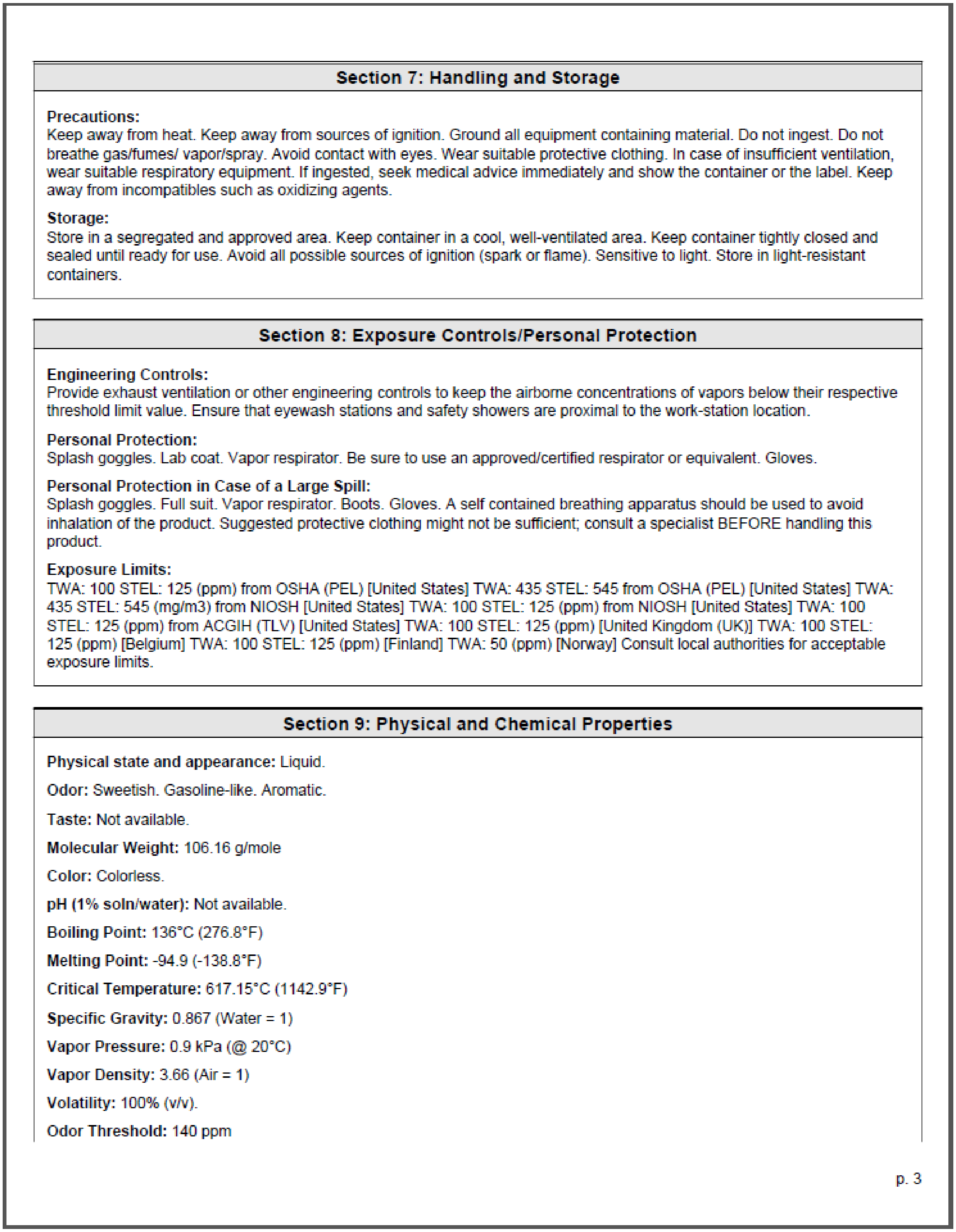
Specific Gravity: 0.867 (Water = 1)

Vapor Pressure: 0.9 kPa (@ 20°C)

Vapor Density: 3.66 (Air = 1)

Volatility: 100% (v/v).

Odor Threshold: 140 ppm



Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Avoid contact with eyes. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibles such as oxidizing agents.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Sensitive to light. Store in light-resistant containers.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 100 STEL: 125 (ppm) from OSHA (PEL) [United States] TWA: 435 STEL: 545 from OSHA (PEL) [United States] TWA: 435 STEL: 545 (mg/m3) from NIOSH [United States] TWA: 100 STEL: 125 (ppm) from NIOSH [United States] TWA: 100 STEL: 125 (ppm) from ACGIH (TLV) [United States] TWA: 100 STEL: 125 (ppm) [United Kingdom (UK)] TWA: 100 STEL: 125 (ppm) [Belgium] TWA: 100 STEL: 125 (ppm) [Finland] TWA: 50 (ppm) [Norway] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Sweetish. Gasoline-like. Aromatic.

Taste: Not available.

Molecular Weight: 106.16 g/mole

Color: Colorless.

pH (1% soln/water): Not available.

Boiling Point: 136°C (276.8°F)

Melting Point: -94.9 (-138.8°F)

Critical Temperature: 617.15°C (1142.9°F)

Specific Gravity: 0.867 (Water = 1)

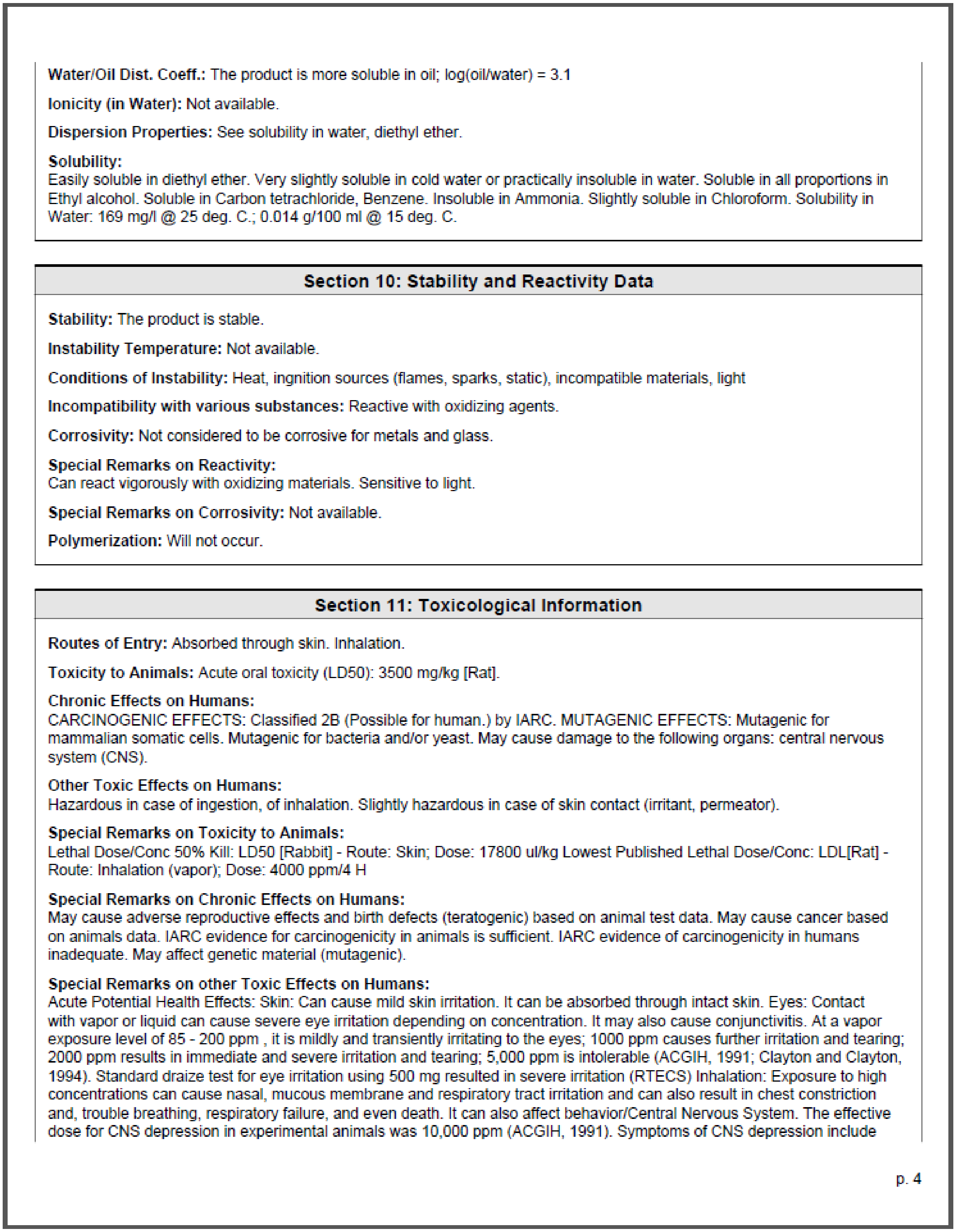
Vapor Pressure: 0.9 kPa (@ 20°C)

Vapor Density: 3.66 (Air = 1)

Volatility: 100% (v/v).

Odor Threshold: 140 ppm

p. 3



Water/Oil Dist. Coeff.: The product is more soluble in oil; log(oil/water) = 3.1

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, diethyl ether.

Solubility:
Easily soluble in diethyl ether. Very slightly soluble in cold water or practically insoluble in water. Soluble in all proportions in Ethyl alcohol. Soluble in Carbon tetrachloride, Benzene. Insoluble in Ammonia. Slightly soluble in Chloroform. Solubility in Water: 169 mg/l @ 25 deg. C.; 0.014 g/100 ml @ 15 deg. C.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Heat, ingnition sources (flames, sparks, static), incompatible materials, light

Incompatibility with various substances: Reactive with oxidizing agents.

Corrosivity: Not considered to be corrosive for metals and glass.

Special Remarks on Reactivity:
Can react vigorously with oxidizing materials. Sensitive to light.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Inhalation.

Toxicity to Animals: Acute oral toxicity (LD50): 3500 mg/kg [Rat].

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: Classified 2B (Possible for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. May cause damage to the following organs: central nervous system (CNS).

Other Toxic Effects on Humans:
Hazardous in case of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant, permeator).

Special Remarks on Toxicity to Animals:
Lethal Dose/Conc 50% Kill: LD50 [Rabbit] - Route: Skin; Dose: 17800 ul/kg Lowest Published Lethal Dose/Conc: LDL[Rat] - Route: Inhalation (vapor); Dose: 4000 ppm/4 H

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects and birth defects (teratogenic) based on animal test data. May cause cancer based on animals data. IARC evidence for carcinogenicity in animals is sufficient. IARC evidence of carcinogenicity in humans inadequate. May affect genetic material (mutagenic).

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Can cause mild skin irritation. It can be absorbed through intact skin. Eyes: Contact with vapor or liquid can cause severe eye irritation depending on concentration. It may also cause conjunctivitis. At a vapor exposure level of 85 - 200 ppm , it is mildly and transiently irritating to the eyes; 1000 ppm causes further irritation and tearing; 2000 ppm results in immediate and severe irritation and tearing; 5,000 ppm is intolerable (ACGIH, 1991; Clayton and Clayton, 1994). Standard draize test for eye irritation using 500 mg resulted in severe irritation (RTECS) Inhalation: Exposure to high concentrations can cause nasal, mucous membrane and respiratory tract irritation and can also result in chest constriction and, trouble breathing, respiratory failure, and even death. It can also affect behavior/Central Nervous System. The effective dose for CNS depression in experimental animals was 10,000 ppm (ACGIH, 1991). Symptoms of CNS depression include

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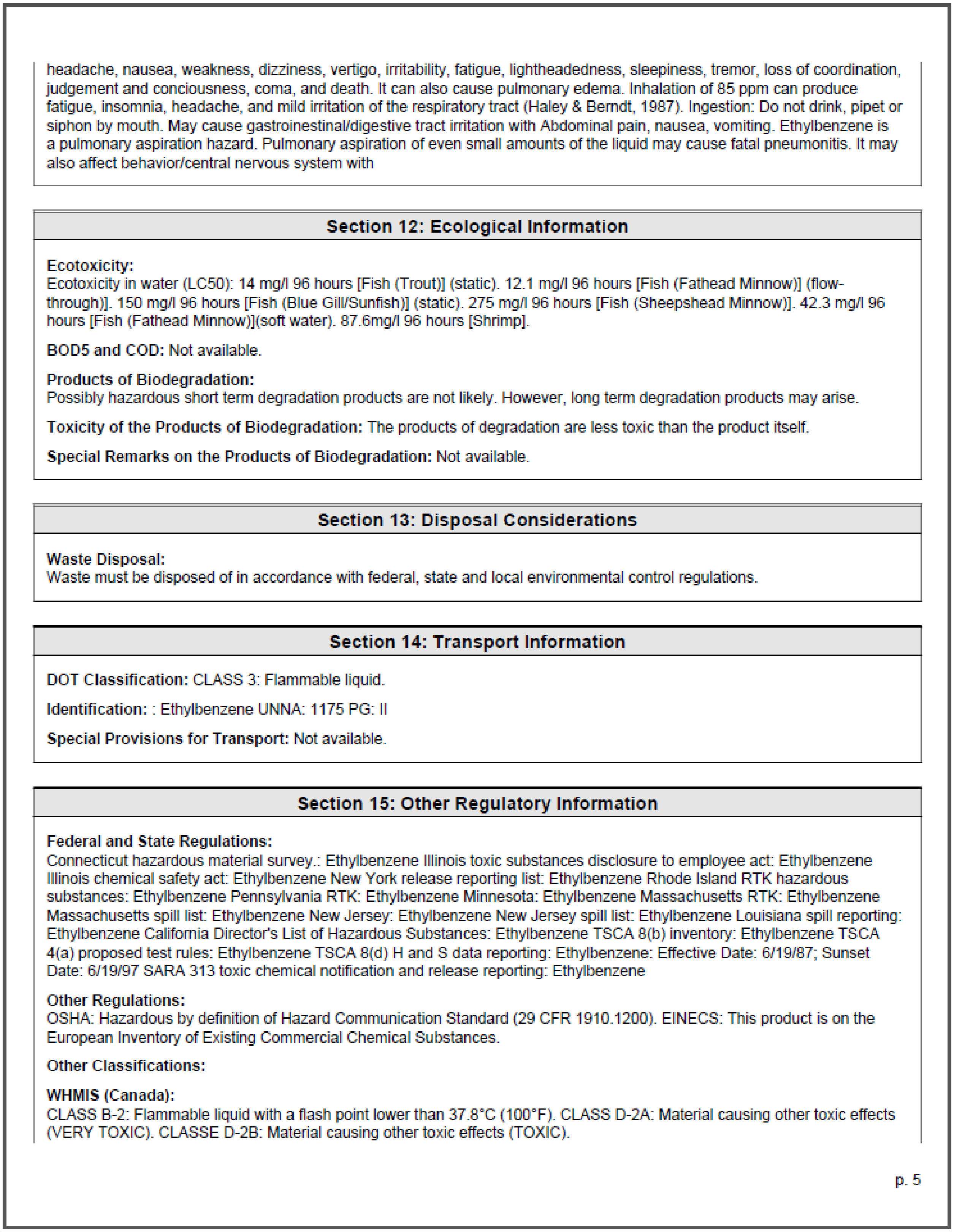

headache, nausea, weakness, dizziness, vertigo, irritability, fatigue, lightheadedness, sleepiness, tremor, loss of coordination, judgement and conciousness, coma, and death. It can also cause pulmonary edema. Inhalation of 85 ppm can produce fatigue, insomnia, headache, and mild irritation of the respiratory tract (Haley & Berndt, 1987). Ingestion: Do not drink, pipet or siphon by mouth. May cause gastroinestinal/digestive tract irritation with Abdominal pain, nausea, vomiting. Ethylbenzene is a pulmonary aspiration hazard. Pulmonary aspiration of even small amounts of the liquid may cause fatal pneumonitis. It may also affect behavior/central nervous system with

Section 12: Ecological Information

Ecotoxicity:
Ecotoxicity in water (LC50): 14 mg/l 96 hours [Fish (Trout)] (static). 12.1 mg/l 96 hours [Fish (Fathead Minnow)] (flow-through)]. 150 mg/l 96 hours [Fish (Blue Gill/Sunfish)] (static). 275 mg/l 96 hours [Fish (Sheepshead Minnow)]. 42.3 mg/l 96 hours [Fish (Fathead Minnow)](soft water). 87.6mg/l 96 hours [Shrimp].

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 3: Flammable liquid.

Identification: : Ethylbenzene UNNA: 1175 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Connecticut hazardous material survey.: Ethylbenzene Illinois toxic substances disclosure to employee act: Ethylbenzene Illinois chemical safety act: Ethylbenzene New York release reporting list: Ethylbenzene Rhode Island RTK hazardous substances: Ethylbenzene Pennsylvania RTK: Ethylbenzene Minnesota: Ethylbenzene Massachusetts RTK: Ethylbenzene Massachusetts spill list: Ethylbenzene New Jersey: Ethylbenzene New Jersey spill list: Ethylbenzene Louisiana spill reporting: Ethylbenzene California Director's List of Hazardous Substances: Ethylbenzene TSCA 8(b) inventory: Ethylbenzene TSCA 4(a) proposed test rules: Ethylbenzene TSCA 8(d) H and S data reporting: Ethylbenzene: Effective Date: 6/19/87; Sunset Date: 6/19/97 SARA 313 toxic chemical notification and release reporting: Ethylbenzene

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2A: Material causing other toxic effects (VERY TOXIC). CLASSE D-2B: Material causing other toxic effects (TOXIC).

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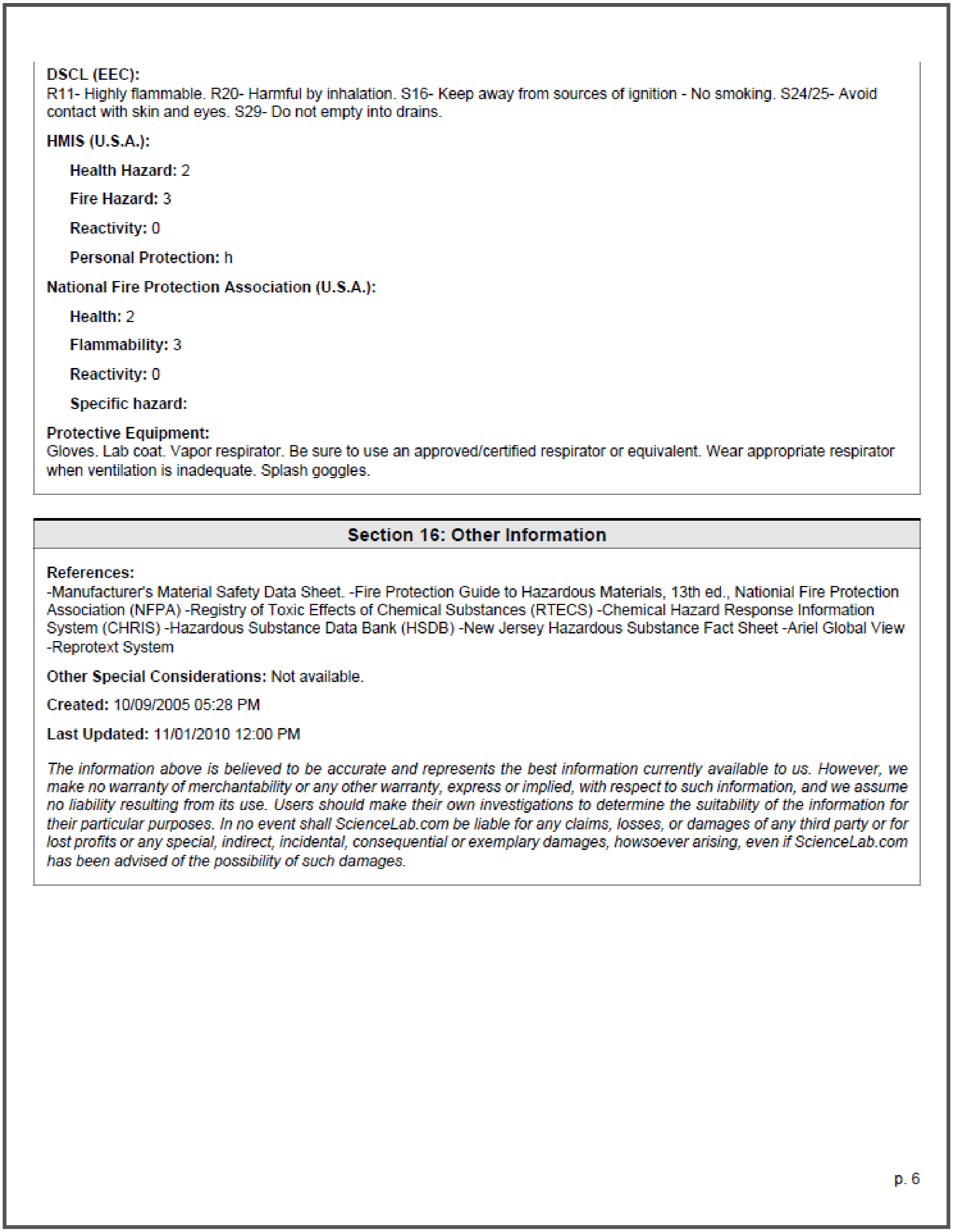

DSCL (EEC):
R11- Highly flammable. R20- Harmful by inhalation. S16- Keep away from sources of ignition - No smoking. S24/25- Avoid contact with skin and eyes. S29- Do not empty into drains.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 3

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References:
-Manufacturer's Material Safety Data Sheet. -Fire Protection Guide to Hazardous Materials, 13th ed., Nationial Fire Protection Association (NFPA) -Registry of Toxic Effects of Chemical Substances (RTECS) -Chemical Hazard Response Information System (CHRIS) -Hazardous Substance Data Bank (HSDB) -New Jersey Hazardous Substance Fact Sheet -Ariel Global View -Reprotext System

Other Special Considerations: Not available.

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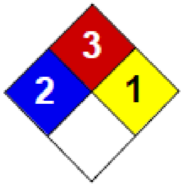


Health	2
Fire	3
Reactivity	0
Personal Protection	H

Material Safety Data Sheet

Cumene MSDS

Section 1: Chemical Product and Company Identification

Product Name: Cumene

Catalog Codes: SLC3052

CAS#: 98-82-8

RTECS: GR8575000

TSCA: TSCA 8(b) inventory: Cumene

CI#: Not available.

Synonym: Isopropyl benzene; Cumol; 2-Phenyl propane; (1-Methylethyl)benzene

Chemical Name: Isopropylbenzene

Chemical Formula: C6H5CH(CH3)2

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Cumene	98-82-8	100

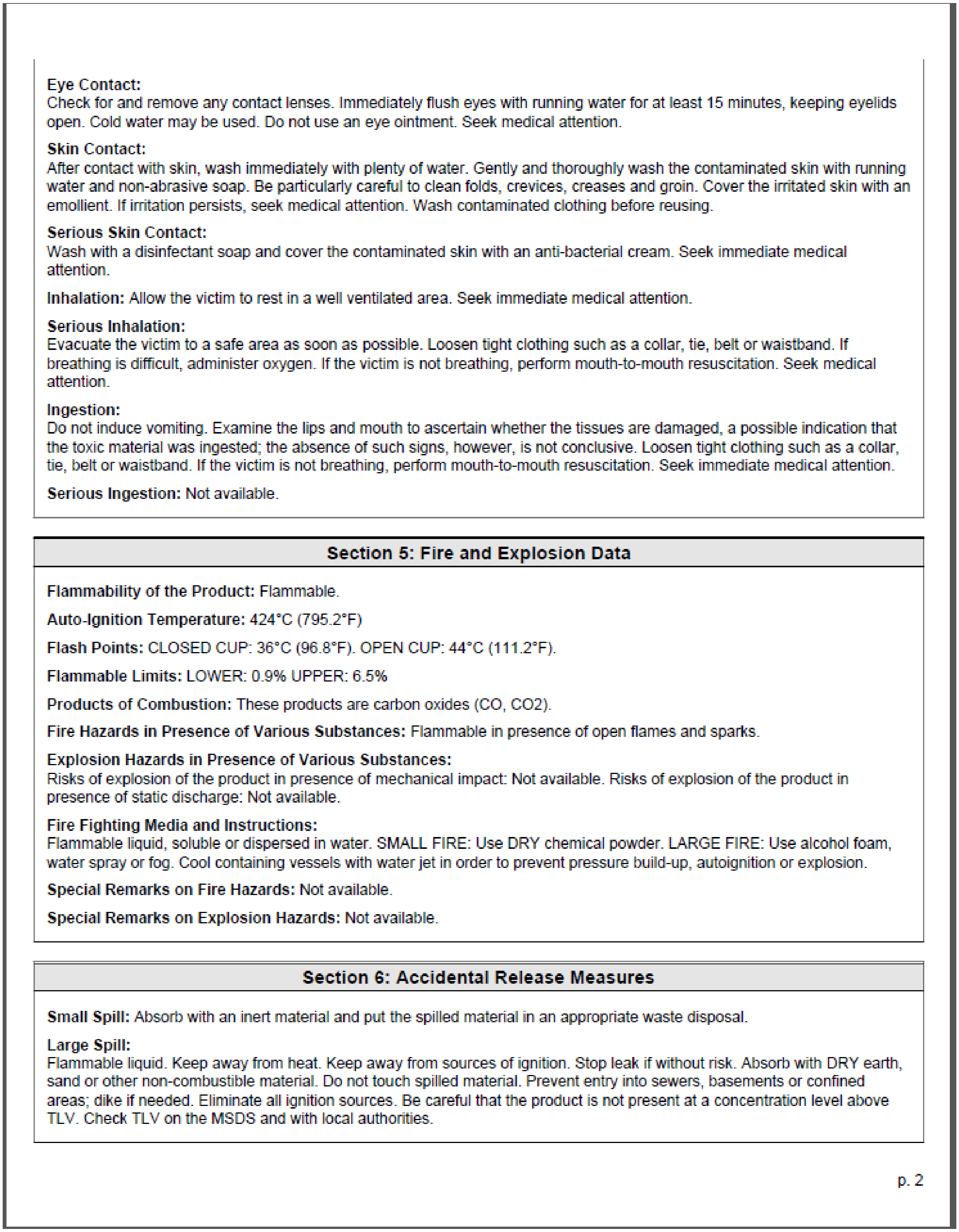
Toxicological Data on Ingredients: Cumene: ORAL (LD50): Acute: 1400 mg/kg [Rat]. 12750 mg/kg [Mouse]. DERMAL (LD50): Acute: 12300 mg/kg [Rabbit].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (irritant, permeator), of eye contact (irritant), of ingestion, of inhalation. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
Very hazardous in case of skin contact (permeator). CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to lungs, the nervous system, mucous membranes. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures



Eye Contact:
Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Do not use an eye ointment. Seek medical attention.

Skin Contact:
After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do not induce vomiting. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 424°C (795.2°F)

Flash Points: CLOSED CUP: 36°C (96.8°F). OPEN CUP: 44°C (111.2°F).

Flammable Limits: LOWER: 0.9% UPPER: 6.5%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Flammable in presence of open flames and sparks.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

Special Remarks on Fire Hazards: Not available.

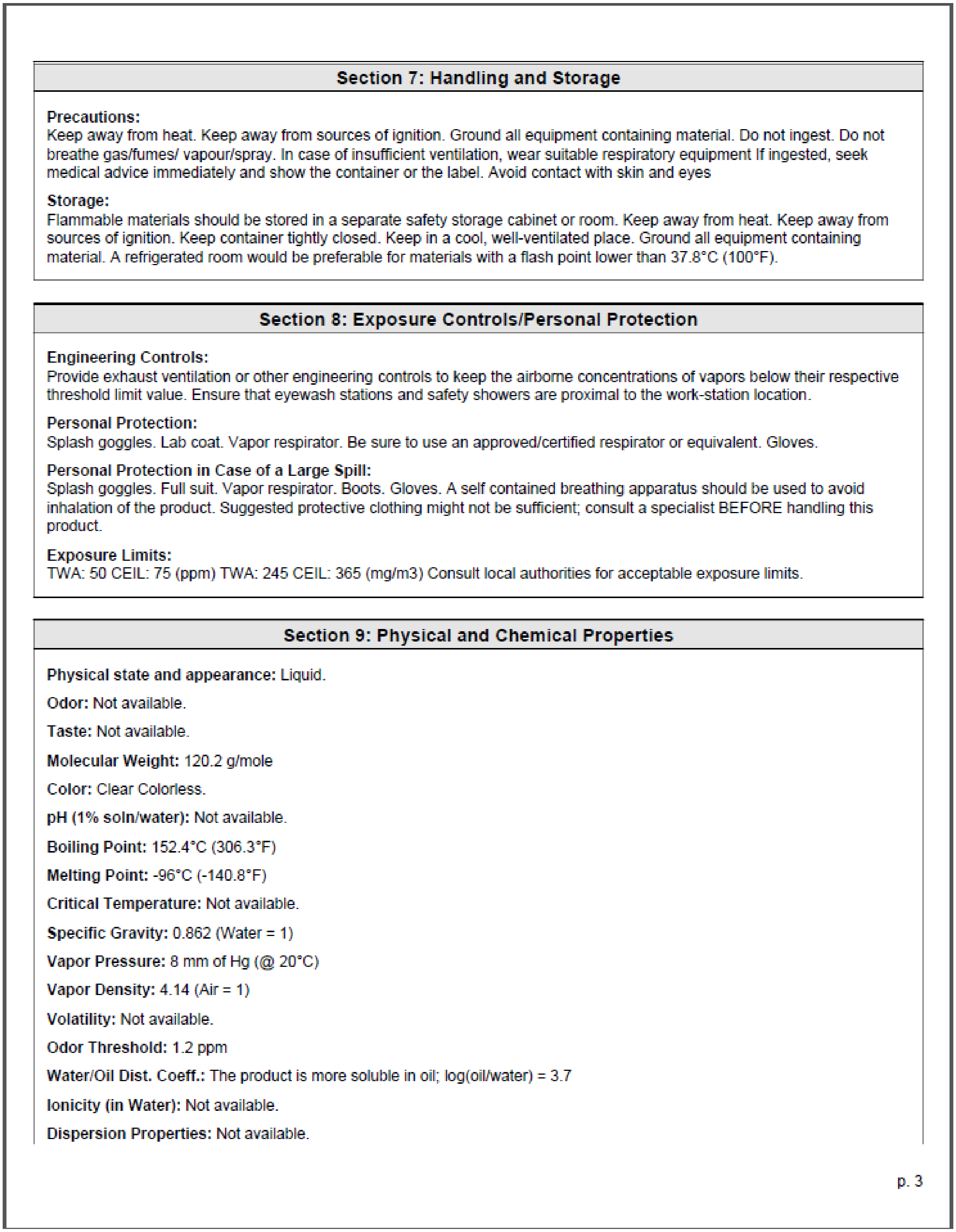
Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:
Flammable liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

p. 2



Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapour/spray. In case of insufficient ventilation, wear suitable respiratory equipment If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes

Storage:
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. A refrigerated room would be preferable for materials with a flash point lower than 37.8°C (100°F).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 50 CEIL: 75 (ppm) TWA: 245 CEIL: 365 (mg/m3) Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Not available.

Taste: Not available.

Molecular Weight: 120.2 g/mole

Color: Clear Colorless.

pH (1% soln/water): Not available.

Boiling Point: 152.4°C (306.3°F)

Melting Point: -96°C (-140.8°F)

Critical Temperature: Not available.

Specific Gravity: 0.862 (Water = 1)

Vapor Pressure: 8 mm of Hg (@ 20°C)

Vapor Density: 4.14 (Air = 1)

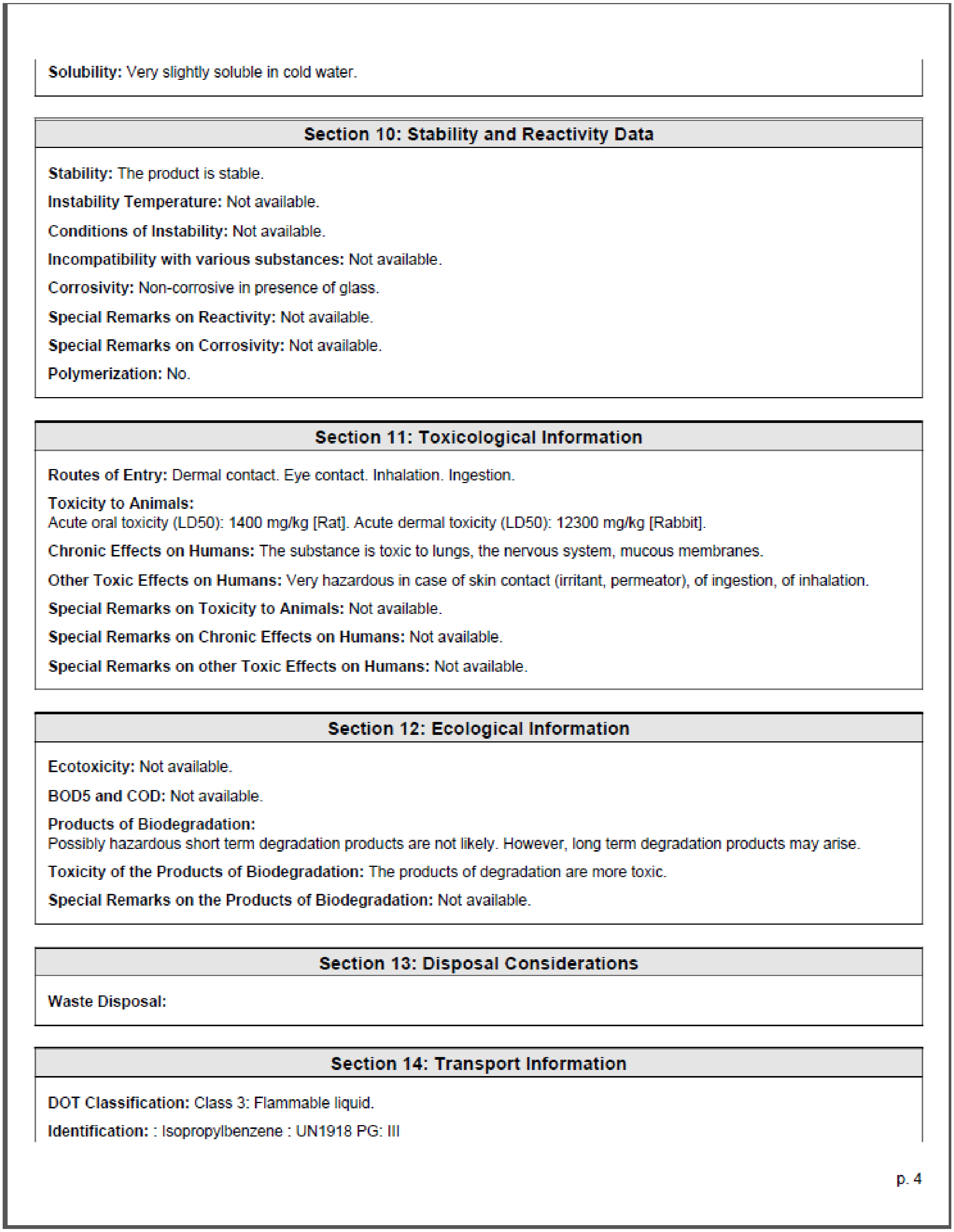
Volatility: Not available.

Odor Threshold: 1.2 ppm

Water/Oil Dist. Coeff.: The product is more soluble in oil; log(oil/water) = 3.7

Ionicity (in Water): Not available.

Dispersion Properties: Not available.



Solubility: Very slightly soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: No.

Section 11: Toxicological Information

Routes of Entry: Dermal contact. Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
Acute oral toxicity (LD50): 1400 mg/kg [Rat]. Acute dermal toxicity (LD50): 12300 mg/kg [Rabbit].

Chronic Effects on Humans: The substance is toxic to lungs, the nervous system, mucous membranes.

Other Toxic Effects on Humans: Very hazardous in case of skin contact (irritant, permeator), of ingestion, of inhalation.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are more toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: Class 3: Flammable liquid.

Identification: : Isopropylbenzene : UN1918 PG: III

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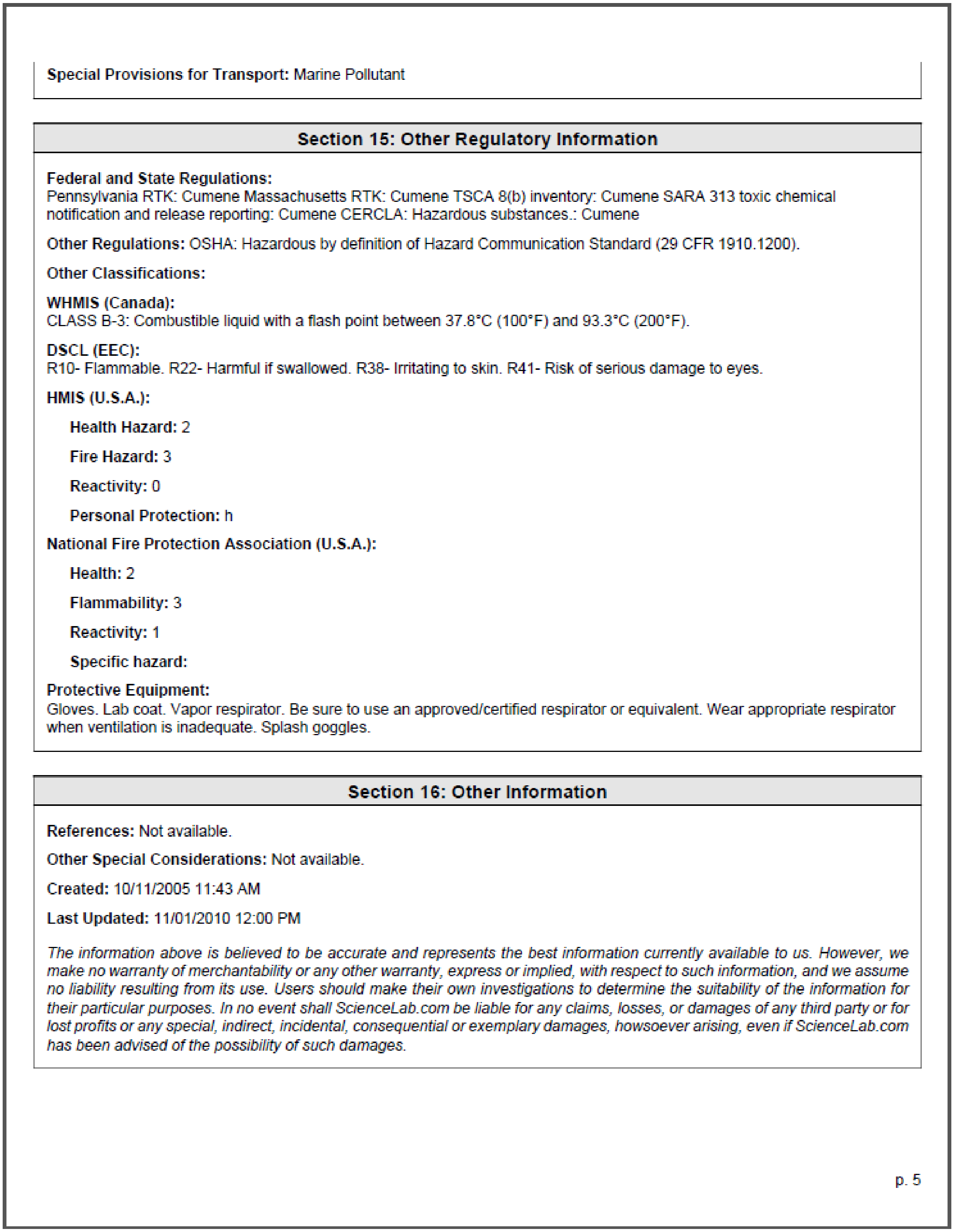

Special Provisions for Transport: Marine Pollutant

Section 15: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK: Cumene Massachusetts RTK: Cumene TSCA 8(b) inventory: Cumene SARA 313 toxic chemical notification and release reporting: Cumene CERCLA: Hazardous substances.: Cumene

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:

WHMIS (Canada):
CLASS B-3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F).

DSCL (EEC):
R10- Flammable. R22- Harmful if swallowed. R38- Irritating to skin. R41- Risk of serious damage to eyes.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 3

Reactivity: 1

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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Last Updated: 11/01/2010 12:00 PM

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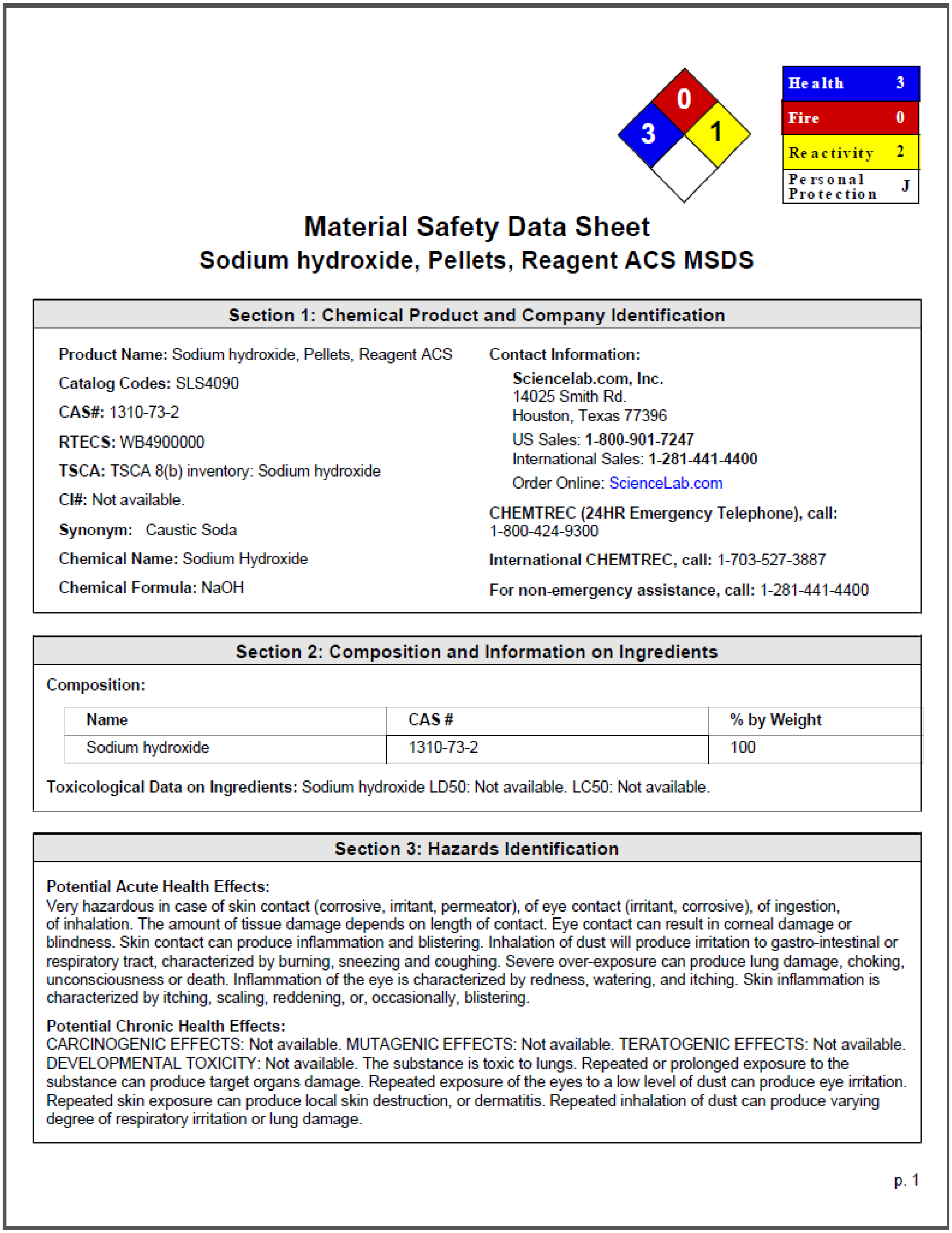

Health	3
Fire	0
Reactivity	2
Personal Protection	J

Material Safety Data Sheet
Sodium hydroxide, Pellets, Reagent ACS MSDS

Section 1: Chemical Product and Company Identification

Product Name: Sodium hydroxide, Pellets, Reagent ACS

Catalog Codes: SLS4090

CAS#: 1310-73-2

RTECS: WB4900000

TSCA: TSCA 8(b) inventory: Sodium hydroxide

CI#: Not available.

Synonym: Caustic Soda

Chemical Name: Sodium Hydroxide

Chemical Formula: NaOH

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Sodium hydroxide	1310-73-2	100

Toxicological Data on Ingredients: Sodium hydroxide LD50: Not available. LC50: Not available.

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (corrosive, irritant, permeator), of eye contact (irritant, corrosive), of ingestion, of inhalation. The amount of tissue damage depends on length of contact. Eye contact can result in corneal damage or blindness. Skin contact can produce inflammation and blistering. Inhalation of dust will produce irritation to gastro-intestinal or respiratory tract, characterized by burning, sneezing and coughing. Severe over-exposure can produce lung damage, choking, unconsciousness or death. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to lungs. Repeated or prolonged exposure to the substance can produce target organs damage. Repeated exposure of the eyes to a low level of dust can produce eye irritation. Repeated skin exposure can produce local skin destruction, or dermatitis. Repeated inhalation of dust can produce varying degree of respiratory irritation or lung damage.

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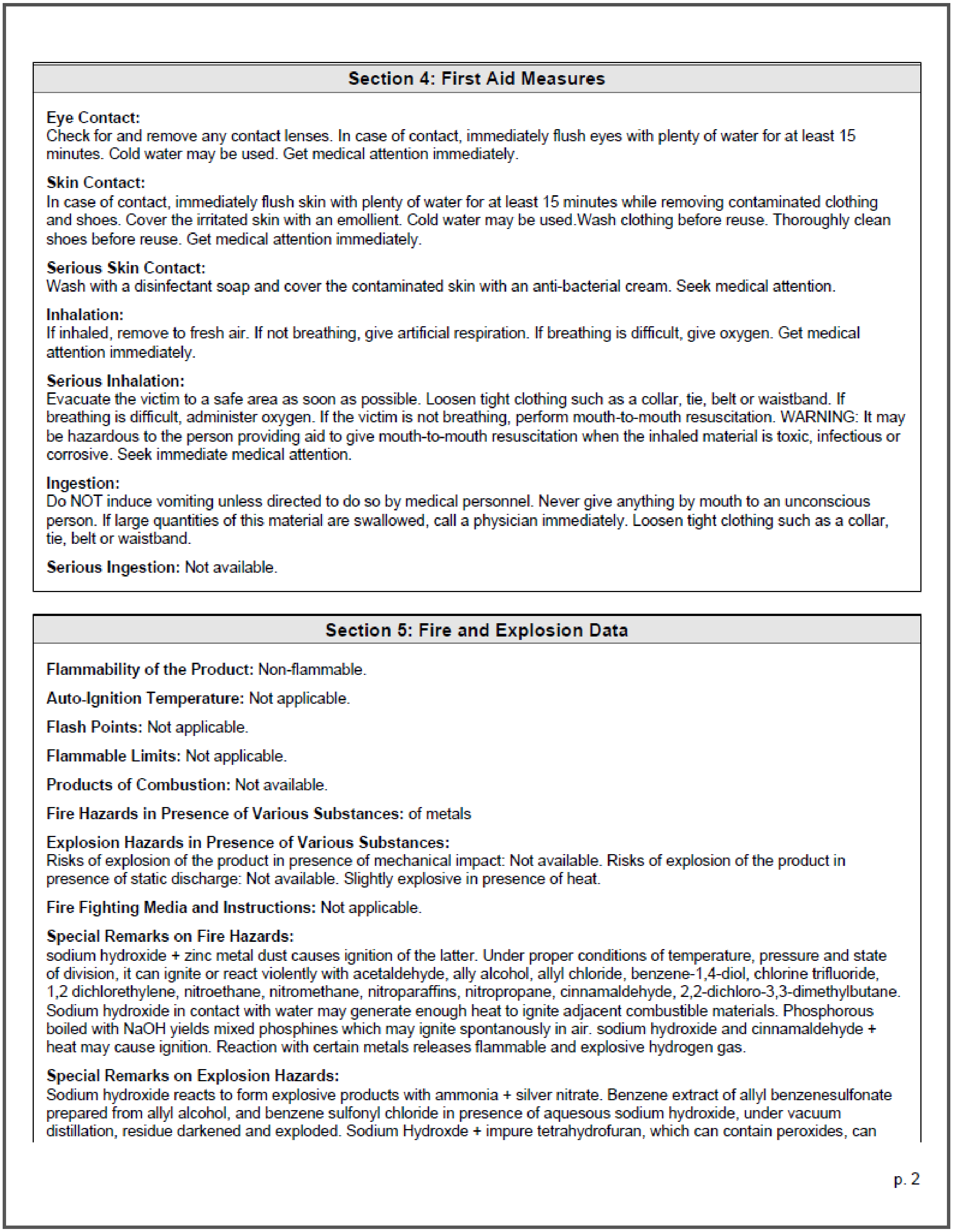


Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention immediately.

Skin Contact:
In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Cover the irritated skin with an emollient. Cold water may be used.Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention immediately.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention immediately.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

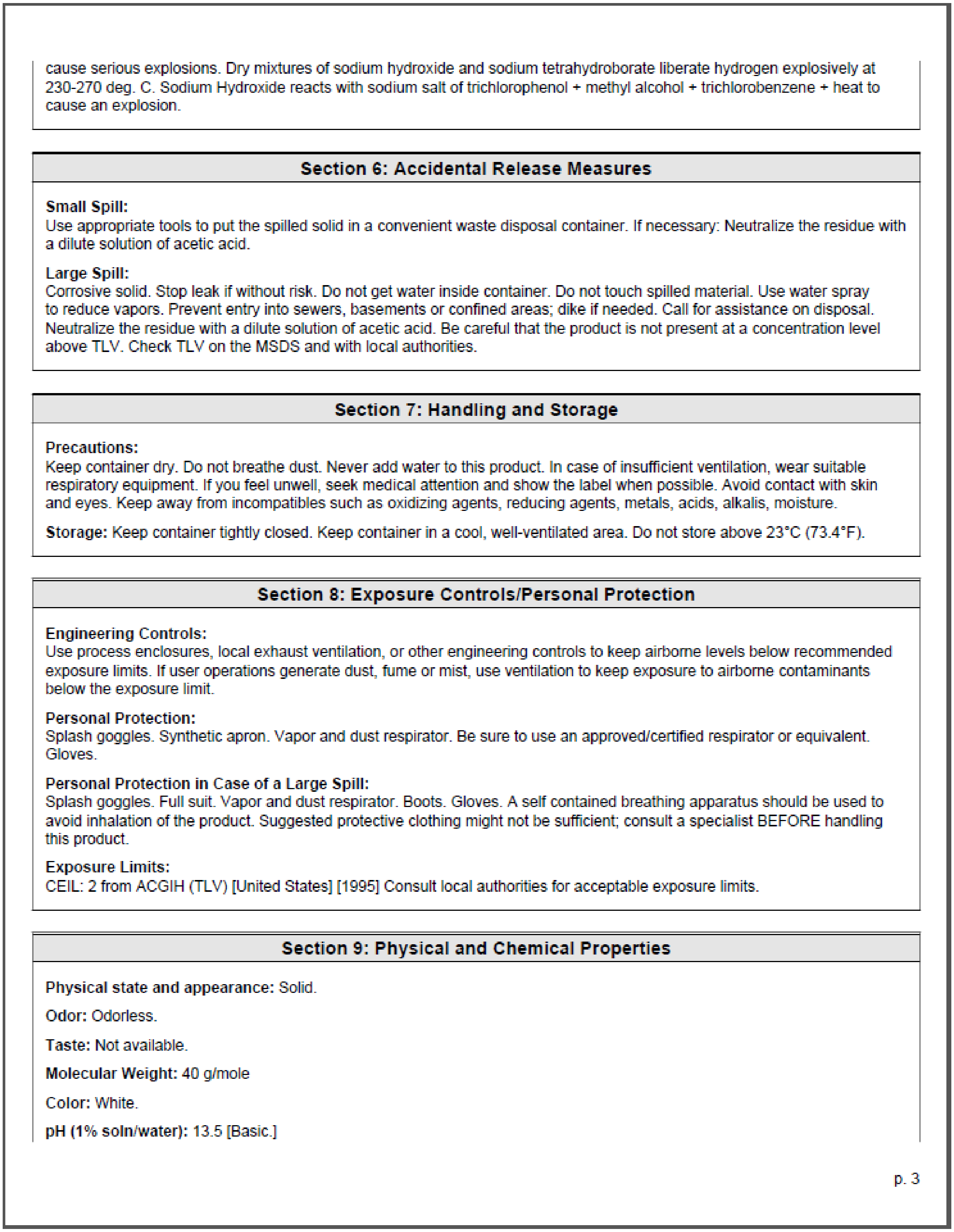
Fire Hazards in Presence of Various Substances: of metals

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available. Slightly explosive in presence of heat.

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards:
sodium hydroxide + zinc metal dust causes ignition of the latter. Under proper conditions of temperature, pressure and state of division, it can ignite or react violently with acetaldehyde, ally alcohol, allyl chloride, benzene-1,4-diol, chlorine trifluoride, 1,2 dichlorethylene, nitroethane, nitromethane, nitroparaffins, nitropropane, cinnamaldehyde, 2,2-dichloro-3,3-dimethylbutane. Sodium hydroxide in contact with water may generate enough heat to ignite adjacent combustible materials. Phosphorous boiled with NaOH yields mixed phosphines which may ignite spontanously in air. sodium hydroxide and cinnamaldehyde + heat may cause ignition. Reaction with certain metals releases flammable and explosive hydrogen gas.

Special Remarks on Explosion Hazards:
Sodium hydroxide reacts to form explosive products with ammonia + silver nitrate. Benzene extract of allyl benzenesulfonate prepared from allyl alcohol, and benzene sulfonyl chloride in presence of aquesous sodium hydroxide, under vacuum distillation, residue darkened and exploded. Sodium Hydroxde + impure tetrahydrofuran, which can contain peroxides, can



cause serious explosions. Dry mixtures of sodium hydroxide and sodium tetrahydroborate liberate hydrogen explosively at 230-270 deg. C. Sodium Hydroxide reacts with sodium salt of trichlorophenol + methyl alcohol + trichlorobenzene + heat to cause an explosion.

Section 6: Accidental Release Measures

Small Spill:
Use appropriate tools to put the spilled solid in a convenient waste disposal container. If necessary: Neutralize the residue with a dilute solution of acetic acid.

Large Spill:
Corrosive solid. Stop leak if without risk. Do not get water inside container. Do not touch spilled material. Use water spray to reduce vapors. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal. Neutralize the residue with a dilute solution of acetic acid. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep container dry. Do not breathe dust. Never add water to this product. In case of insufficient ventilation, wear suitable respiratory equipment. If you feel unwell, seek medical attention and show the label when possible. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, reducing agents, metals, acids, alkalis, moisture.

Storage: Keep container tightly closed. Keep container in a cool, well-ventilated area. Do not store above 23°C (73.4°F).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Synthetic apron. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor and dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
CEIL: 2 from ACGIH (TLV) [United States] [1995] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid.

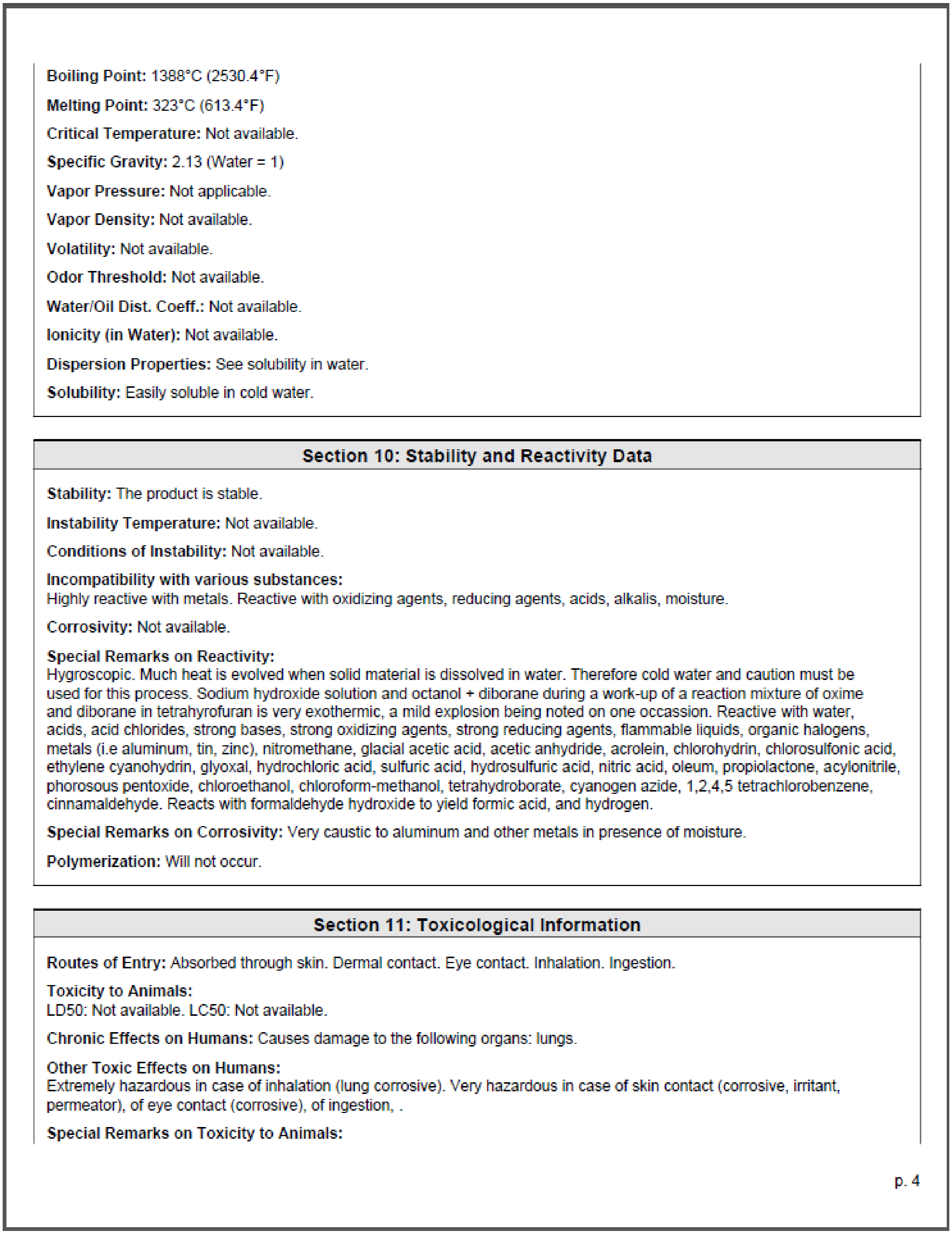
Odor: Odorless.

Taste: Not available.

Molecular Weight: 40 g/mole

Color: White.

pH (1% soln/water): 13.5 [Basic.]



Boiling Point: 1388°C (2530.4°F)

Melting Point: 323°C (613.4°F)

Critical Temperature: Not available.

Specific Gravity: 2.13 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water.

Solubility: Easily soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances:
Highly reactive with metals. Reactive with oxidizing agents, reducing agents, acids, alkalis, moisture.

Corrosivity: Not available.

Special Remarks on Reactivity:
Hygroscopic. Much heat is evolved when solid material is dissolved in water. Therefore cold water and caution must be used for this process. Sodium hydroxide solution and octanol + diborane during a work-up of a reaction mixture of oxime and diborane in tetrahyrofuran is very exothermic, a mild explosion being noted on one occassion. Reactive with water, acids, acid chlorides, strong bases, strong oxidizing agents, strong reducing agents, flammable liquids, organic halogens, metals (i.e aluminum, tin, zinc), nitromethane, glacial acetic acid, acetic anhydride, acrolein, chlorohydrin, chlorosulfonic acid, ethylene cyanohydrin, glyoxal, hydrochloric acid, sulfuric acid, hydrosulfuric acid, nitric acid, oleum, propiolactone, acylonitrile, phorosous pentoxide, chloroethanol, chloroform-methanol, tetrahydroborate, cyanogen azide, 1,2,4,5 tetrachlorobenzene, cinnamaldehyde. Reacts with formaldehyde hydroxide to yield formic acid, and hydrogen.

Special Remarks on Corrosivity: Very caustic to aluminum and other metals in presence of moisture.

Polymerization: Will not occur.

Section 11: Toxicological Information

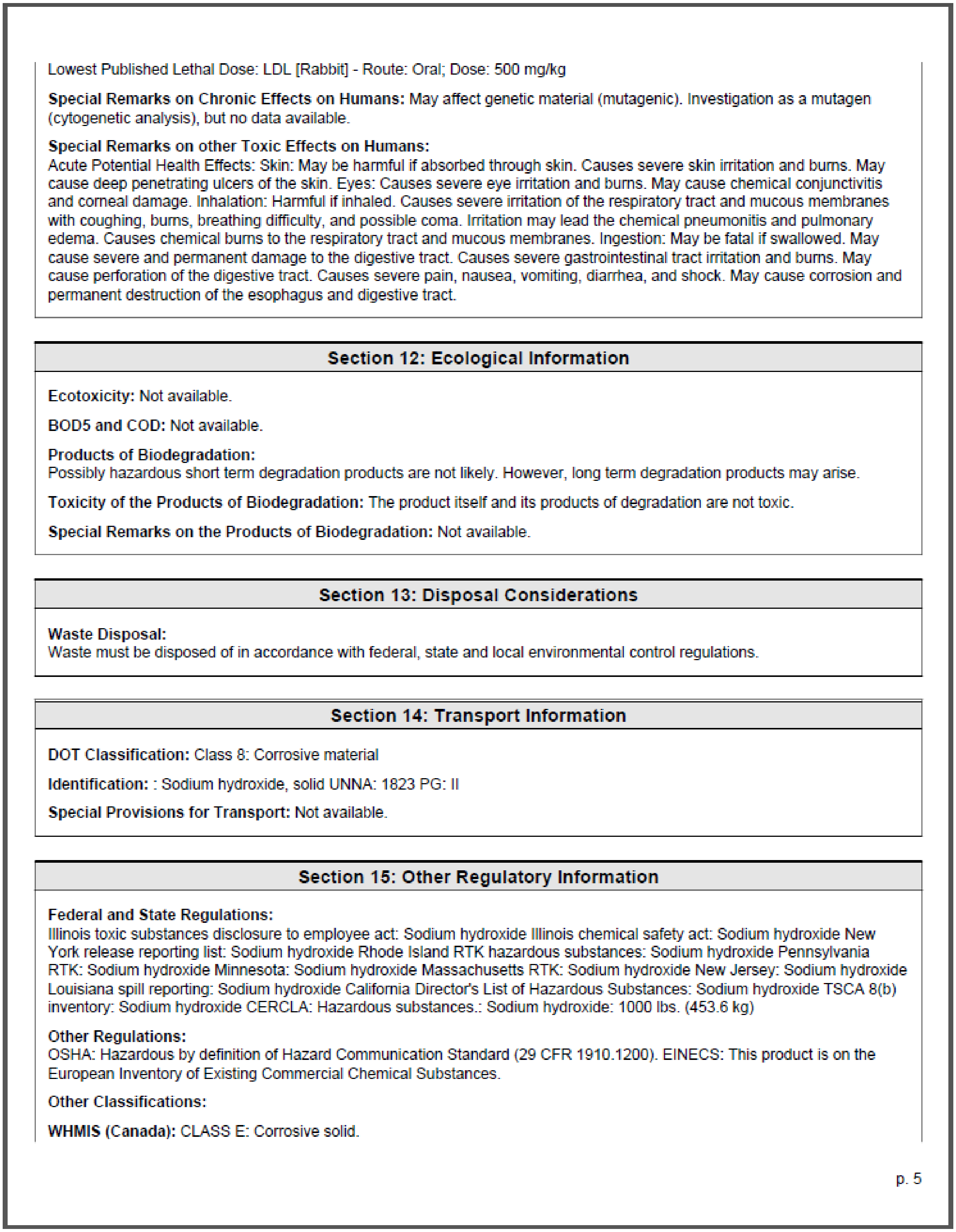
Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
LD50: Not available. LC50: Not available.

Chronic Effects on Humans: Causes damage to the following organs: lungs.

Other Toxic Effects on Humans:
Extremely hazardous in case of inhalation (lung corrosive). Very hazardous in case of skin contact (corrosive, irritant, permeator), of eye contact (corrosive), of ingestion, .

Special Remarks on Toxicity to Animals:



Lowest Published Lethal Dose: LDL [Rabbit] - Route: Oral; Dose: 500 mg/kg

Special Remarks on Chronic Effects on Humans: May affect genetic material (mutagenic). Investigation as a mutagen (cytogenetic analysis), but no data available.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: May be harmful if absorbed through skin. Causes severe skin irritation and burns. May cause deep penetrating ulcers of the skin. Eyes: Causes severe eye irritation and burns. May cause chemical conjunctivitis and corneal damage. Inhalation: Harmful if inhaled. Causes severe irritation of the respiratory tract and mucous membranes with coughing, burns, breathing difficulty, and possible coma. Irritation may lead the chemical pneumonitis and pulmonary edema. Causes chemical burns to the respiratory tract and mucous membranes. Ingestion: May be fatal if swallowed. May cause severe and permanent damage to the digestive tract. Causes severe gastrointestinal tract irritation and burns. May cause perforation of the digestive tract. Causes severe pain, nausea, vomiting, diarrhea, and shock. May cause corrosion and permanent destruction of the esophagus and digestive tract.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The product itself and its products of degradation are not toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: Class 8: Corrosive material

Identification: : Sodium hydroxide, solid UNNA: 1823 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Illinois toxic substances disclosure to employee act: Sodium hydroxide Illinois chemical safety act: Sodium hydroxide New York release reporting list: Sodium hydroxide Rhode Island RTK hazardous substances: Sodium hydroxide Pennsylvania RTK: Sodium hydroxide Minnesota: Sodium hydroxide Massachusetts RTK: Sodium hydroxide New Jersey: Sodium hydroxide Louisiana spill reporting: Sodium hydroxide California Director's List of Hazardous Substances: Sodium hydroxide TSCA 8(b) inventory: Sodium hydroxide CERCLA: Hazardous substances.: Sodium hydroxide: 1000 lbs. (453.6 kg)

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada): CLASS E: Corrosive solid.

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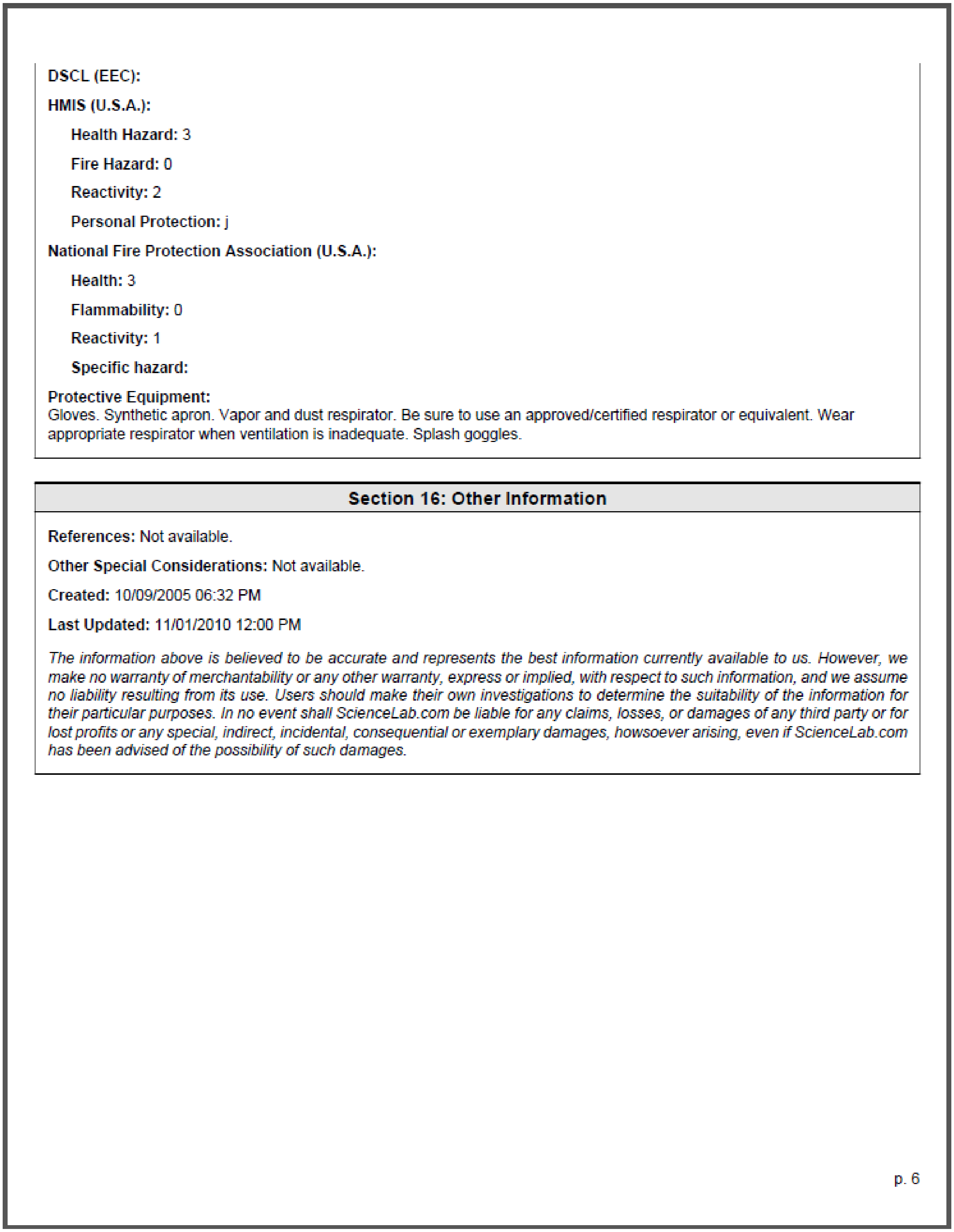

DSCL (EEC):

HMIS (U.S.A.):

Health Hazard: 3

Fire Hazard: 0

Reactivity: 2

Personal Protection: j

National Fire Protection Association (U.S.A.):

Health: 3

Flammability: 0

Reactivity: 1

Specific hazard:

Protective Equipment:
Gloves. Synthetic apron. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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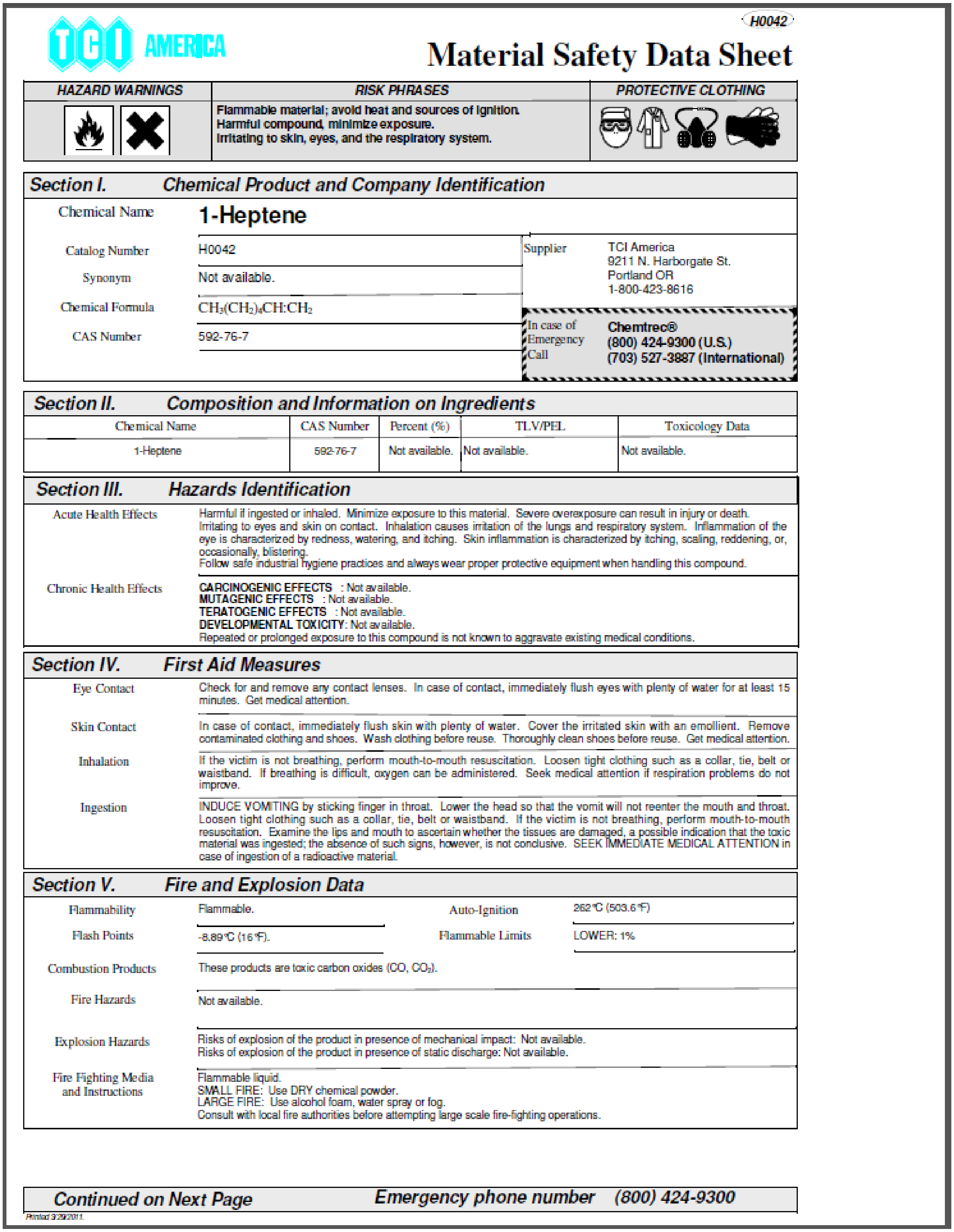

H0042

TCI AMERICA

Material Safety Data Sheet

HAZARD WARNINGS	RISK PHRASES	PROTECTIVE CLOTHING
	Flammable material; avoid heat and sources of ignition. **Harmful compound, minimize exposure.** **Irritating to skin, eyes, and the respiratory system.**	

Section I. Chemical Product and Company Identification

Chemical Name	**1-Heptene**
Catalog Number	H0042
Synonym	Not available.
Chemical Formula	$CH_3(CH_2)_4CH{:}CH_2$
CAS Number	592-76-7
Supplier	TCI America 9211 N. Harborgate St. Portland OR 1-800-423-8616
In case of Emergency Call	**Chemtrec®** **(800) 424-9300 (U.S.)** **(703) 527-3887 (International)**

Section II. Composition and Information on Ingredients

Chemical Name	CAS Number	Percent (%)	TLV/PEL	Toxicology Data
1-Heptene	592-76-7	Not available.	Not available.	Not available.

Section III. Hazards Identification

Acute Health Effects	Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.
Chronic Health Effects	**CARCINOGENIC EFFECTS** : Not available. **MUTAGENIC EFFECTS** : Not available. **TERATOGENIC EFFECTS** : Not available. **DEVELOPMENTAL TOXICITY**: Not available. Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.

Section IV. First Aid Measures

Eye Contact	Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Get medical attention.
Skin Contact	In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.
Inhalation	If the victim is not breathing, perform mouth-to-mouth resuscitation. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, oxygen can be administered. Seek medical attention if respiration problems do not improve.
Ingestion	INDUCE VOMITING by sticking finger in throat. Lower the head so that the vomit will not reenter the mouth and throat. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. SEEK IMMEDIATE MEDICAL ATTENTION in case of ingestion of a radioactive material.

Section V. Fire and Explosion Data

Flammability	Flammable.	Auto-Ignition	262°C (503.6°F)
Flash Points	-8.89°C (16°F).	Flammable Limits	LOWER: 1%
Combustion Products	These products are toxic carbon oxides (CO, CO_2).		
Fire Hazards	Not available.		
Explosion Hazards	Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.		
Fire Fighting Media and Instructions	Flammable liquid. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog. Consult with local fire authorities before attempting large scale fire-fighting operations.		

Continued on Next Page **Emergency phone number (800) 424-9300**

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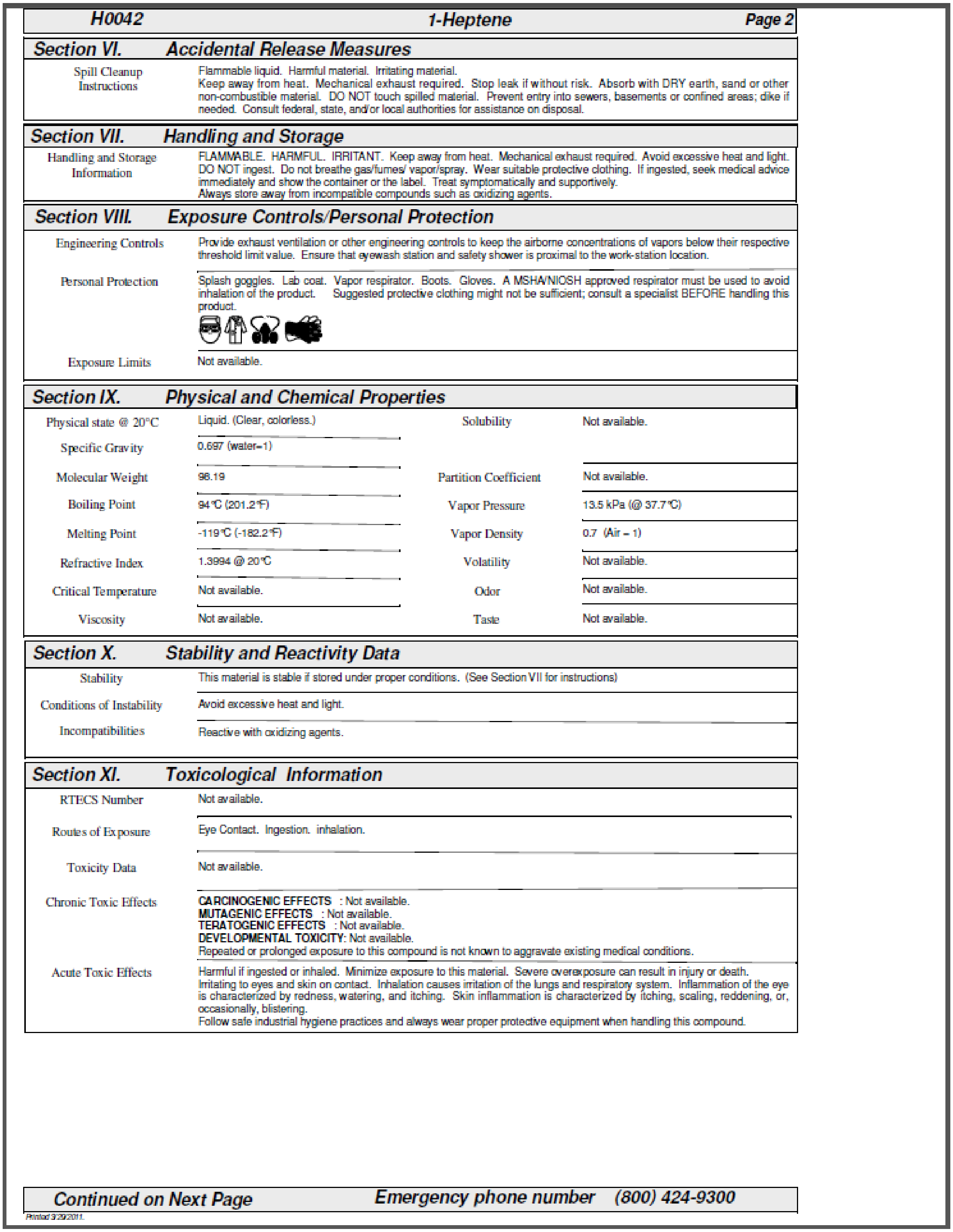

H0042 **1-Heptene** **Page 2**

Section VI. Accidental Release Measures

Spill Cleanup Instructions	Flammable liquid. Harmful material. Irritating material. Keep away from heat. Mechanical exhaust required. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. DO NOT touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Consult federal, state, and/or local authorities for assistance on disposal.

Section VII. Handling and Storage

Handling and Storage Information	FLAMMABLE. HARMFUL. IRRITANT. Keep away from heat. Mechanical exhaust required. Avoid excessive heat and light. DO NOT ingest. Do not breathe gas/fumes/ vapor/spray. Wear suitable protective clothing. If ingested, seek medical advice immediately and show the container or the label. Treat symptomatically and supportively. Always store away from incompatible compounds such as oxidizing agents.

Section VIII. Exposure Controls/Personal Protection

Engineering Controls	Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash station and safety shower is proximal to the work-station location.
Personal Protection	Splash goggles. Lab coat. Vapor respirator. Boots. Gloves. A MSHA/NIOSH approved respirator must be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.
Exposure Limits	Not available.

Section IX. Physical and Chemical Properties

Physical state @ 20°C	Liquid. (Clear, colorless.)	Solubility	Not available.
Specific Gravity	0.697 (water=1)		
Molecular Weight	98.19	Partition Coefficient	Not available.
Boiling Point	94°C (201.2°F)	Vapor Pressure	13.5 kPa (@ 37.7°C)
Melting Point	-119°C (-182.2°F)	Vapor Density	0.7 (Air = 1)
Refractive Index	1.3994 @ 20°C	Volatility	Not available.
Critical Temperature	Not available.	Odor	Not available.
Viscosity	Not available.	Taste	Not available.

Section X. Stability and Reactivity Data

Stability	This material is stable if stored under proper conditions. (See Section VII for instructions)
Conditions of Instability	Avoid excessive heat and light.
Incompatibilities	Reactive with oxidizing agents.

Section XI. Toxicological Information

RTECS Number	Not available.
Routes of Exposure	Eye Contact. Ingestion. inhalation.
Toxicity Data	Not available.
Chronic Toxic Effects	**CARCINOGENIC EFFECTS** : Not available. **MUTAGENIC EFFECTS** : Not available. **TERATOGENIC EFFECTS** : Not available. **DEVELOPMENTAL TOXICITY**: Not available. Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.
Acute Toxic Effects	Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.

Continued on Next Page **Emergency phone number (800) 424-9300**

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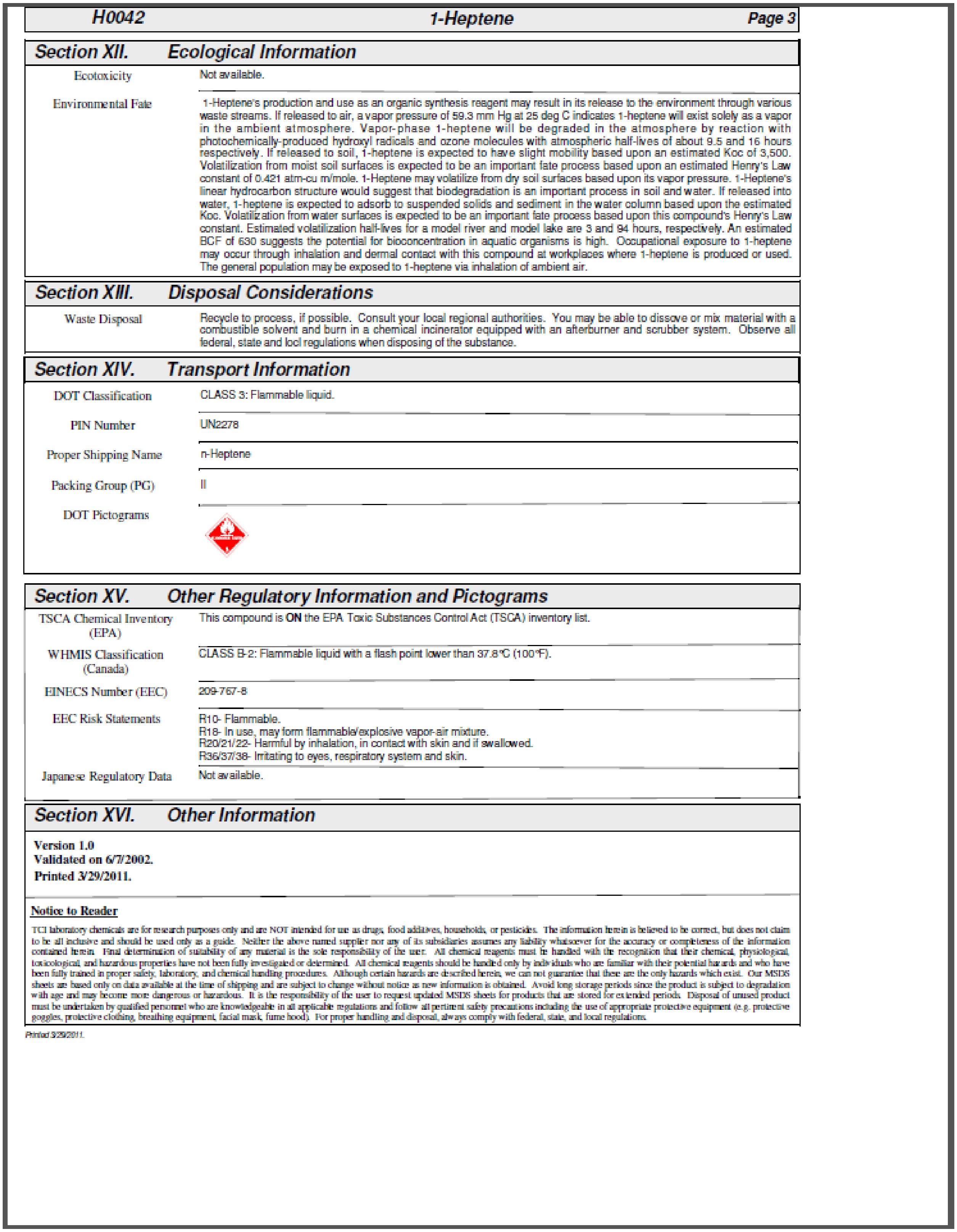

H0042 **1-Heptene** **Page 3**

Section XII. Ecological Information

Ecotoxicity	Not available.
Environmental Fate	1-Heptene's production and use as an organic synthesis reagent may result in its release to the environment through various waste streams. If released to air, a vapor pressure of 59.3 mm Hg at 25 deg C indicates 1-heptene will exist solely as a vapor in the ambient atmosphere. Vapor-phase 1-heptene will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals and ozone molecules with atmospheric half-lives of about 9.5 and 16 hours respectively. If released to soil, 1-heptene is expected to have slight mobility based upon an estimated Koc of 3,500. Volatilization from moist soil surfaces is expected to be an important fate process based upon an estimated Henry's Law constant of 0.421 atm-cu m/mole. 1-Heptene may volatilize from dry soil surfaces based upon its vapor pressure. 1-Heptene's linear hydrocarbon structure would suggest that biodegradation is an important process in soil and water. If released into water, 1-heptene is expected to adsorb to suspended solids and sediment in the water column based upon the estimated Koc. Volatilization from water surfaces is expected to be an important fate process based upon this compound's Henry's Law constant. Estimated volatilization half-lives for a model river and model lake are 3 and 94 hours, respectively. An estimated BCF of 630 suggests the potential for bioconcentration in aquatic organisms is high. Occupational exposure to 1-heptene may occur through inhalation and dermal contact with this compound at workplaces where 1-heptene is produced or used. The general population may be exposed to 1-heptene via inhalation of ambient air.

Section XIII. Disposal Considerations

Waste Disposal	Recycle to process, if possible. Consult your local regional authorities. You may be able to dissove or mix material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. Observe all federal, state and locl regulations when disposing of the substance.

Section XIV. Transport Information

DOT Classification	CLASS 3: Flammable liquid.
PIN Number	UN2278
Proper Shipping Name	n-Heptene
Packing Group (PG)	II
DOT Pictograms	

Section XV. Other Regulatory Information and Pictograms

TSCA Chemical Inventory (EPA)	This compound is **ON** the EPA Toxic Substances Control Act (TSCA) inventory list.
WHMIS Classification (Canada)	CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F).
EINECS Number (EEC)	209-767-8
EEC Risk Statements	R10- Flammable. R18- In use, may form flammable/explosive vapor-air mixture. R20/21/22- Harmful by inhalation, in contact with skin and if swallowed. R36/37/38- Irritating to eyes, respiratory system and skin.
Japanese Regulatory Data	Not available.

Section XVI. Other Information

Version 1.0
Validated on 6/7/2002.
Printed 3/29/2011.

Notice to Reader

TCI laboratory chemicals are for research purposes only and are NOT intended for use as drugs, food additives, households, or pesticides. The information herein is believed to be correct, but does not claim to be all inclusive and should be used only as a guide. Neither the above named supplier nor any of its subsidiaries assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All chemical reagents must be handled with the recognition that their chemical, physiological, toxicological, and hazardous properties have not been fully investigated or determined. All chemical reagents should be handled only by individuals who are familiar with their potential hazards and who have been fully trained in proper safety, laboratory, and chemical handling procedures. Although certain hazards are described herein, we can not guarantee that these are the only hazards which exist. Our MSDS sheets are based only on data available at the time of shipping and are subject to change without notice as new information is obtained. Avoid long storage periods since the product is subject to degradation with age and may become more dangerous or hazardous. It is the responsibility of the user to request updated MSDS sheets for products that are stored for extended periods. Disposal of unused product must be undertaken by qualified personnel who are knowledgeable in all applicable regulations and follow all pertinent safety precautions including the use of appropriate protective equipment (e.g. protective goggles, protective clothing, breathing equipment, facial mask, fume hood). For proper handling and disposal, always comply with federal, state, and local regulations.

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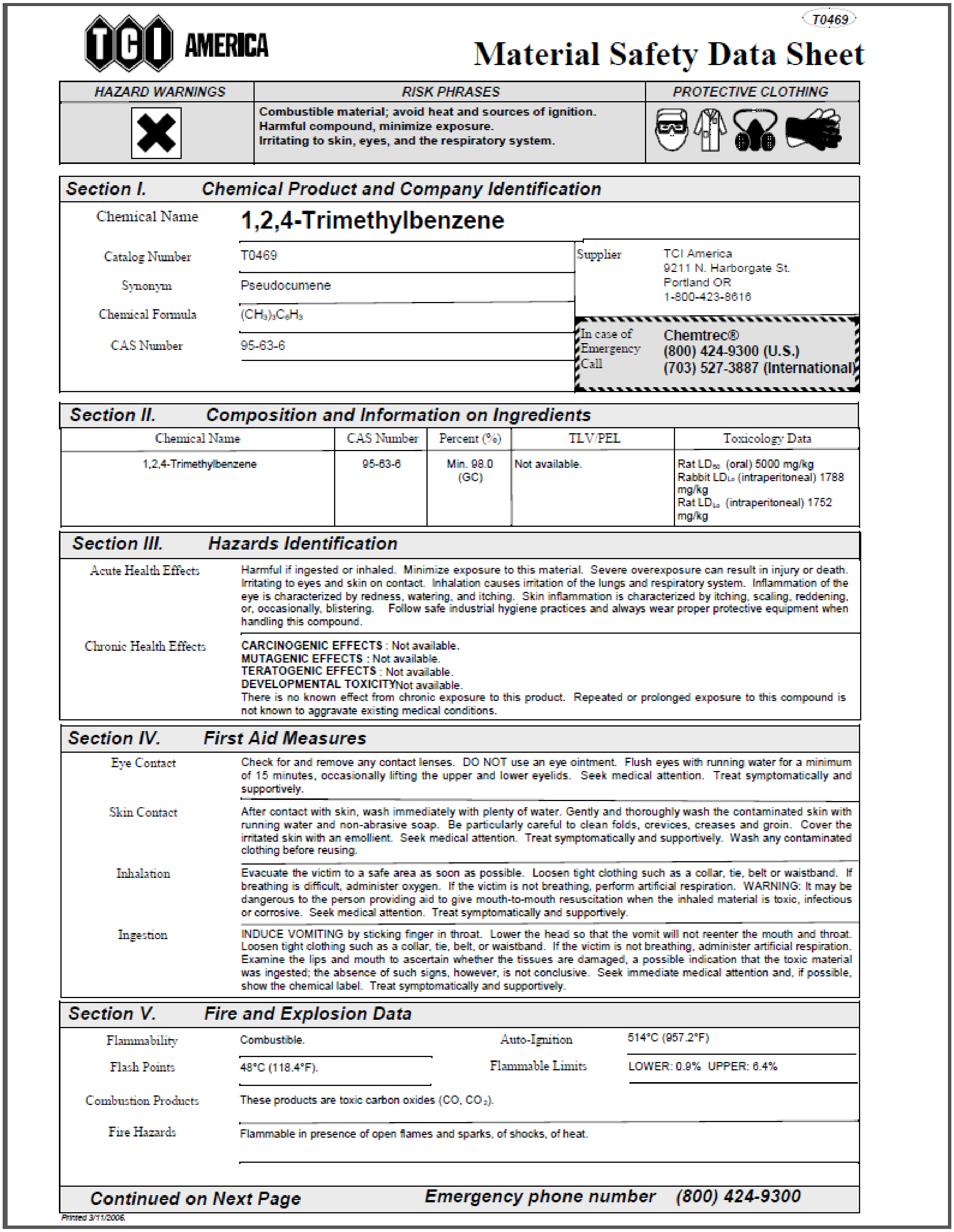

T0469

Material Safety Data Sheet

HAZARD WARNINGS	RISK PHRASES	PROTECTIVE CLOTHING
✖	**Combustible material; avoid heat and sources of ignition.** **Harmful compound, minimize exposure.** **Irritating to skin, eyes, and the respiratory system.**	

Section I. Chemical Product and Company Identification

Chemical Name	**1,2,4-Trimethylbenzene**
Catalog Number	T0469
Synonym	Pseudocumene
Chemical Formula	$(CH_3)_3C_6H_3$
CAS Number	95-63-6
Supplier	TCI America 9211 N. Harborgate St. Portland OR 1-800-423-8616
In case of Emergency Call	Chemtrec® (800) 424-9300 (U.S.) (703) 527-3887 (International)

Section II. Composition and Information on Ingredients

Chemical Name	CAS Number	Percent (%)	TLV/PEL	Toxicology Data
1,2,4-Trimethylbenzene	95-63-6	Min. 98.0 (GC)	Not available.	Rat LD$_{50}$ (oral) 5000 mg/kg Rabbit LD$_{Lo}$ (intraperitoneal) 1788 mg/kg Rat LD$_{Lo}$ (intraperitoneal) 1752 mg/kg

Section III. Hazards Identification

Acute Health Effects	Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.
Chronic Health Effects	**CARCINOGENIC EFFECTS** : Not available. **MUTAGENIC EFFECTS** : Not available. **TERATOGENIC EFFECTS** : Not available. **DEVELOPMENTAL TOXICITY**Not available. There is no known effect from chronic exposure to this product. Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.

Section IV. First Aid Measures

Eye Contact	Check for and remove any contact lenses. DO NOT use an eye ointment. Flush eyes with running water for a minimum of 15 minutes, occasionally lifting the upper and lower eyelids. Seek medical attention. Treat symptomatically and supportively.
Skin Contact	After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. Seek medical attention. Treat symptomatically and supportively. Wash any contaminated clothing before reusing.
Inhalation	Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform artificial respiration. WARNING: It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek medical attention. Treat symptomatically and supportively.
Ingestion	INDUCE VOMITING by sticking finger in throat. Lower the head so that the vomit will not reenter the mouth and throat. Loosen tight clothing such as a collar, tie, belt, or waistband. If the victim is not breathing, administer artificial respiration. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. Seek immediate medical attention and, if possible, show the chemical label. Treat symptomatically and supportively.

Section V. Fire and Explosion Data

Flammability	Combustible.	Auto-Ignition	514°C (957.2°F)
Flash Points	48°C (118.4°F).	Flammable Limits	LOWER: 0.9% UPPER: 6.4%
Combustion Products	These products are toxic carbon oxides (CO, CO_2).		
Fire Hazards	Flammable in presence of open flames and sparks, of shocks, of heat.		

Continued on Next Page **Emergency phone number (800) 424-9300**

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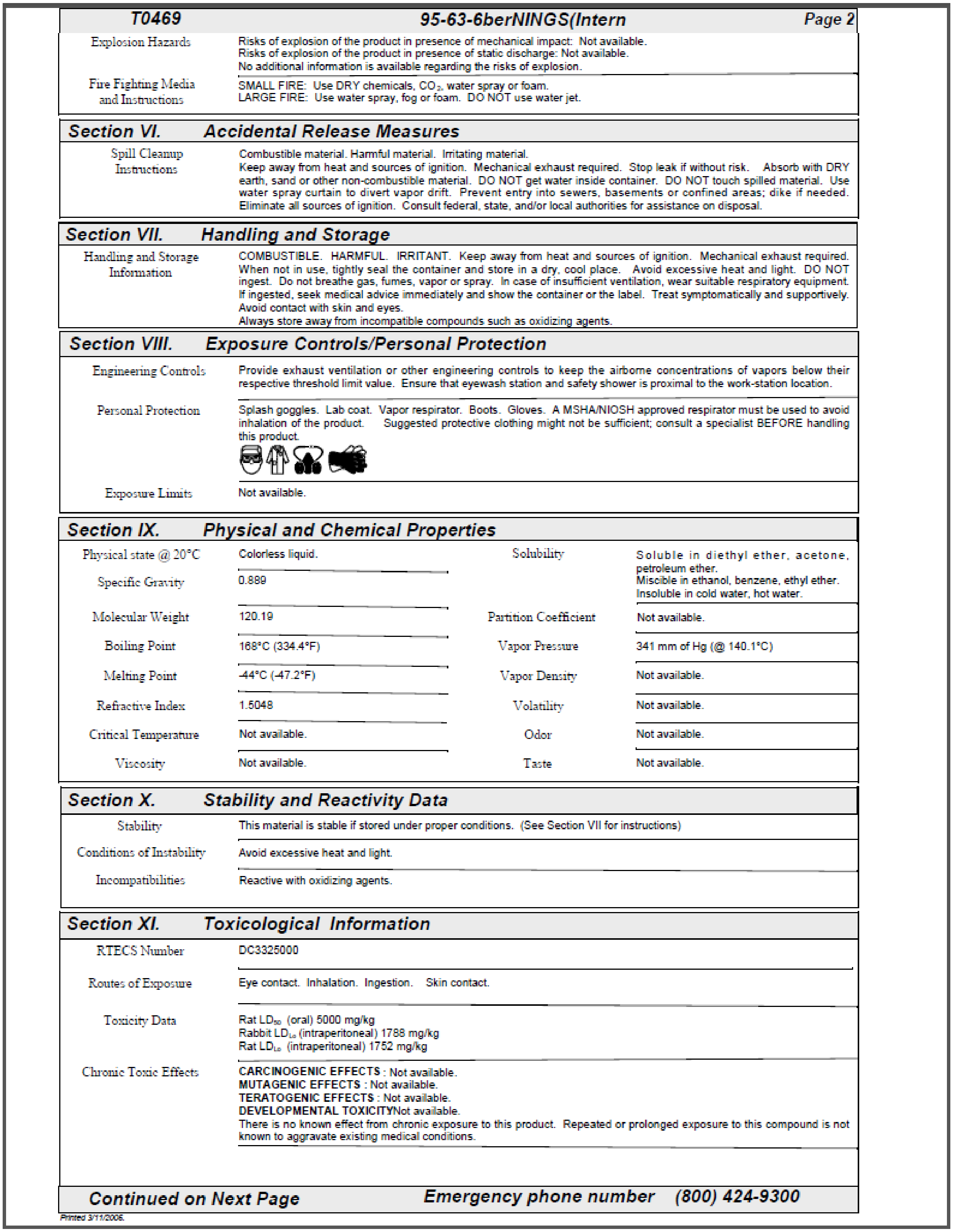

T0469 **95-63-6berNINGS(Intern** **Page 2**

Explosion Hazards	Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available. No additional information is available regarding the risks of explosion.
Fire Fighting Media and Instructions	SMALL FIRE: Use DRY chemicals, CO_2, water spray or foam. LARGE FIRE: Use water spray, fog or foam. DO NOT use water jet.

Section VI. Accidental Release Measures

Spill Cleanup Instructions	Combustible material. Harmful material. Irritating material. Keep away from heat and sources of ignition. Mechanical exhaust required. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. DO NOT get water inside container. DO NOT touch spilled material. Use water spray curtain to divert vapor drift. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all sources of ignition. Consult federal, state, and/or local authorities for assistance on disposal.

Section VII. Handling and Storage

Handling and Storage Information	COMBUSTIBLE. HARMFUL. IRRITANT. Keep away from heat and sources of ignition. Mechanical exhaust required. When not in use, tightly seal the container and store in a dry, cool place. Avoid excessive heat and light. DO NOT ingest. Do not breathe gas, fumes, vapor or spray. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Treat symptomatically and supportively. Avoid contact with skin and eyes. Always store away from incompatible compounds such as oxidizing agents.

Section VIII. Exposure Controls/Personal Protection

Engineering Controls	Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash station and safety shower is proximal to the work-station location.
Personal Protection	Splash goggles. Lab coat. Vapor respirator. Boots. Gloves. A MSHA/NIOSH approved respirator must be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.
Exposure Limits	Not available.

Section IX. Physical and Chemical Properties

Physical state @ 20°C	Colorless liquid.	Solubility	Soluble in diethyl ether, acetone, petroleum ether. Miscible in ethanol, benzene, ethyl ether. Insoluble in cold water, hot water.
Specific Gravity	0.889		
Molecular Weight	120.19	Partition Coefficient	Not available.
Boiling Point	168°C (334.4°F)	Vapor Pressure	341 mm of Hg (@ 140.1°C)
Melting Point	-44°C (-47.2°F)	Vapor Density	Not available.
Refractive Index	1.5048	Volatility	Not available.
Critical Temperature	Not available.	Odor	Not available.
Viscosity	Not available.	Taste	Not available.

Section X. Stability and Reactivity Data

Stability	This material is stable if stored under proper conditions. (See Section VII for instructions)
Conditions of Instability	Avoid excessive heat and light.
Incompatibilities	Reactive with oxidizing agents.

Section XI. Toxicological Information

RTECS Number	DC3325000
Routes of Exposure	Eye contact. Inhalation. Ingestion. Skin contact.
Toxicity Data	Rat LD_{50} (oral) 5000 mg/kg Rabbit LD_{Lo} (intraperitoneal) 1788 mg/kg Rat LD_{Lo} (intraperitoneal) 1752 mg/kg
Chronic Toxic Effects	**CARCINOGENIC EFFECTS** : Not available. **MUTAGENIC EFFECTS** : Not available. **TERATOGENIC EFFECTS** : Not available. **DEVELOPMENTAL TOXICITY**Not available. There is no known effect from chronic exposure to this product. Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.

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Emergency phone number (800) 424-9300

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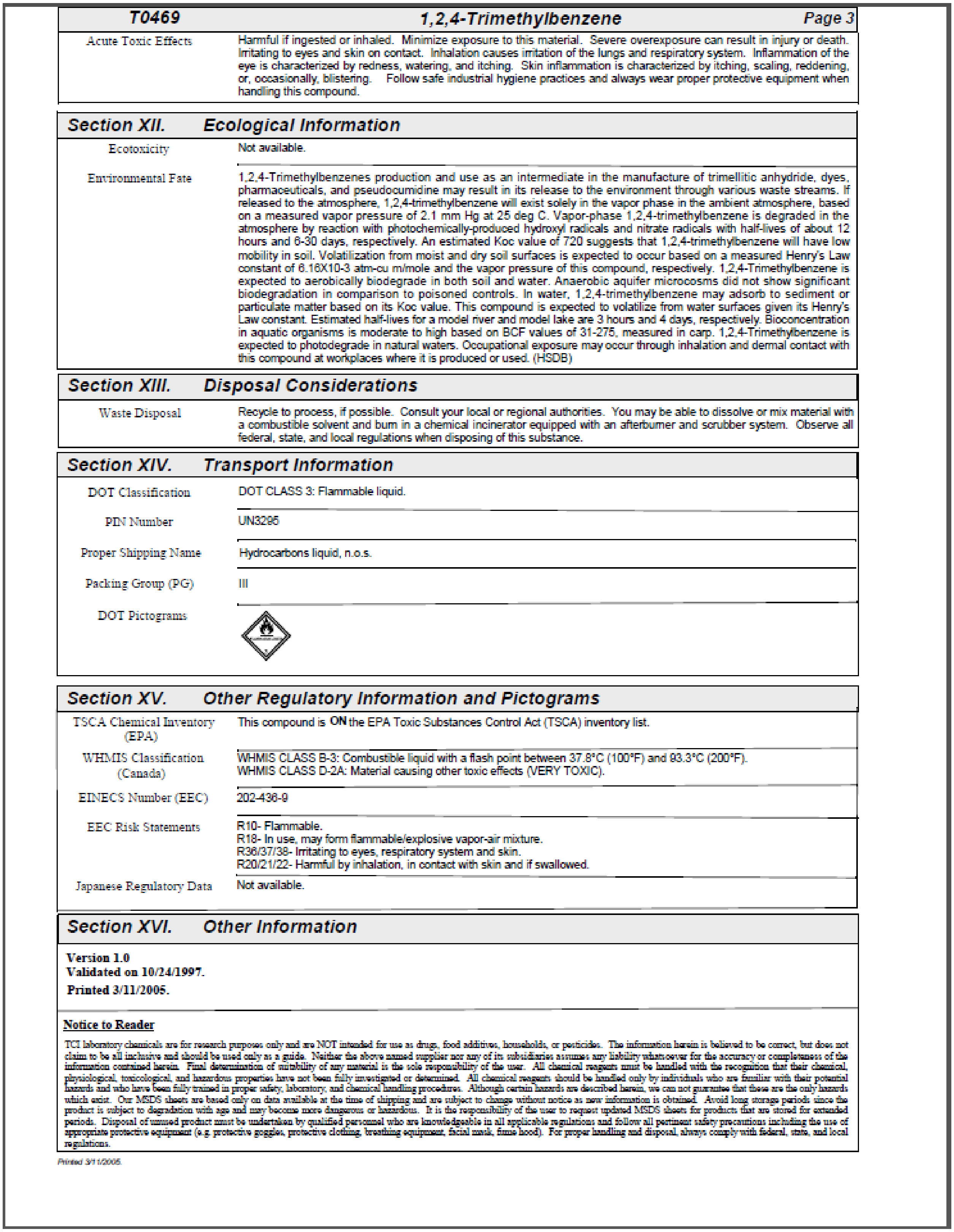


Acute Toxic Effects	Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.

Section XII. Ecological Information

Ecotoxicity	Not available.
Environmental Fate	1,2,4-Trimethylbenzenes production and use as an intermediate in the manufacture of trimellitic anhydride, dyes, pharmaceuticals, and pseudocumidine may result in its release to the environment through various waste streams. If released to the atmosphere, 1,2,4-trimethylbenzene will exist solely in the vapor phase in the ambient atmosphere, based on a measured vapor pressure of 2.1 mm Hg at 25 deg C. Vapor-phase 1,2,4-trimethylbenzene is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals and nitrate radicals with half-lives of about 12 hours and 6-30 days, respectively. An estimated Koc value of 720 suggests that 1,2,4-trimethylbenzene will have low mobility in soil. Volatilization from moist and dry soil surfaces is expected to occur based on a measured Henry's Law constant of 6.16X10-3 atm-cu m/mole and the vapor pressure of this compound, respectively. 1,2,4-Trimethylbenzene is expected to aerobically biodegrade in both soil and water. Anaerobic aquifer microcosms did not show significant biodegradation in comparison to poisoned controls. In water, 1,2,4-trimethylbenzene may adsorb to sediment or particulate matter based on its Koc value. This compound is expected to volatilize from water surfaces given its Henry's Law constant. Estimated half-lives for a model river and model lake are 3 hours and 4 days, respectively. Bioconcentration in aquatic organisms is moderate to high based on BCF values of 31-275, measured in carp. 1,2,4-Trimethylbenzene is expected to photodegrade in natural waters. Occupational exposure may occur through inhalation and dermal contact with this compound at workplaces where it is produced or used. (HSDB)

Section XIII. Disposal Considerations

Waste Disposal	Recycle to process, if possible. Consult your local or regional authorities. You may be able to dissolve or mix material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. Observe all federal, state, and local regulations when disposing of this substance.

Section XIV. Transport Information

DOT Classification	DOT CLASS 3: Flammable liquid.
PIN Number	UN3295
Proper Shipping Name	Hydrocarbons liquid, n.o.s.
Packing Group (PG)	III
DOT Pictograms	

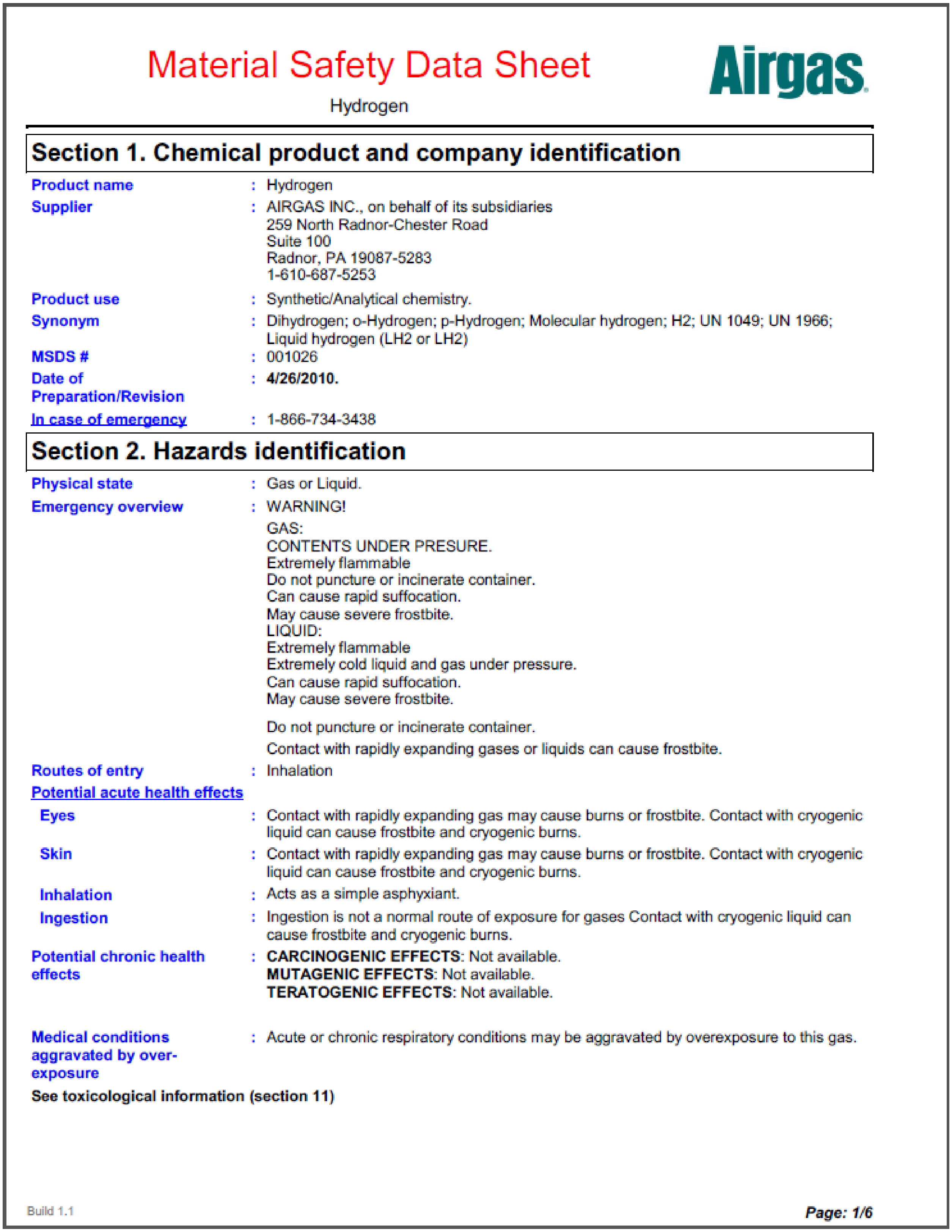
Section XV. Other Regulatory Information and Pictograms

TSCA Chemical Inventory (EPA)	This compound is ON the EPA Toxic Substances Control Act (TSCA) inventory list.
WHMIS Classification (Canada)	WHMIS CLASS B-3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F). WHMIS CLASS D-2A: Material causing other toxic effects (VERY TOXIC).
EINECS Number (EEC)	202-436-9
EEC Risk Statements	R10- Flammable. R18- In use, may form flammable/explosive vapor-air mixture. R36/37/38- Irritating to eyes, respiratory system and skin. R20/21/22- Harmful by inhalation, in contact with skin and if swallowed.
Japanese Regulatory Data	Not available.

Section XVI. Other Information

Version 1.0
Validated on 10/24/1997.
Printed 3/11/2005.

Notice to Reader



Material Safety Data Sheet

Airgas

Hydrogen

Section 1. Chemical product and company identification

Product name : Hydrogen

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : Dihydrogen; o-Hydrogen; p-Hydrogen; Molecular hydrogen; H2; UN 1049; UN 1966; Liquid hydrogen (LH2 or LH2)

MSDS # : 001026

Date of Preparation/Revision : **4/26/2010.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas or Liquid.

Emergency overview : WARNING!

GAS:
CONTENTS UNDER PRESURE.
Extremely flammable
Do not puncture or incinerate container.
Can cause rapid suffocation.
May cause severe frostbite.
LIQUID:
Extremely flammable
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.

Do not puncture or incinerate container.

Contact with rapidly expanding gases or liquids can cause frostbite.

Routes of entry : Inhalation

Potential acute health effects

Eyes : Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Skin : Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Inhalation : Acts as a simple asphyxiant.

Ingestion : Ingestion is not a normal route of exposure for gases Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Potential chronic health effects : **CARCINOGENIC EFFECTS**: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.

Medical conditions aggravated by over-exposure : Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.

See toxicological information (section 11)

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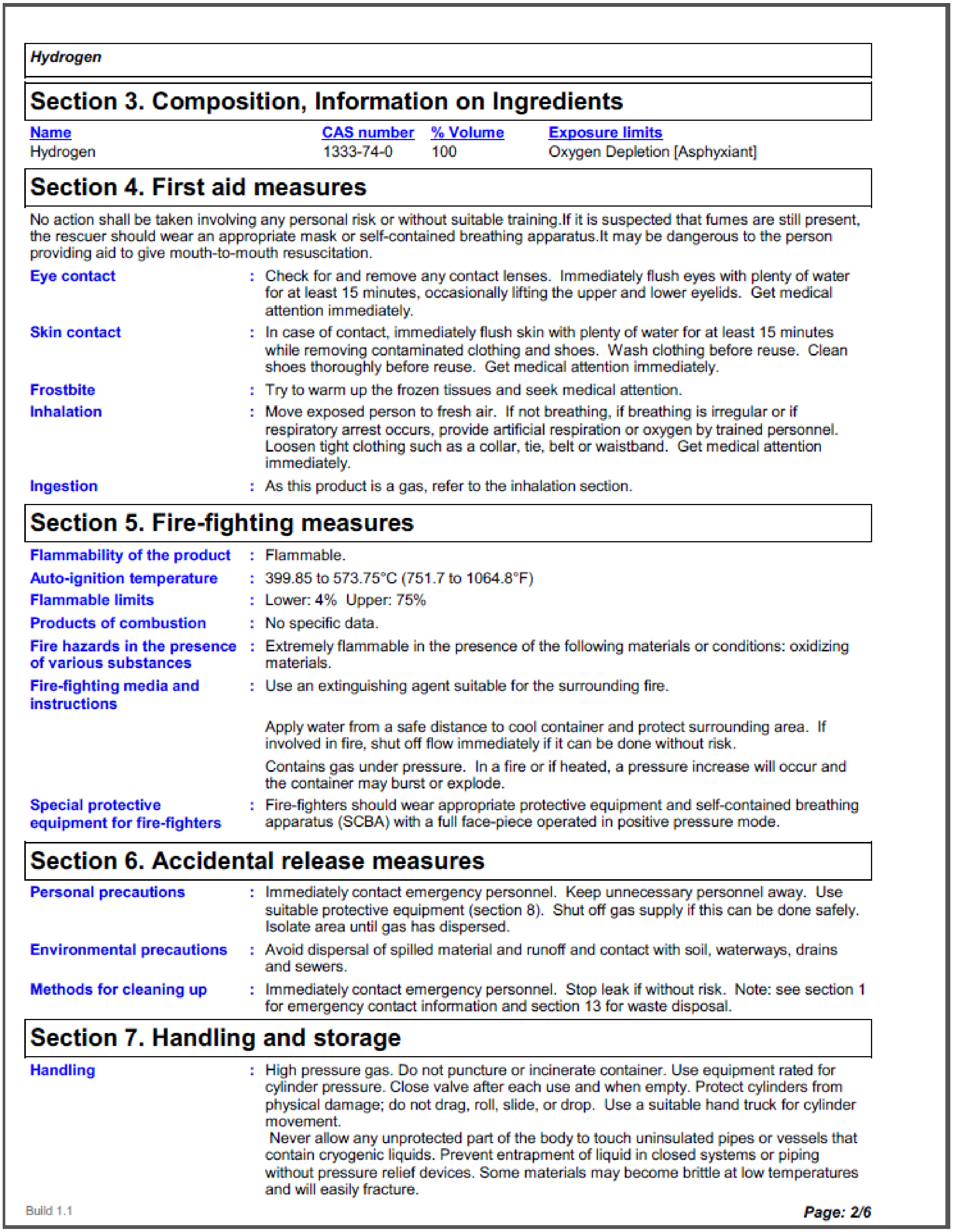


Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Hydrogen	1333-74-0	100	Oxygen Depletion [Asphyxiant]

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 399.85 to 573.75°C (751.7 to 1064.8°F)

Flammable limits : Lower: 4% Upper: 75%

Products of combustion : No specific data.

Fire hazards in the presence of various substances : Extremely flammable in the presence of the following materials or conditions: oxidizing materials.

Fire-fighting media and instructions : Use an extinguishing agent suitable for the surrounding fire.

Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. In a fire or if heated, a pressure increase will occur and the container may burst or explode.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

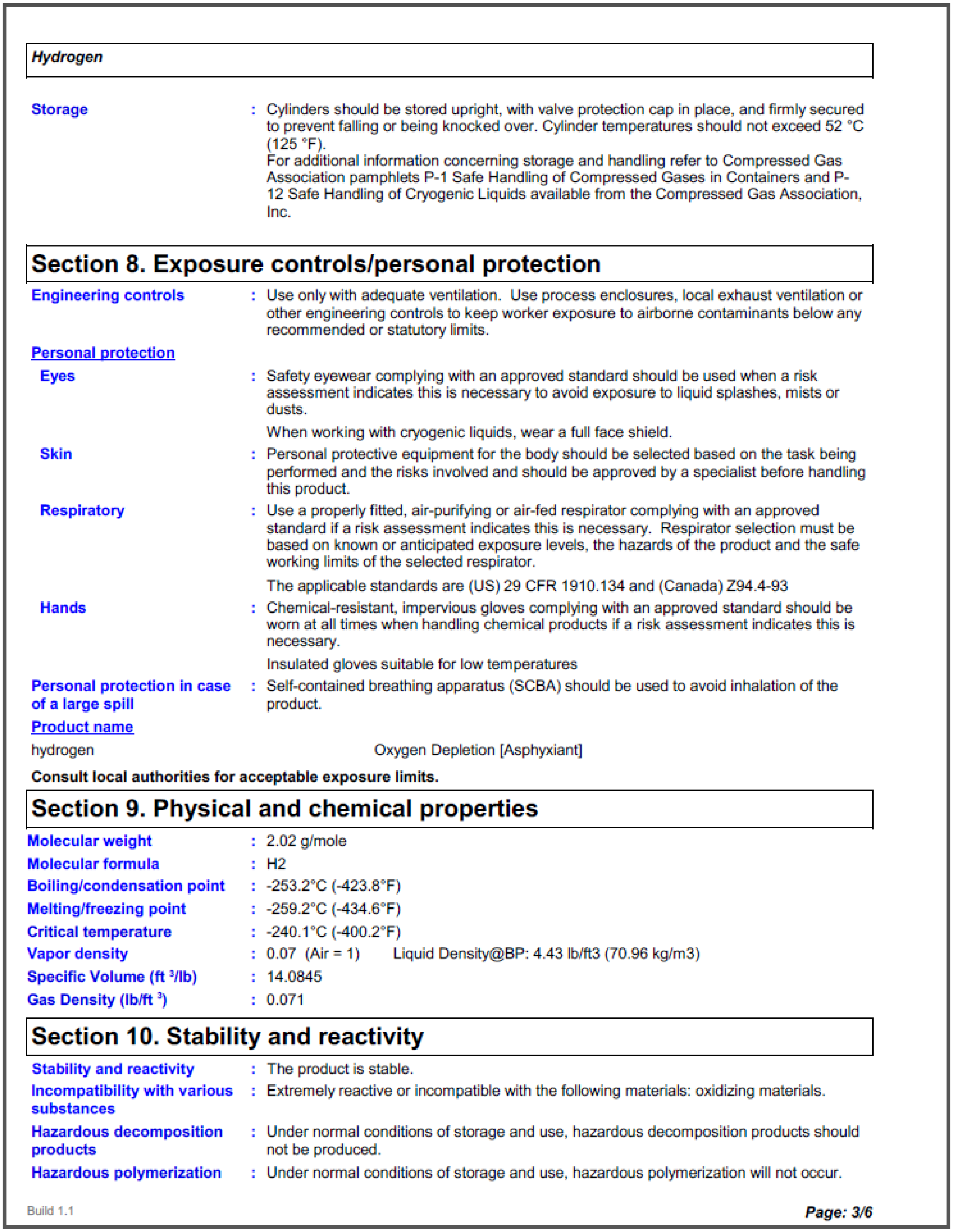
Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.



Hydrogen

Storage : Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).
For additional information concerning storage and handling refer to Compressed Gas Association pamphlets P-1 Safe Handling of Compressed Gases in Containers and P-12 Safe Handling of Cryogenic Liquids available from the Compressed Gas Association, Inc.

Section 8. Exposure controls/personal protection

Engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

When working with cryogenic liquids, wear a full face shield.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Insulated gloves suitable for low temperatures

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name	
hydrogen	Oxygen Depletion [Asphyxiant]

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight : 2.02 g/mole

Molecular formula : H2

Boiling/condensation point : -253.2°C (-423.8°F)

Melting/freezing point : -259.2°C (-434.6°F)

Critical temperature : -240.1°C (-400.2°F)

Vapor density : 0.07 (Air = 1) Liquid Density@BP: 4.43 lb/ft3 (70.96 kg/m3)

Specific Volume (ft ^{3}/lb) : 14.0845

Gas Density (lb/ft ^{3}) : 0.071

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.

Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.

Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

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Section 11. Toxicological information

Toxicity data

Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

- **Carcinogenic effects** : No known significant effects or critical hazards.
- **Mutagenic effects** : No known significant effects or critical hazards.
- **Reproduction toxicity** : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Environmental fate : Not available.

Environmental hazards : No known significant effects or critical hazards.

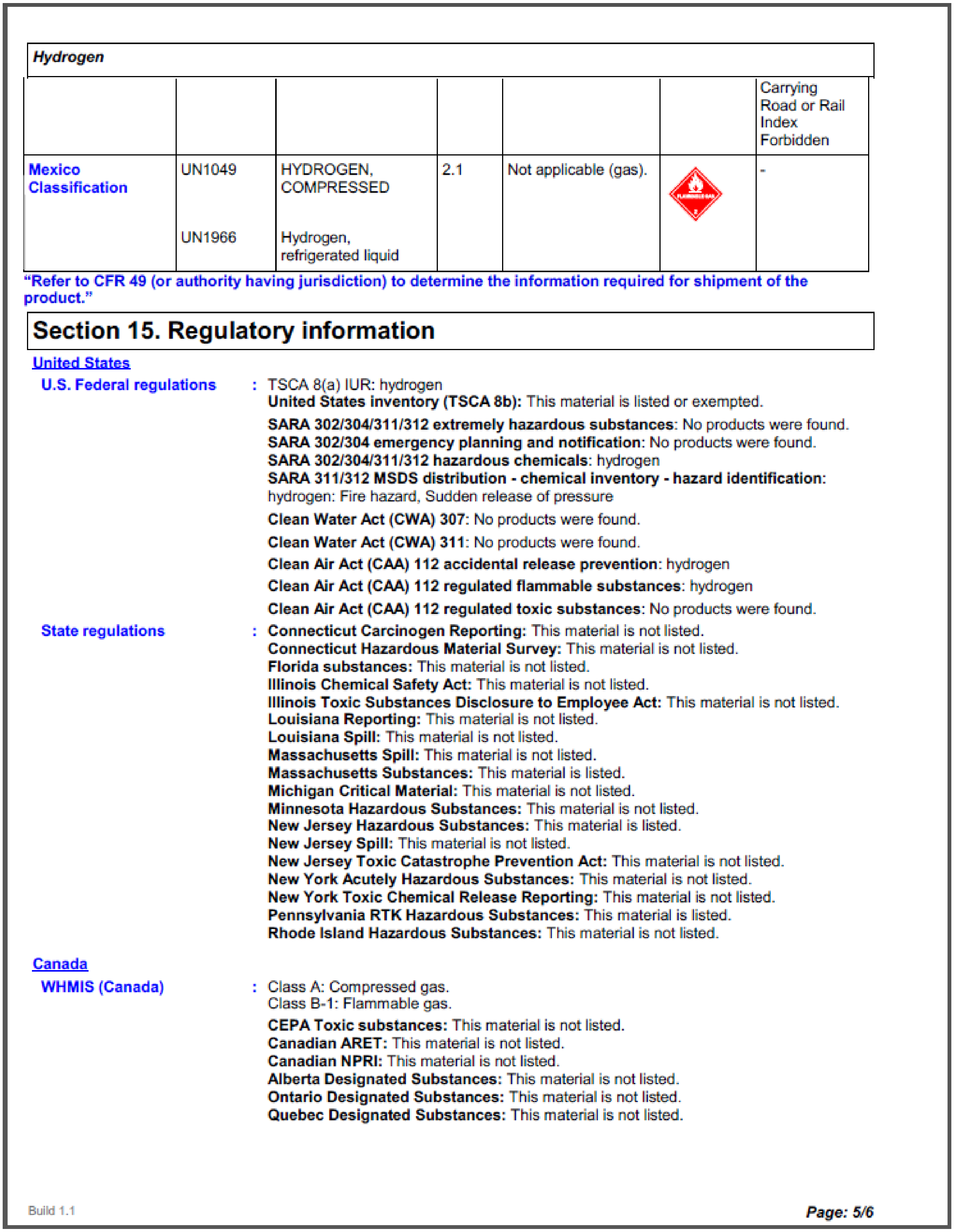
Toxicity to the environment : Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1049 UN1966	HYDROGEN, COMPRESSED Hydrogen, refrigerated liquid	2.1	Not applicable (gas).		**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: Forbidden. **Cargo aircraft** Quantity limitation: 150 kg
TDG Classification	UN1049 UN1966	HYDROGEN, COMPRESSED Hydrogen, refrigerated liquid	2.1	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0.125 **ERAP Index** 3000 **Passenger Carrying Ship Index** Forbidden **Passenger**



Hydrogen

						Carrying Road or Rail Index Forbidden
Mexico Classification	UN1049 UN1966	HYDROGEN, COMPRESSED Hydrogen, refrigerated liquid	2.1	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

U.S. Federal regulations : TSCA 8(a) IUR: hydrogen
United States inventory (TSCA 8b): This material is listed or exempted.
SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: hydrogen
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: hydrogen: Fire hazard, Sudden release of pressure
Clean Water Act (CWA) 307: No products were found.
Clean Water Act (CWA) 311: No products were found.
Clean Air Act (CAA) 112 accidental release prevention: hydrogen
Clean Air Act (CAA) 112 regulated flammable substances: hydrogen
Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

State regulations : **Connecticut Carcinogen Reporting:** This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class B-1: Flammable gas.
CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is not listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

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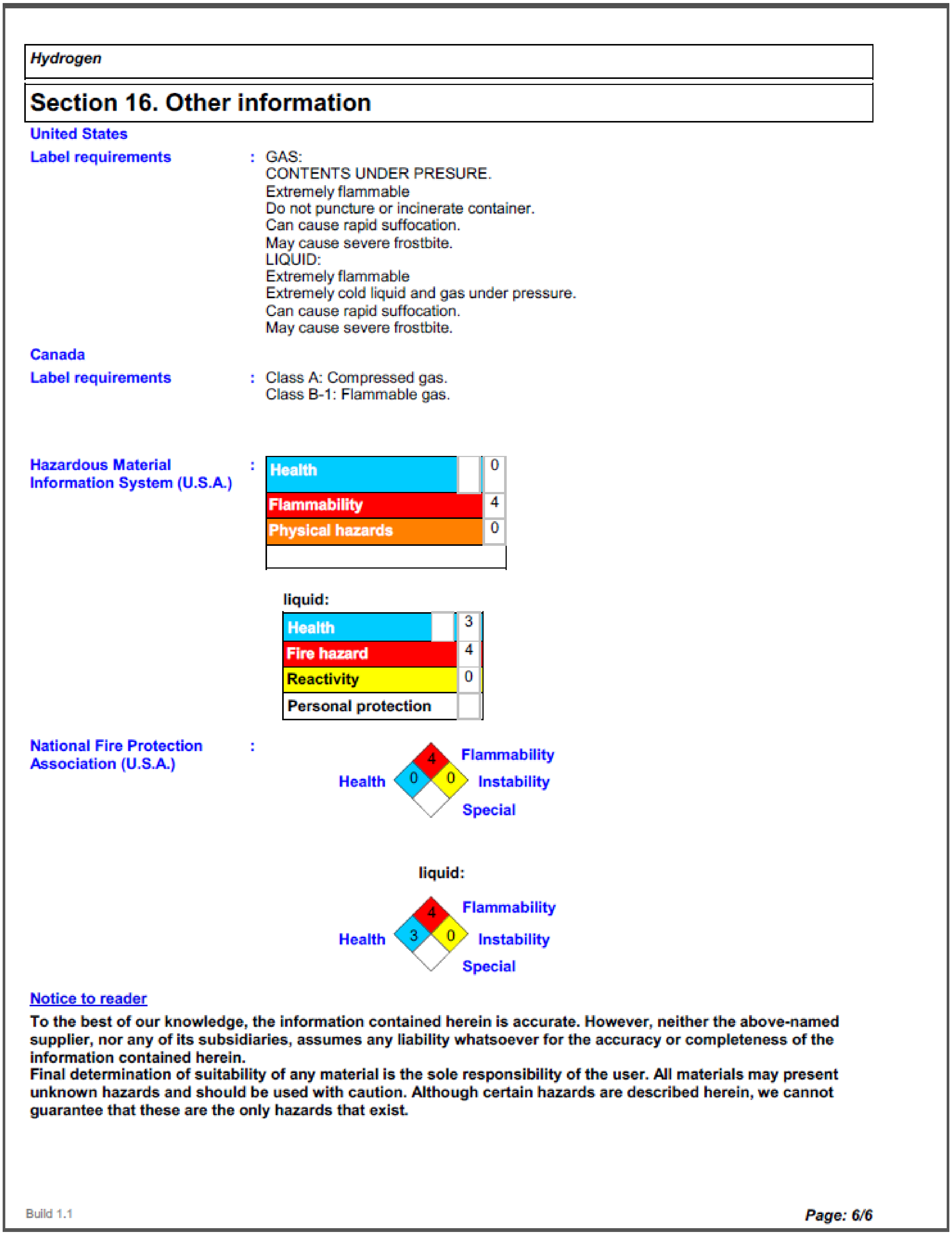

Hydrogen

Section 16. Other information

United States

Label requirements : GAS:
CONTENTS UNDER PRESURE.
Extremely flammable
Do not puncture or incinerate container.
Can cause rapid suffocation.
May cause severe frostbite.
LIQUID:
Extremely flammable
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.

Canada

Label requirements : Class A: Compressed gas.
Class B-1: Flammable gas.

Hazardous Material Information System (U.S.A.) :

Health	0
Flammability	4
Physical hazards	0

liquid:

Health	3
Fire hazard	4
Reactivity	0
Personal protection	

National Fire Protection Association (U.S.A.) :

Flammability 4
Health 0
Instability 0
Special

liquid:

Flammability 4
Health 3
Instability 0
Special

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

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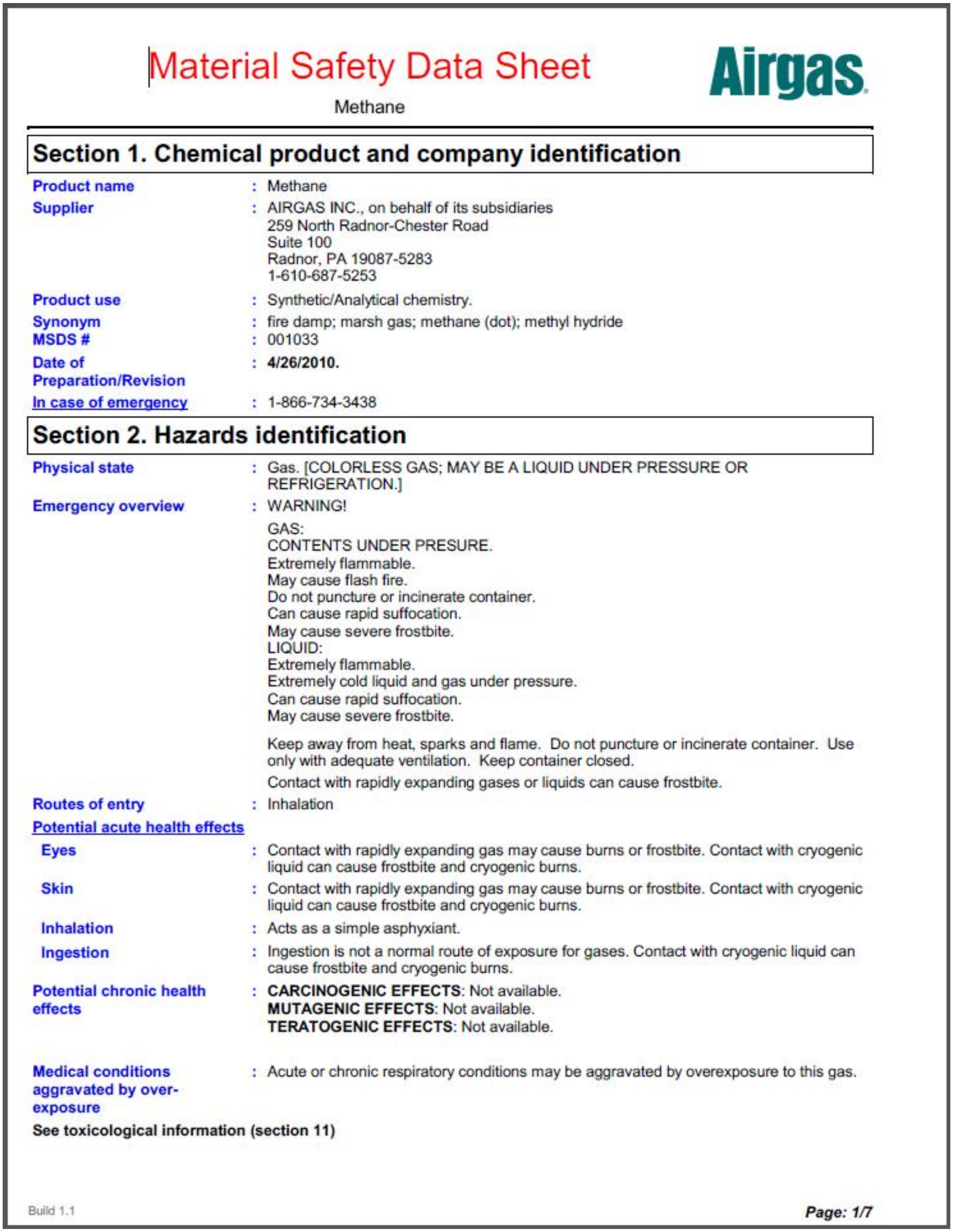

Material Safety Data Sheet

Airgas

Methane

Section 1. Chemical product and company identification

Product name	: Methane
Supplier	: AIRGAS INC., on behalf of its subsidiaries 259 North Radnor-Chester Road Suite 100 Radnor, PA 19087-5283 1-610-687-5253
Product use	: Synthetic/Analytical chemistry.
Synonym	: fire damp; marsh gas; methane (dot); methyl hydride
MSDS #	: 001033
Date of Preparation/Revision	: **4/26/2010.**
In case of emergency	: 1-866-734-3438

Section 2. Hazards identification

Physical state	: Gas. [COLORLESS GAS; MAY BE A LIQUID UNDER PRESSURE OR REFRIGERATION.]
Emergency overview	: WARNING! GAS: CONTENTS UNDER PRESURE. Extremely flammable. May cause flash fire. Do not puncture or incinerate container. Can cause rapid suffocation. May cause severe frostbite. LIQUID: Extremely flammable. Extremely cold liquid and gas under pressure. Can cause rapid suffocation. May cause severe frostbite. Keep away from heat, sparks and flame. Do not puncture or incinerate container. Use only with adequate ventilation. Keep container closed. Contact with rapidly expanding gases or liquids can cause frostbite.
Routes of entry	: Inhalation
Potential acute health effects	
Eyes	: Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.
Skin	: Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.
Inhalation	: Acts as a simple asphyxiant.
Ingestion	: Ingestion is not a normal route of exposure for gases. Contact with cryogenic liquid can cause frostbite and cryogenic burns.
Potential chronic health effects	: **CARCINOGENIC EFFECTS**: Not available. **MUTAGENIC EFFECTS**: Not available. **TERATOGENIC EFFECTS**: Not available.
Medical conditions aggravated by over-exposure	: Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.

See toxicological information (section 11)

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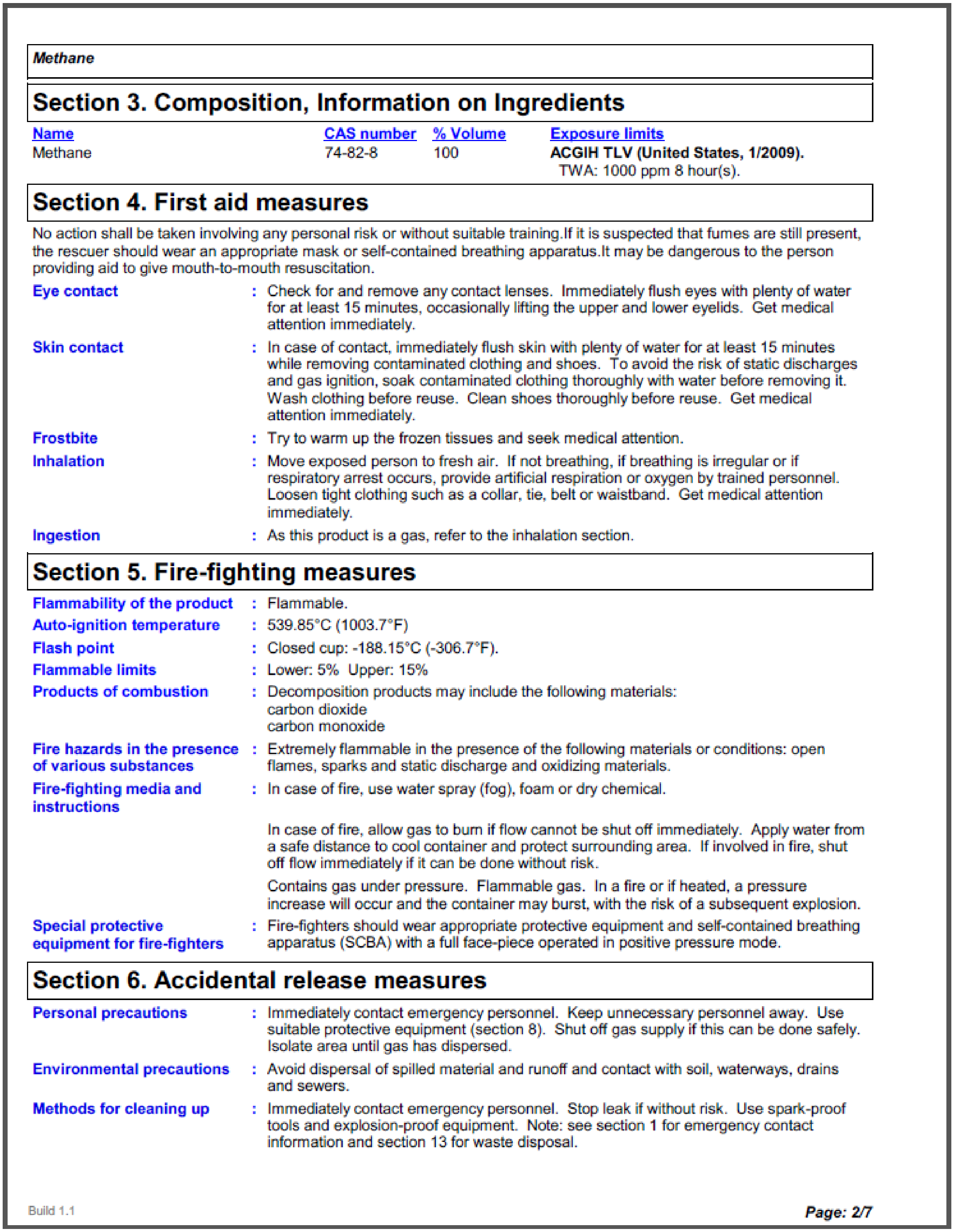


Methane

Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Methane	74-82-8	100	**ACGIH TLV (United States, 1/2009).** TWA: 1000 ppm 8 hour(s).

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 539.85°C (1003.7°F)

Flash point : Closed cup: -188.15°C (-306.7°F).

Flammable limits : Lower: 5% Upper: 15%

Products of combustion : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Fire hazards in the presence of various substances : Extremely flammable in the presence of the following materials or conditions: open flames, sparks and static discharge and oxidizing materials.

Fire-fighting media and instructions : In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

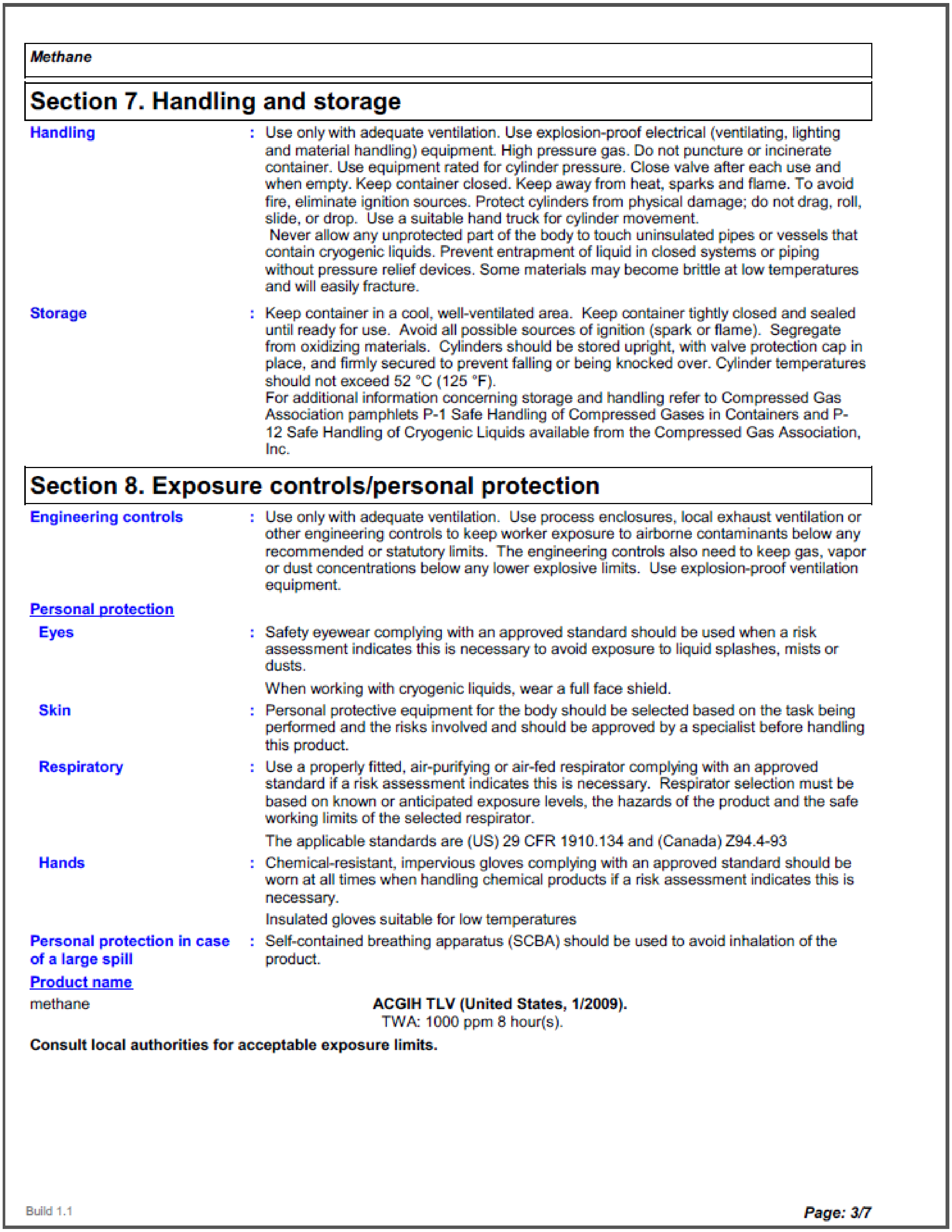
Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.



Methane

Section 7. Handling and storage

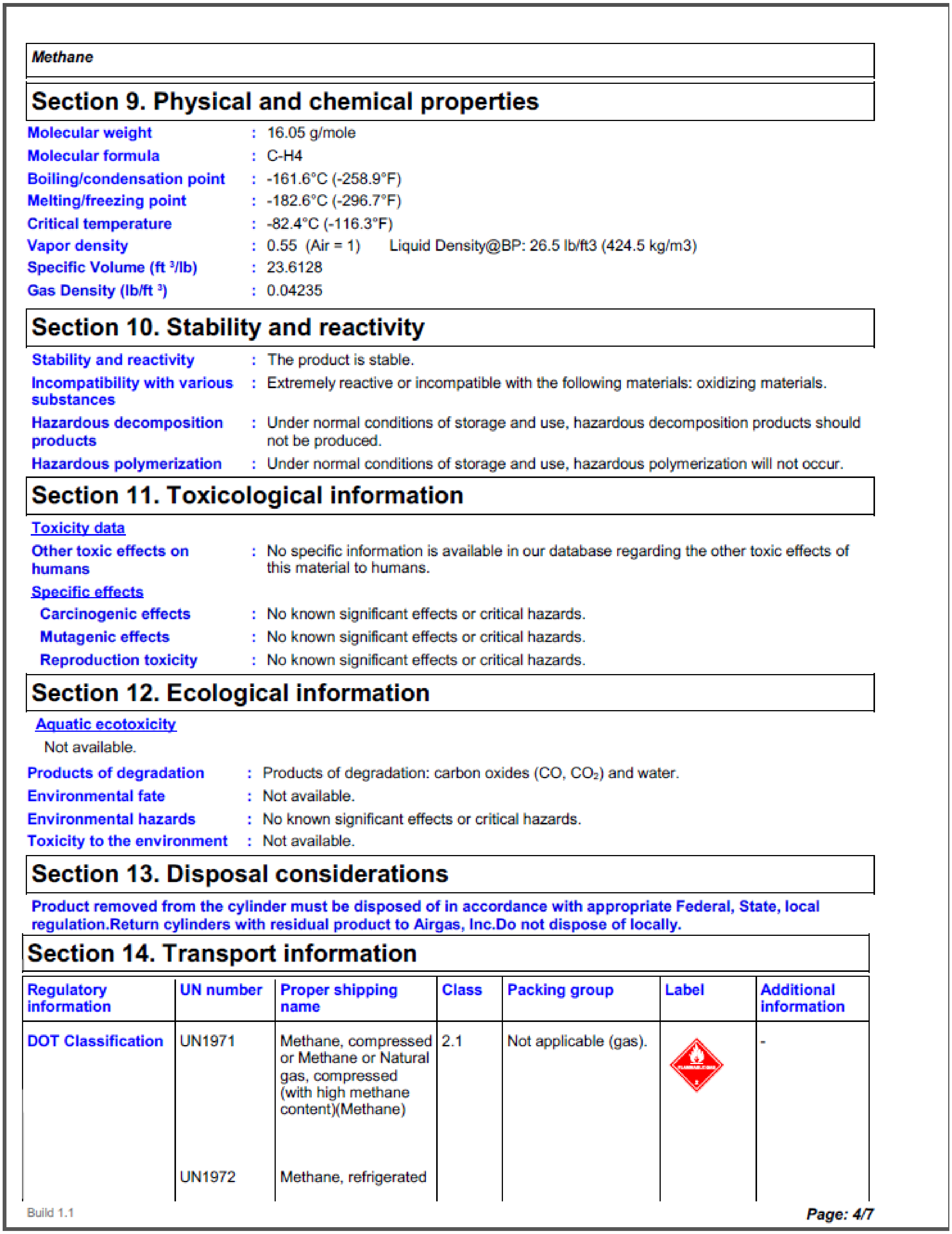
Handling	Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement. Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.
Storage	Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F). For additional information concerning storage and handling refer to Compressed Gas Association pamphlets P-1 Safe Handling of Compressed Gases in Containers and P-12 Safe Handling of Cryogenic Liquids available from the Compressed Gas Association, Inc.

Section 8. Exposure controls/personal protection

Engineering controls	Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.
Personal protection	
Eyes	Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts. When working with cryogenic liquids, wear a full face shield.
Skin	Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.
Respiratory	Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator. The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93
Hands	Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Insulated gloves suitable for low temperatures
Personal protection in case of a large spill	Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name	
methane	**ACGIH TLV (United States, 1/2009).** TWA: 1000 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.



Methane

Section 9. Physical and chemical properties

Molecular weight : 16.05 g/mole
Molecular formula : C-H4
Boiling/condensation point : -161.6°C (-258.9°F)
Melting/freezing point : -182.6°C (-296.7°F)
Critical temperature : -82.4°C (-116.3°F)
Vapor density : 0.55 (Air = 1) Liquid Density@BP: 26.5 lb/ft3 (424.5 kg/m3)
Specific Volume (ft^3/lb) : 23.6128
Gas Density (lb/ft^3) : 0.04235

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.
Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.
Mutagenic effects : No known significant effects or critical hazards.
Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Products of degradation : Products of degradation: carbon oxides (CO, CO_2) and water.
Environmental fate : Not available.
Environmental hazards : No known significant effects or critical hazards.
Toxicity to the environment : Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1971	Methane, compressed or Methane or Natural gas, compressed (with high methane content)(Methane)	2.1	Not applicable (gas).		-
	UN1972	Methane, refrigerated				

Build 1.1

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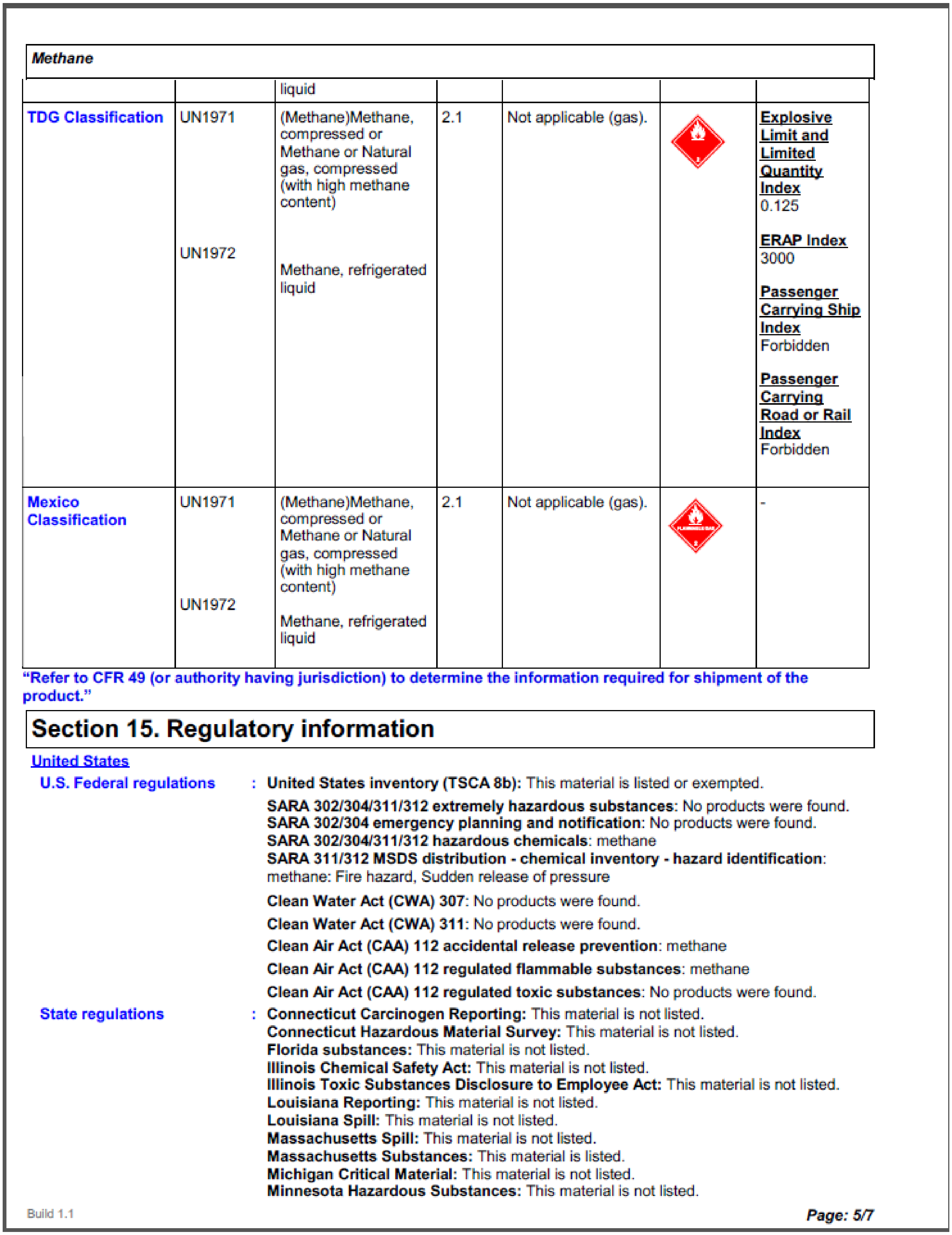


Methane

		liquid				
TDG Classification	UN1971 UN1972	(Methane)Methane, compressed or Methane or Natural gas, compressed (with high methane content) Methane, refrigerated liquid	2.1	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0.125 **ERAP Index** 3000 **Passenger Carrying Ship Index** Forbidden **Passenger Carrying Road or Rail Index** Forbidden
Mexico Classification	UN1971 UN1972	(Methane)Methane, compressed or Methane or Natural gas, compressed (with high methane content) Methane, refrigerated liquid	2.1	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

U.S. Federal regulations : **United States inventory (TSCA 8b):** This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: methane
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: methane: Fire hazard, Sudden release of pressure

Clean Water Act (CWA) 307: No products were found.

Clean Water Act (CWA) 311: No products were found.

Clean Air Act (CAA) 112 accidental release prevention: methane

Clean Air Act (CAA) 112 regulated flammable substances: methane

Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

State regulations : **Connecticut Carcinogen Reporting:** This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.

New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class B-1: Flammable gas.

CEPA Toxic substances: This material is listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

United States

Label requirements : GAS:
CONTENTS UNDER PRESURE.
Extremely flammable.
May cause flash fire.
Do not puncture or incinerate container.
Can cause rapid suffocation.
May cause severe frostbite.
LIQUID:
Extremely flammable.
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.

Canada

Label requirements : Class A: Compressed gas.
Class B-1: Flammable gas.

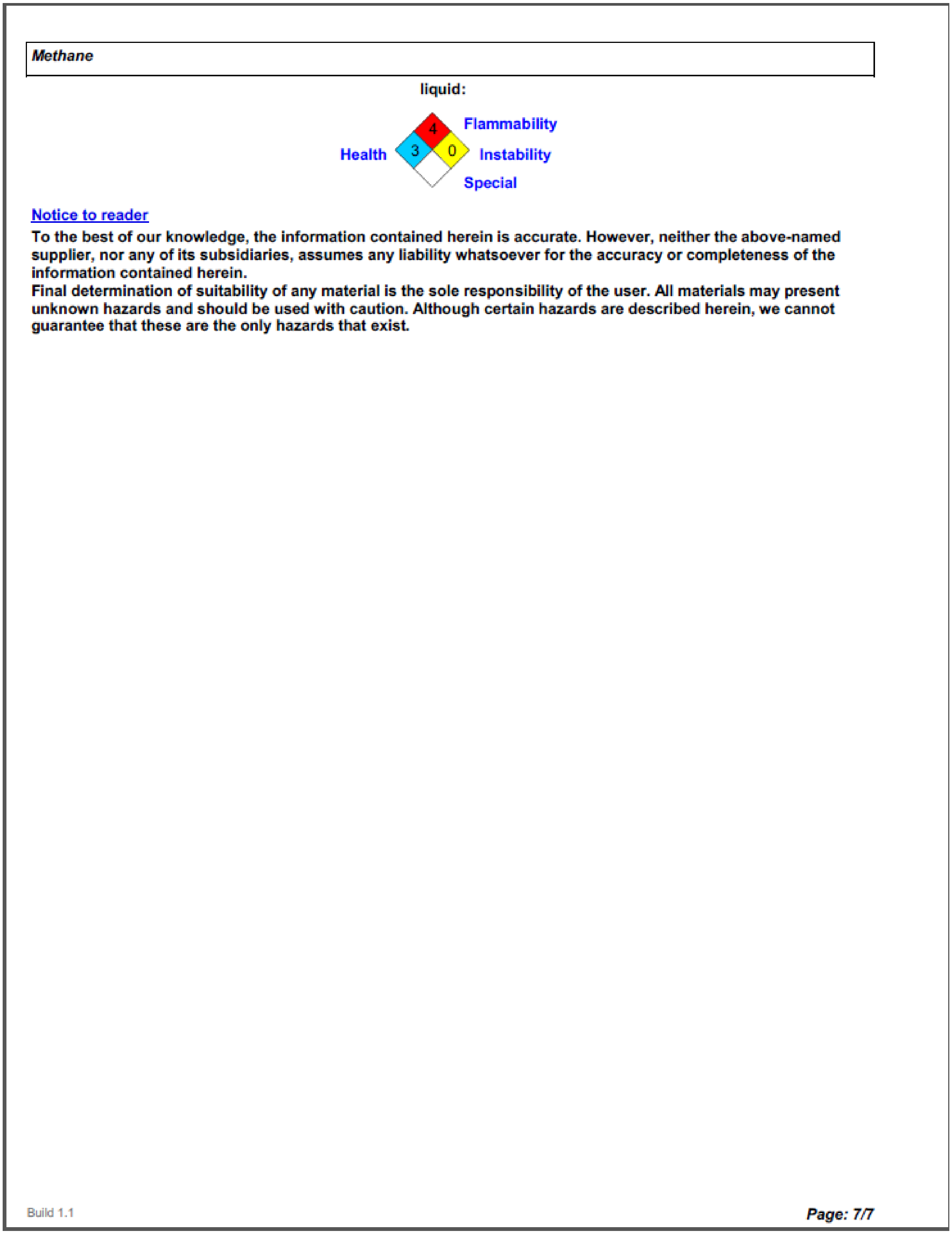
Hazardous Material Information System (U.S.A.) :

Health	1
Flammability	4
Physical hazards	0

liquid:

Health	3
Fire hazard	4
Reactivity	1
Personal protection	

National Fire Protection Association (U.S.A.) :



Methane

liquid:

Flammability 4
Health 3
Instability 0
Special

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

Build 1.1

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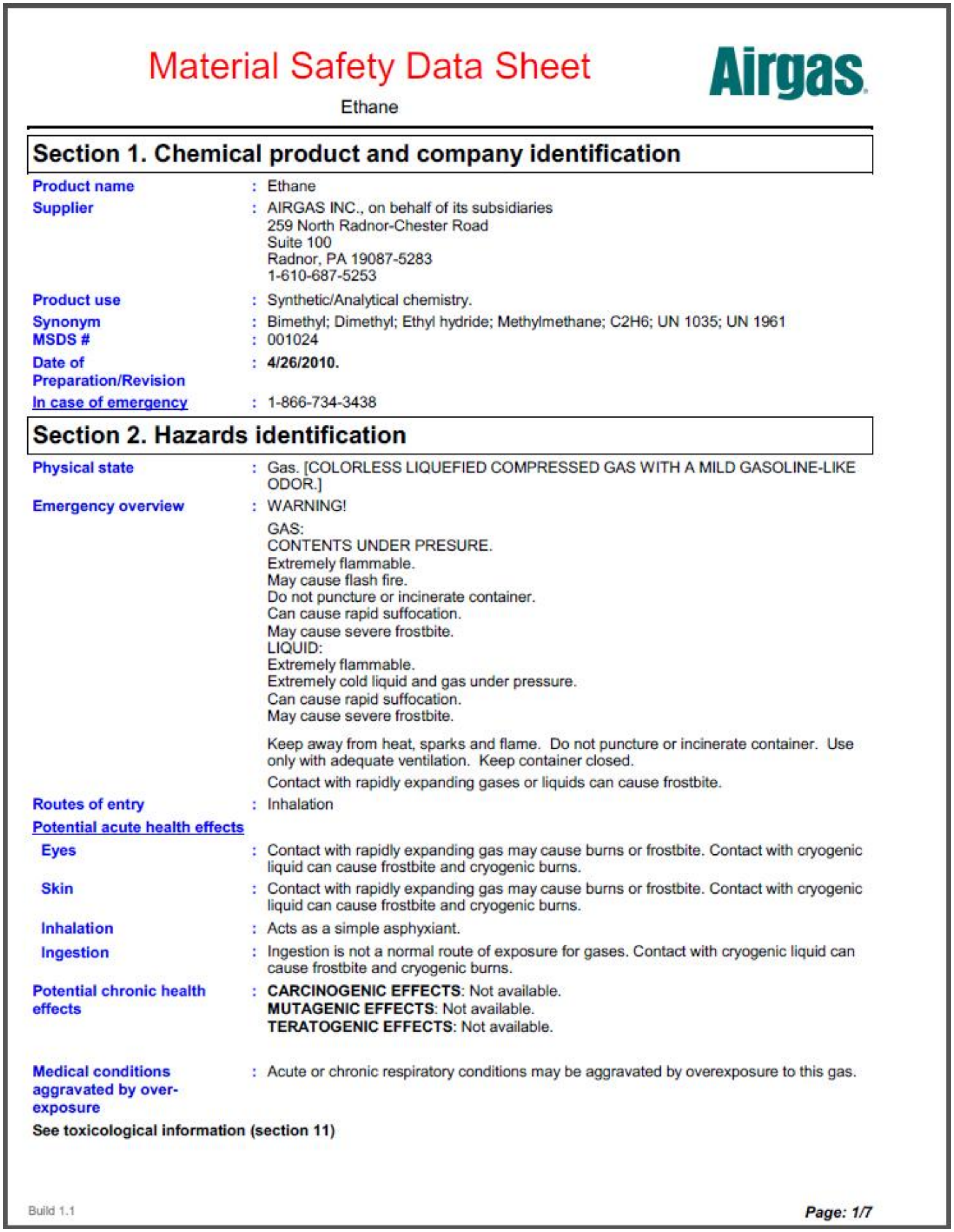

Material Safety Data Sheet

Ethane

Section 1. Chemical product and company identification

Product name : Ethane

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : Bimethyl; Dimethyl; Ethyl hydride; Methylmethane; C2H6; UN 1035; UN 1961

MSDS # : 001024

Date of Preparation/Revision : **4/26/2010.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas. [COLORLESS LIQUEFIED COMPRESSED GAS WITH A MILD GASOLINE-LIKE ODOR.]

Emergency overview : WARNING!

GAS:
CONTENTS UNDER PRESURE.
Extremely flammable.
May cause flash fire.
Do not puncture or incinerate container.
Can cause rapid suffocation.
May cause severe frostbite.
LIQUID:
Extremely flammable.
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.

Keep away from heat, sparks and flame. Do not puncture or incinerate container. Use only with adequate ventilation. Keep container closed.

Contact with rapidly expanding gases or liquids can cause frostbite.

Routes of entry : Inhalation

Potential acute health effects

Eyes : Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Skin : Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Inhalation : Acts as a simple asphyxiant.

Ingestion : Ingestion is not a normal route of exposure for gases. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Potential chronic health effects : **CARCINOGENIC EFFECTS**: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.

Medical conditions aggravated by over-exposure : Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.

See toxicological information (section 11)

Build 1.1

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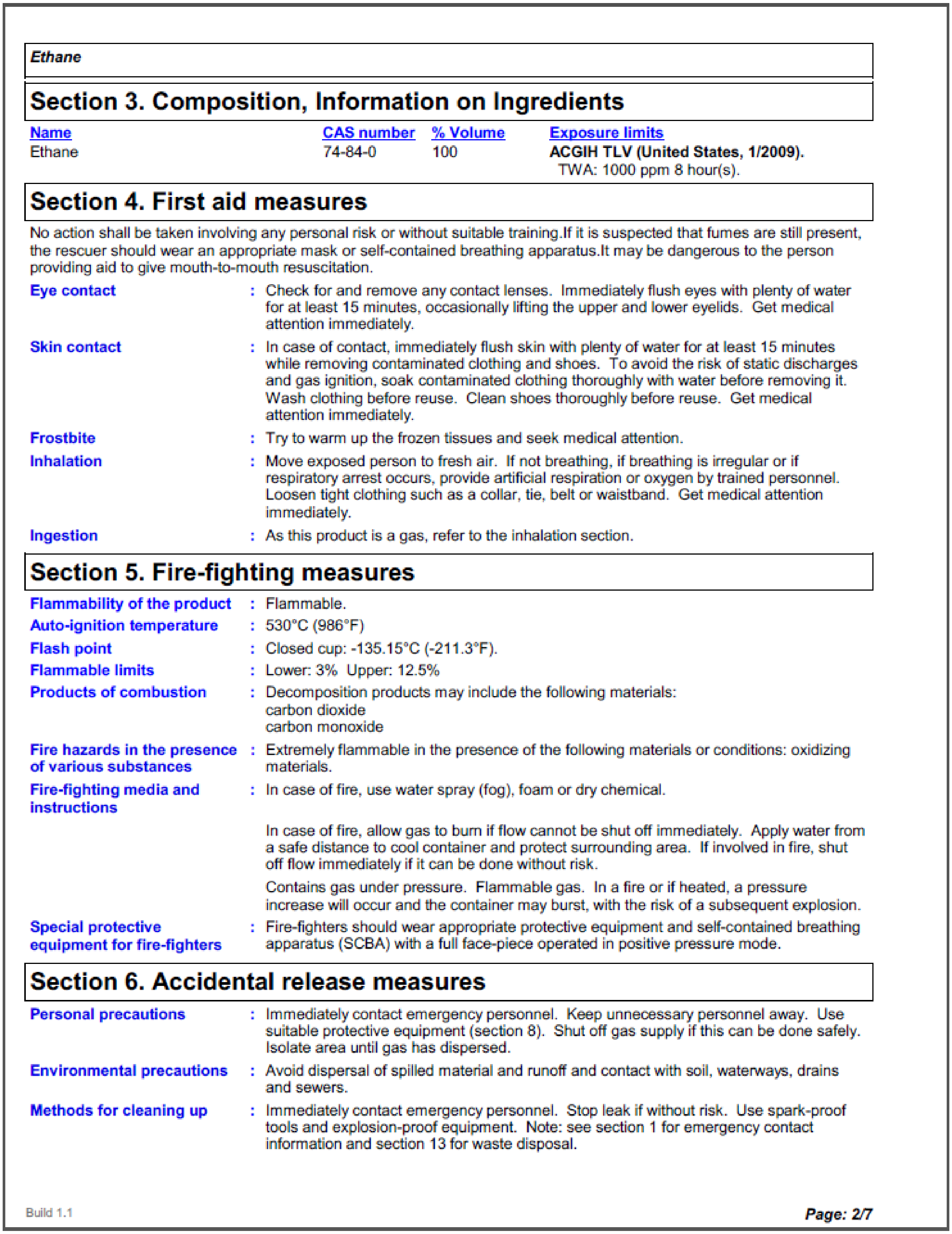

Ethane

Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Ethane	74-84-0	100	**ACGIH TLV (United States, 1/2009).** TWA: 1000 ppm 8 hour(s).

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 530°C (986°F)

Flash point : Closed cup: -135.15°C (-211.3°F).

Flammable limits : Lower: 3% Upper: 12.5%

Products of combustion : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Fire hazards in the presence of various substances : Extremely flammable in the presence of the following materials or conditions: oxidizing materials.

Fire-fighting media and instructions : In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.

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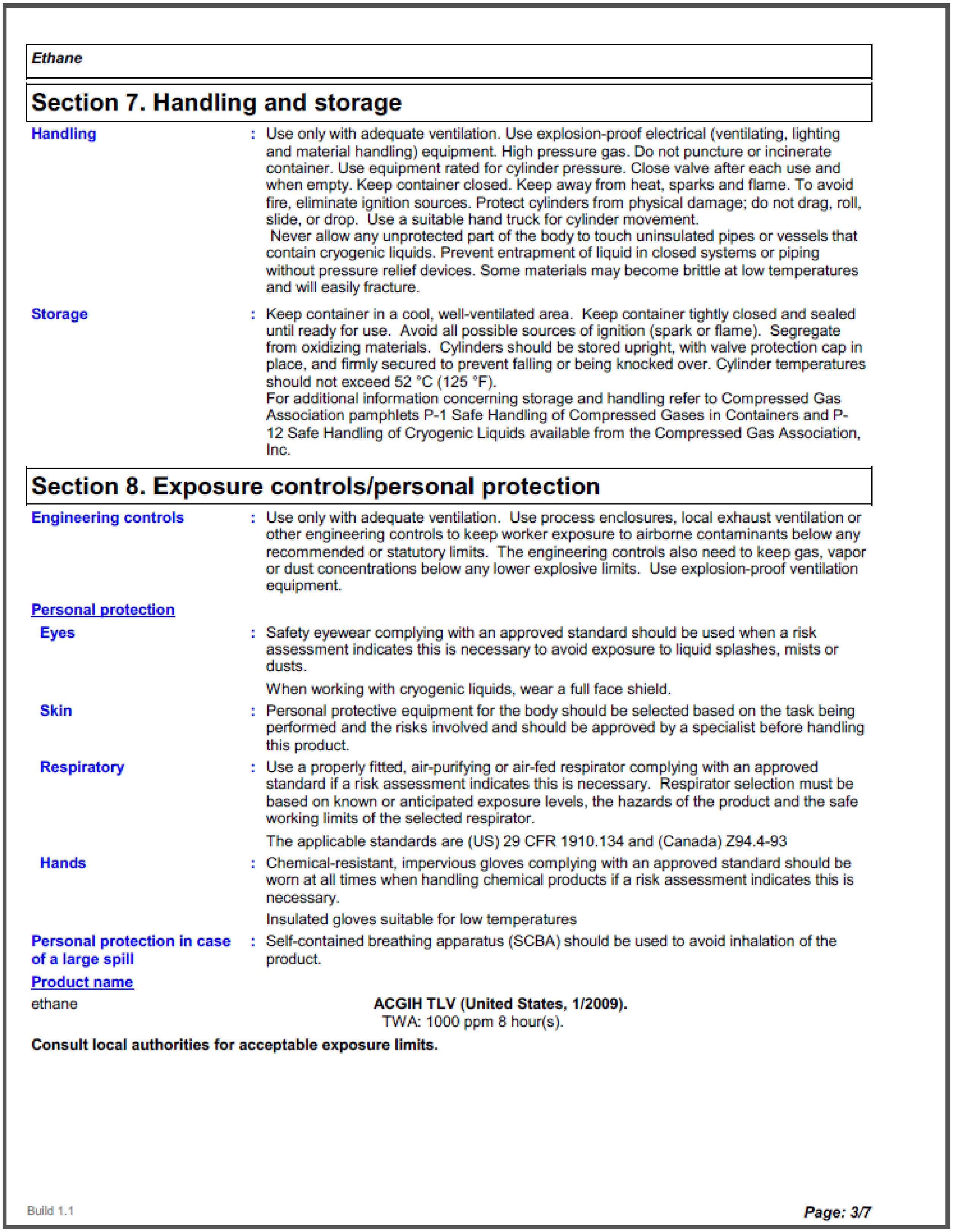


Section 7. Handling and storage

Handling : Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.
Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.

Storage : Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).
For additional information concerning storage and handling refer to Compressed Gas Association pamphlets P-1 Safe Handling of Compressed Gases in Containers and P-12 Safe Handling of Cryogenic Liquids available from the Compressed Gas Association, Inc.

Section 8. Exposure controls/personal protection

Engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

When working with cryogenic liquids, wear a full face shield.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

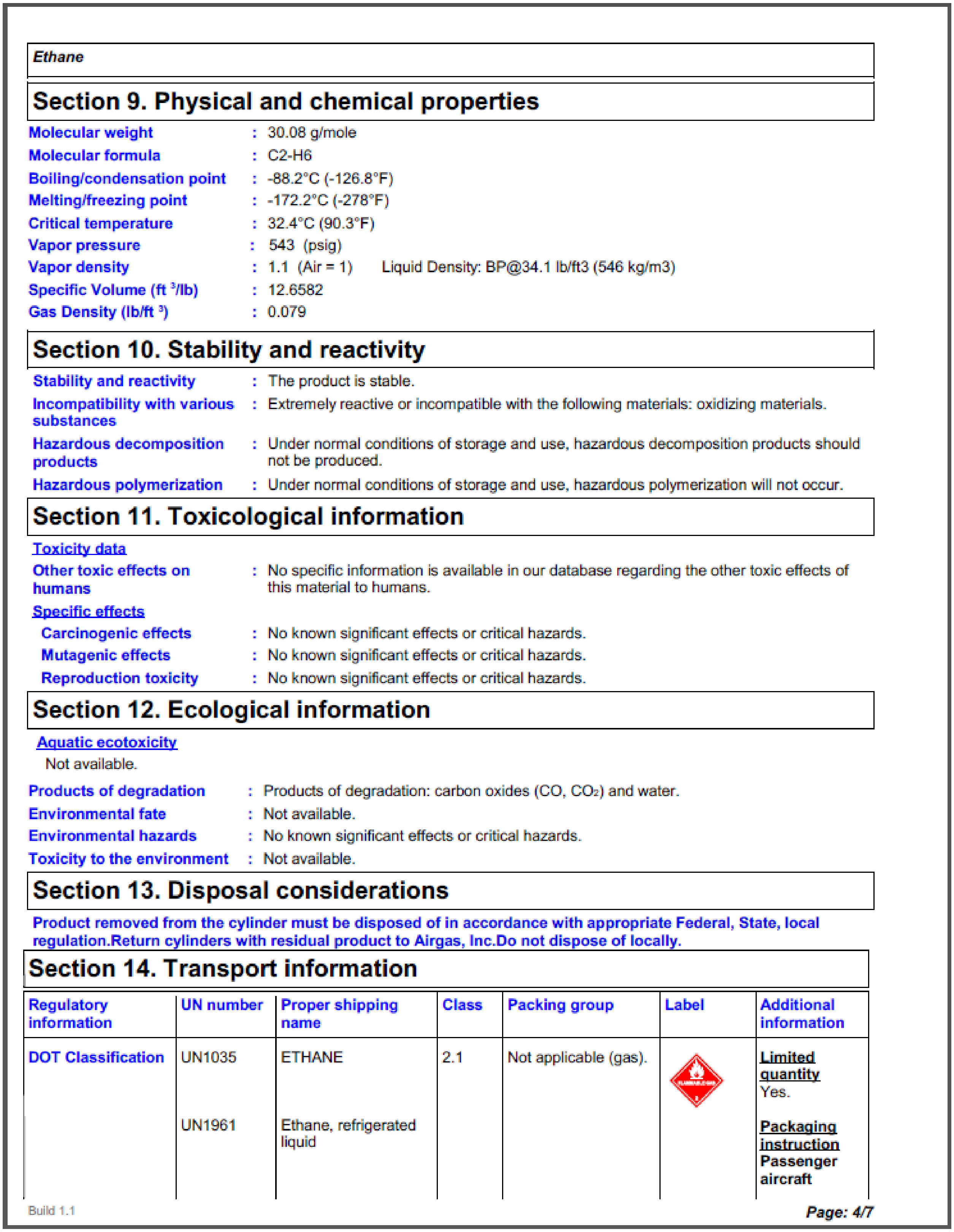
Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Insulated gloves suitable for low temperatures

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name	
ethane	**ACGIH TLV (United States, 1/2009).** TWA: 1000 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.



Ethane

Section 9. Physical and chemical properties

Molecular weight	: 30.08 g/mole
Molecular formula	: C2-H6
Boiling/condensation point	: -88.2°C (-126.8°F)
Melting/freezing point	: -172.2°C (-278°F)
Critical temperature	: 32.4°C (90.3°F)
Vapor pressure	: 543 (psig)
Vapor density	: 1.1 (Air = 1) Liquid Density: BP@34.1 lb/ft3 (546 kg/m3)
Specific Volume (ft^3/lb)	: 12.6582
Gas Density (lb/ft^3)	: 0.079

Section 10. Stability and reactivity

Stability and reactivity	: The product is stable.
Incompatibility with various substances	: Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products	: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization	: Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Other toxic effects on humans	: No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects	: No known significant effects or critical hazards.
Mutagenic effects	: No known significant effects or critical hazards.
Reproduction toxicity	: No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Products of degradation	: Products of degradation: carbon oxides (CO, CO_2) and water.
Environmental fate	: Not available.
Environmental hazards	: No known significant effects or critical hazards.
Toxicity to the environment	: Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1035	ETHANE	2.1	Not applicable (gas).		**Limited quantity** Yes.
	UN1961	Ethane, refrigerated liquid				**Packaging instruction** **Passenger aircraft**

Build 1.1

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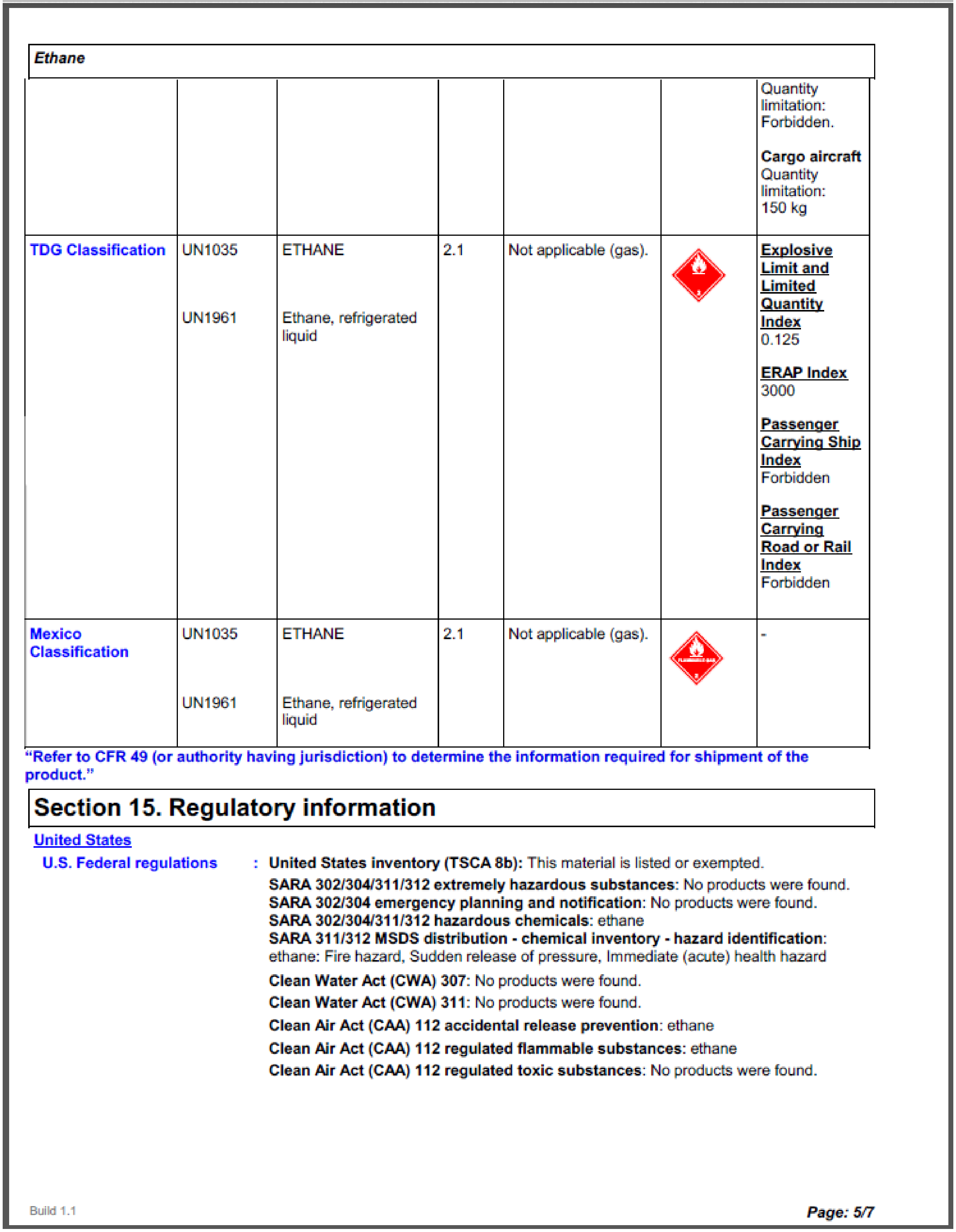

Ethane

						Quantity limitation: Forbidden. **Cargo aircraft** Quantity limitation: 150 kg
TDG Classification	UN1035 UN1961	ETHANE Ethane, refrigerated liquid	2.1	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0.125 **ERAP Index** 3000 **Passenger Carrying Ship Index** Forbidden **Passenger Carrying Road or Rail Index** Forbidden
Mexico Classification	UN1035 UN1961	ETHANE Ethane, refrigerated liquid	2.1	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

U.S. Federal regulations : **United States inventory (TSCA 8b):** This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: ethane
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: ethane: Fire hazard, Sudden release of pressure, Immediate (acute) health hazard

Clean Water Act (CWA) 307: No products were found.

Clean Water Act (CWA) 311: No products were found.

Clean Air Act (CAA) 112 accidental release prevention: ethane

Clean Air Act (CAA) 112 regulated flammable substances: ethane

Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

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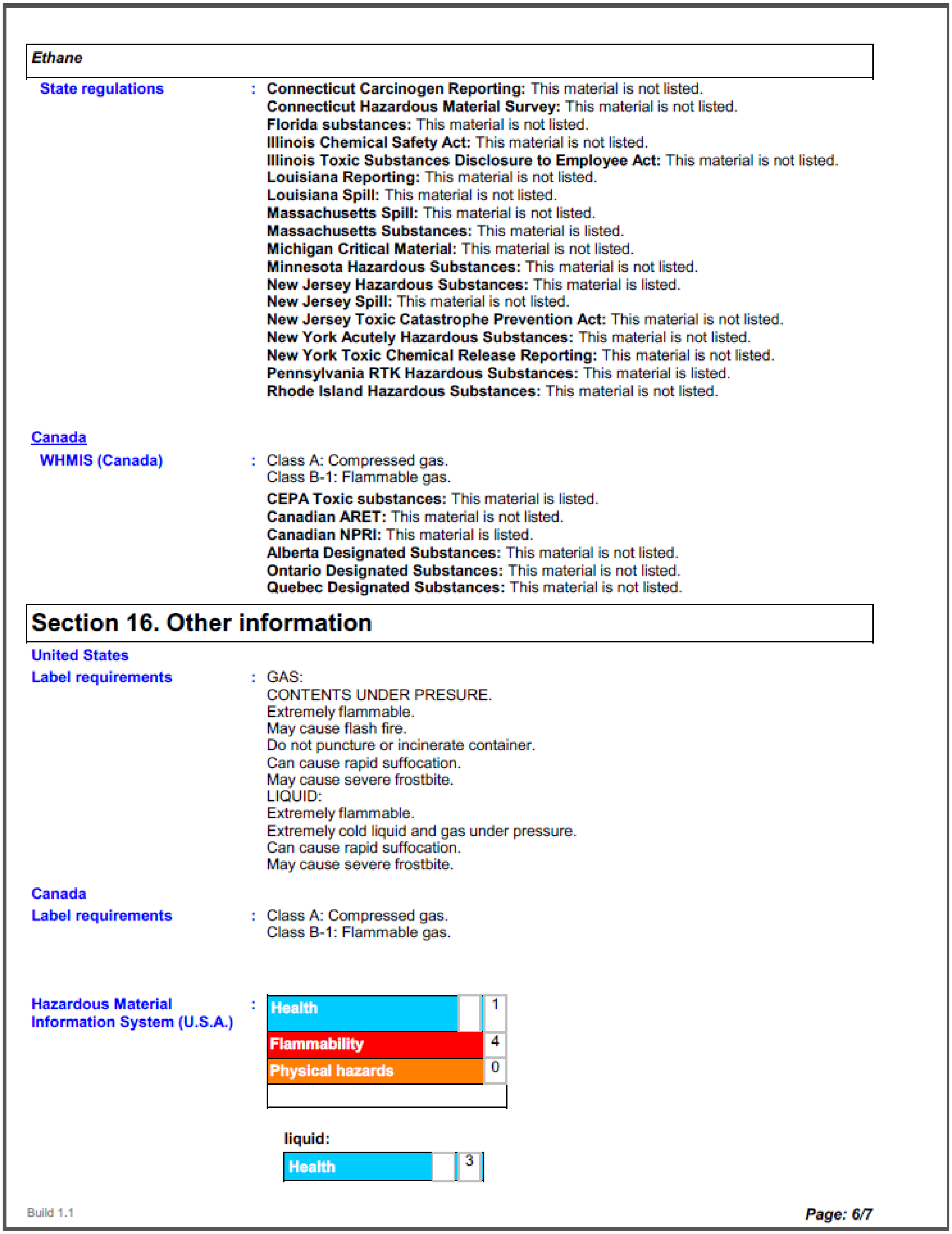

Ethane

State regulations : **Connecticut Carcinogen Reporting:** This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class B-1: Flammable gas.

CEPA Toxic substances: This material is listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

United States

Label requirements : GAS:
CONTENTS UNDER PRESURE.
Extremely flammable.
May cause flash fire.
Do not puncture or incinerate container.
Can cause rapid suffocation.
May cause severe frostbite.
LIQUID:
Extremely flammable.
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.

Canada

Label requirements : Class A: Compressed gas.
Class B-1: Flammable gas.

Hazardous Material Information System (U.S.A.) :

Health	1
Flammability	4
Physical hazards	0

liquid:

Health	3

Build 1.1

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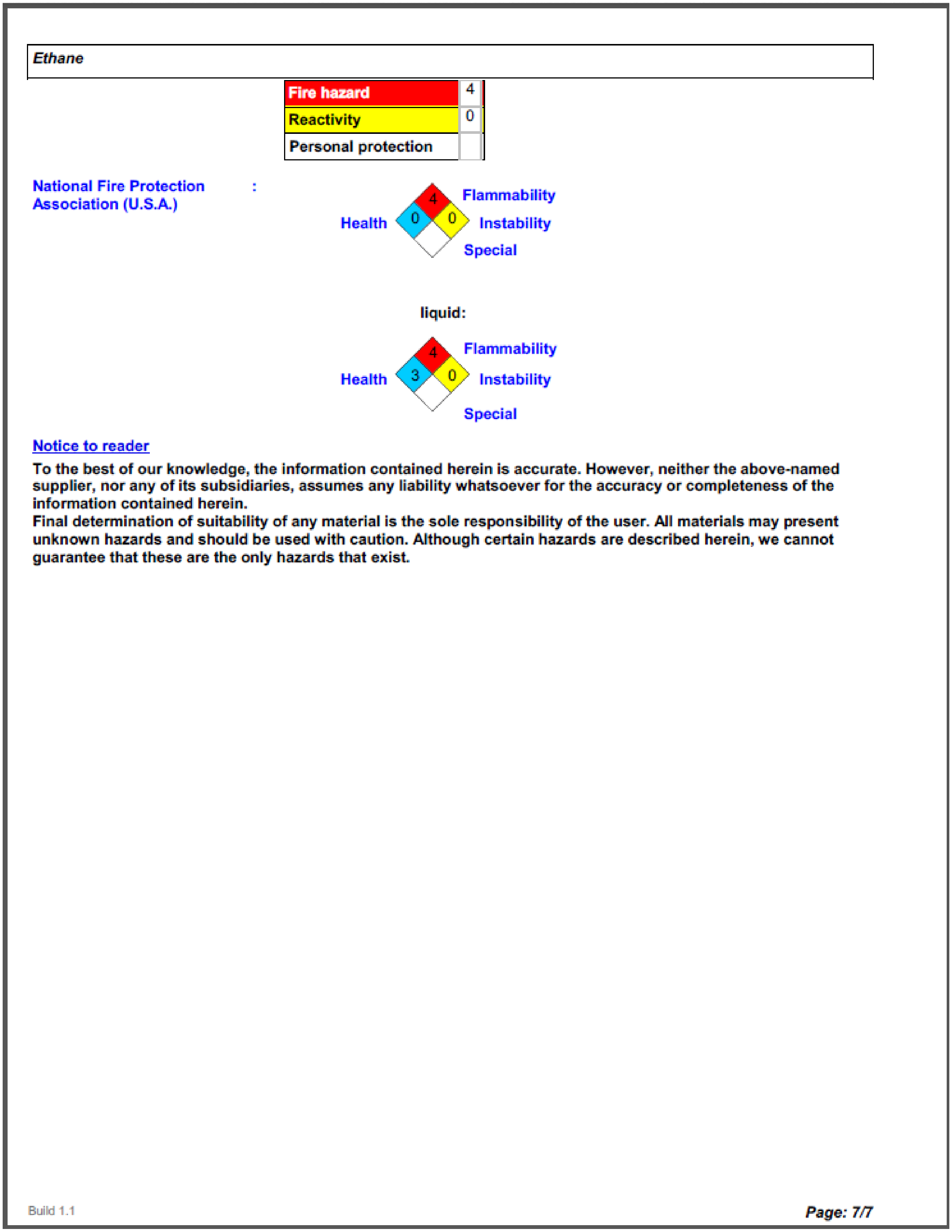

Ethane

Fire hazard	4
Reactivity	0
Personal protection	

National Fire Protection Association (U.S.A.) :

Flammability 4
Health 0
Instability 0
Special

liquid:

Flammability 4
Health 3
Instability 0
Special

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

Build 1.1

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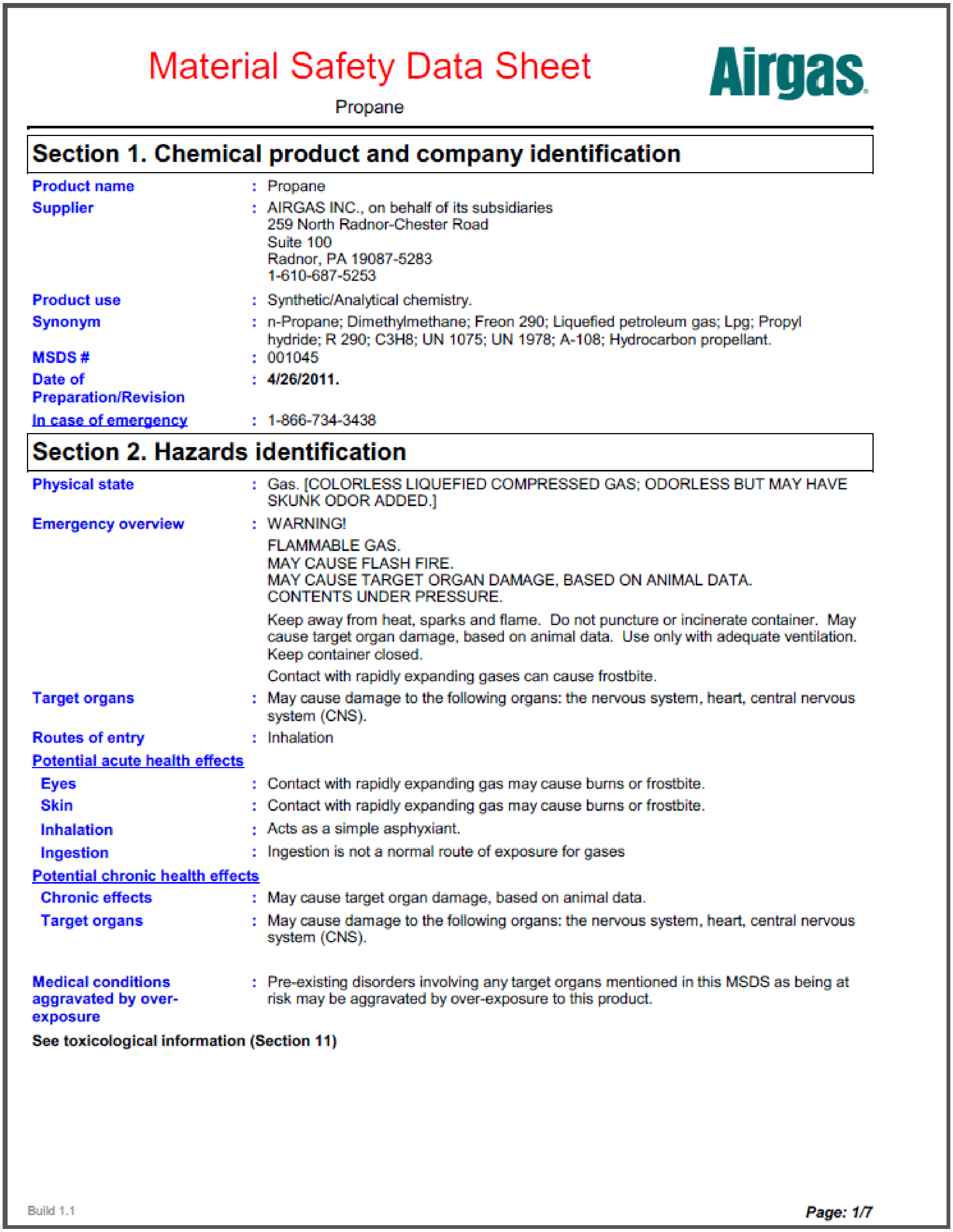

Material Safety Data Sheet

Airgas

Propane

Section 1. Chemical product and company identification

Product name : Propane

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : n-Propane; Dimethylmethane; Freon 290; Liquefied petroleum gas; Lpg; Propyl hydride; R 290; C3H8; UN 1075; UN 1978; A-108; Hydrocarbon propellant.

MSDS # : 001045

Date of Preparation/Revision : **4/26/2011.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas. [COLORLESS LIQUEFIED COMPRESSED GAS; ODORLESS BUT MAY HAVE SKUNK ODOR ADDED.]

Emergency overview : WARNING!

FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.

Keep away from heat, sparks and flame. Do not puncture or incinerate container. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container closed.

Contact with rapidly expanding gases can cause frostbite.

Target organs : May cause damage to the following organs: the nervous system, heart, central nervous system (CNS).

Routes of entry : Inhalation

Potential acute health effects

- **Eyes** : Contact with rapidly expanding gas may cause burns or frostbite.
- **Skin** : Contact with rapidly expanding gas may cause burns or frostbite.
- **Inhalation** : Acts as a simple asphyxiant.
- **Ingestion** : Ingestion is not a normal route of exposure for gases

Potential chronic health effects

- **Chronic effects** : May cause target organ damage, based on animal data.
- **Target organs** : May cause damage to the following organs: the nervous system, heart, central nervous system (CNS).

Medical conditions aggravated by over-exposure : Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (Section 11)

Build 1.1

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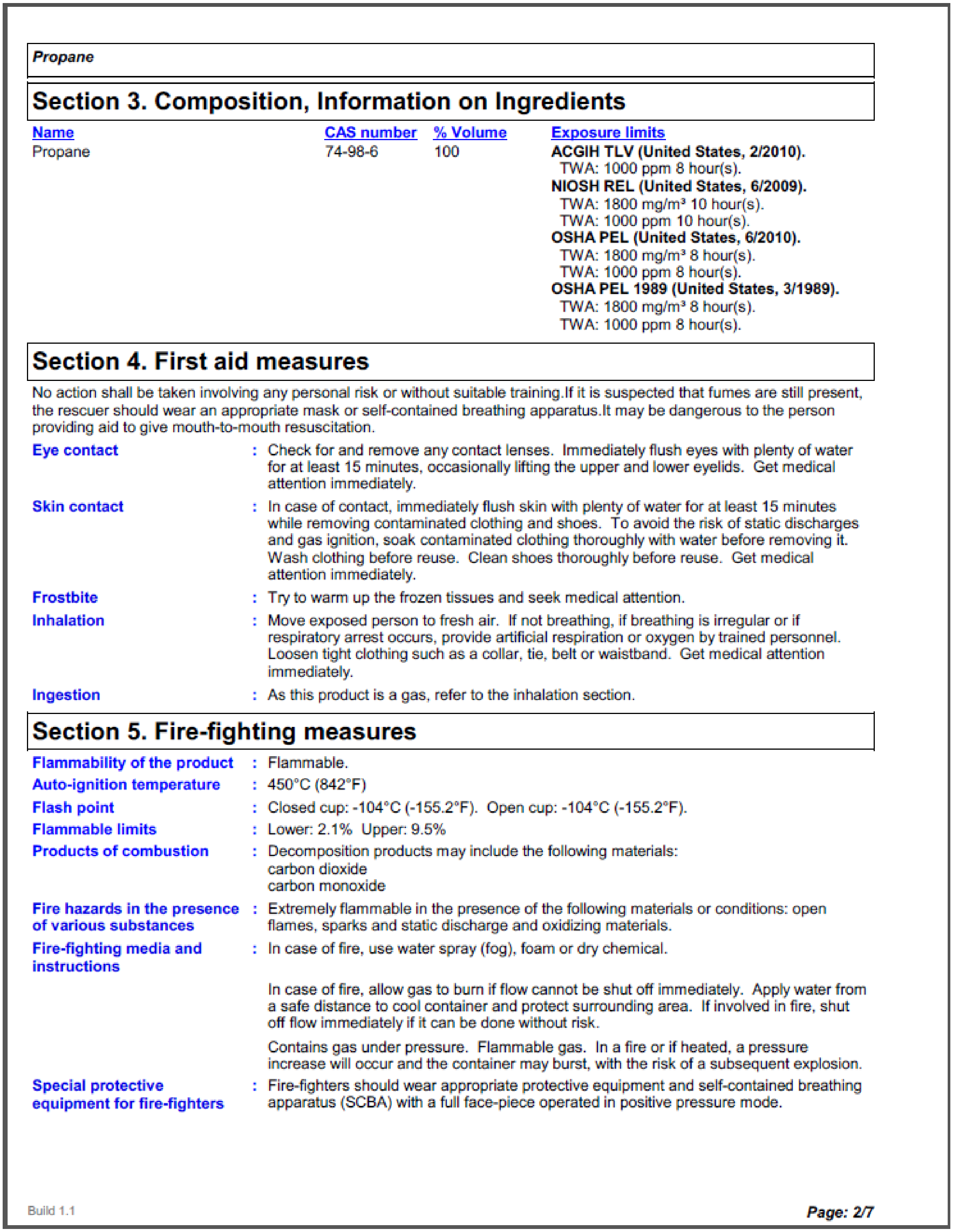


Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Propane	74-98-6	100	**ACGIH TLV (United States, 2/2010).** TWA: 1000 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** TWA: 1800 mg/m³ 10 hour(s). TWA: 1000 ppm 10 hour(s). **OSHA PEL (United States, 6/2010).** TWA: 1800 mg/m³ 8 hour(s). TWA: 1000 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** TWA: 1800 mg/m³ 8 hour(s). TWA: 1000 ppm 8 hour(s).

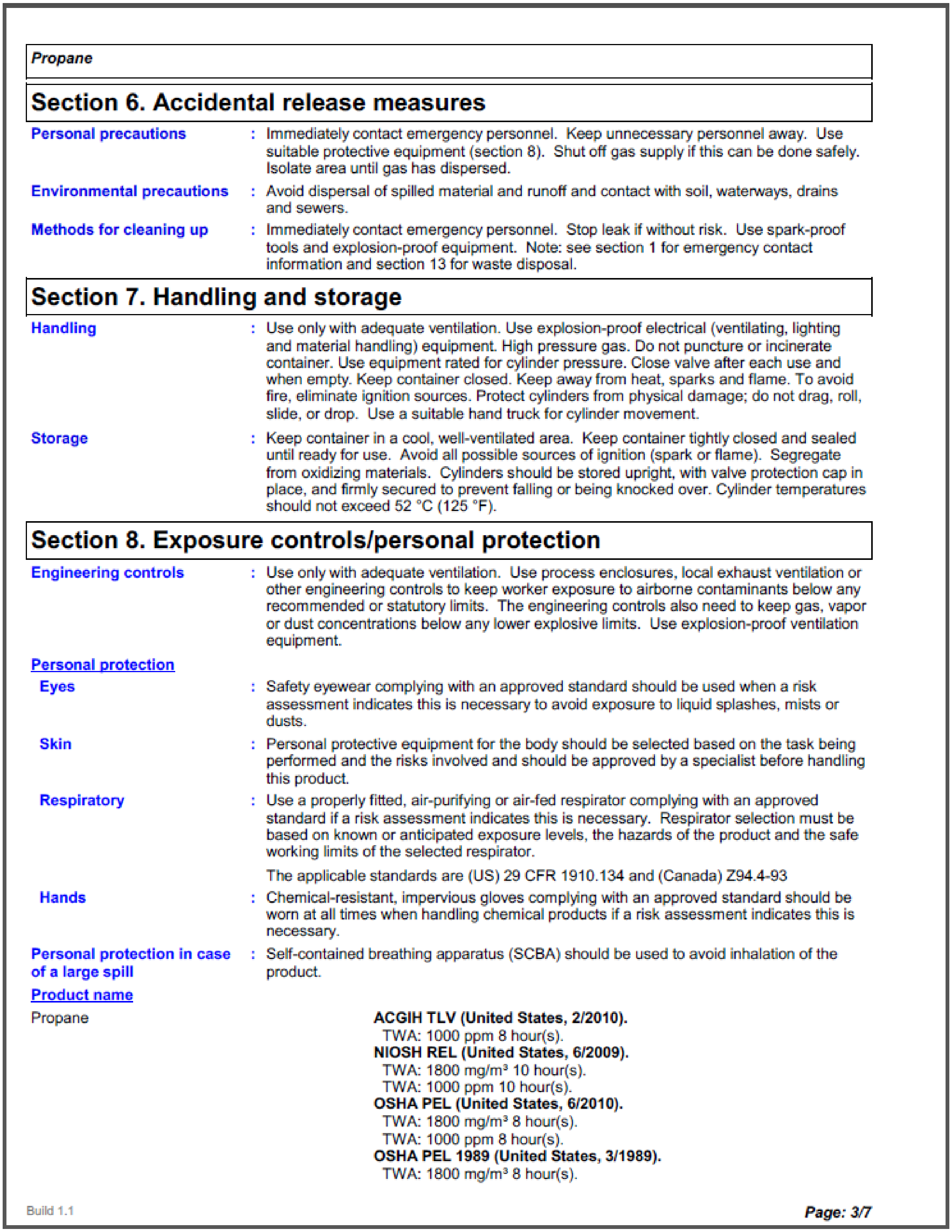
Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact	Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.
Skin contact	In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.
Frostbite	Try to warm up the frozen tissues and seek medical attention.
Inhalation	Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.
Ingestion	As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product	Flammable.
Auto-ignition temperature	450°C (842°F)
Flash point	Closed cup: -104°C (-155.2°F). Open cup: -104°C (-155.2°F).
Flammable limits	Lower: 2.1% Upper: 9.5%
Products of combustion	Decomposition products may include the following materials: carbon dioxide carbon monoxide
Fire hazards in the presence of various substances	Extremely flammable in the presence of the following materials or conditions: open flames, sparks and static discharge and oxidizing materials.
Fire-fighting media and instructions	In case of fire, use water spray (fog), foam or dry chemical. In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk. Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.
Special protective equipment for fire-fighters	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.



Propane

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Storage : Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

Section 8. Exposure controls/personal protection

Engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name

Propane	**ACGIH TLV (United States, 2/2010).** TWA: 1000 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** TWA: 1800 mg/m³ 10 hour(s). TWA: 1000 ppm 10 hour(s). **OSHA PEL (United States, 6/2010).** TWA: 1800 mg/m³ 8 hour(s). TWA: 1000 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** TWA: 1800 mg/m³ 8 hour(s).

Build 1.1

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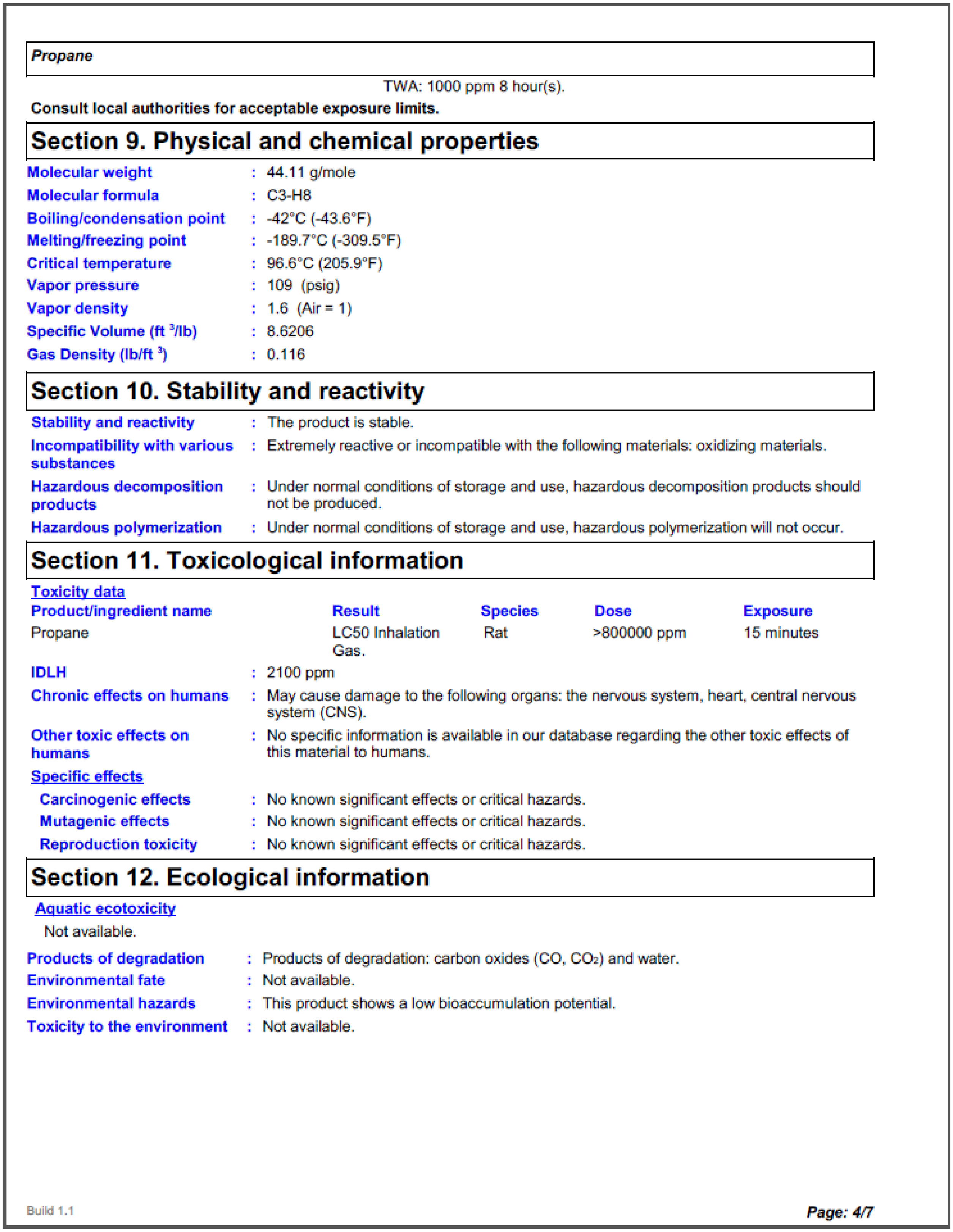


TWA: 1000 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight	44.11 g/mole
Molecular formula	C3-H8
Boiling/condensation point	-42°C (-43.6°F)
Melting/freezing point	-189.7°C (-309.5°F)
Critical temperature	96.6°C (205.9°F)
Vapor pressure	109 (psig)
Vapor density	1.6 (Air = 1)
Specific Volume (ft ^{3}/lb)	8.6206
Gas Density (lb/ft ^{3})	0.116

Section 10. Stability and reactivity

Stability and reactivity	The product is stable.
Incompatibility with various substances	Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization	Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Product/ingredient name	**Result**	**Species**	**Dose**	**Exposure**
Propane	LC50 Inhalation Gas.	Rat	>800000 ppm	15 minutes

IDLH	2100 ppm
Chronic effects on humans	May cause damage to the following organs: the nervous system, heart, central nervous system (CNS).
Other toxic effects on humans	No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

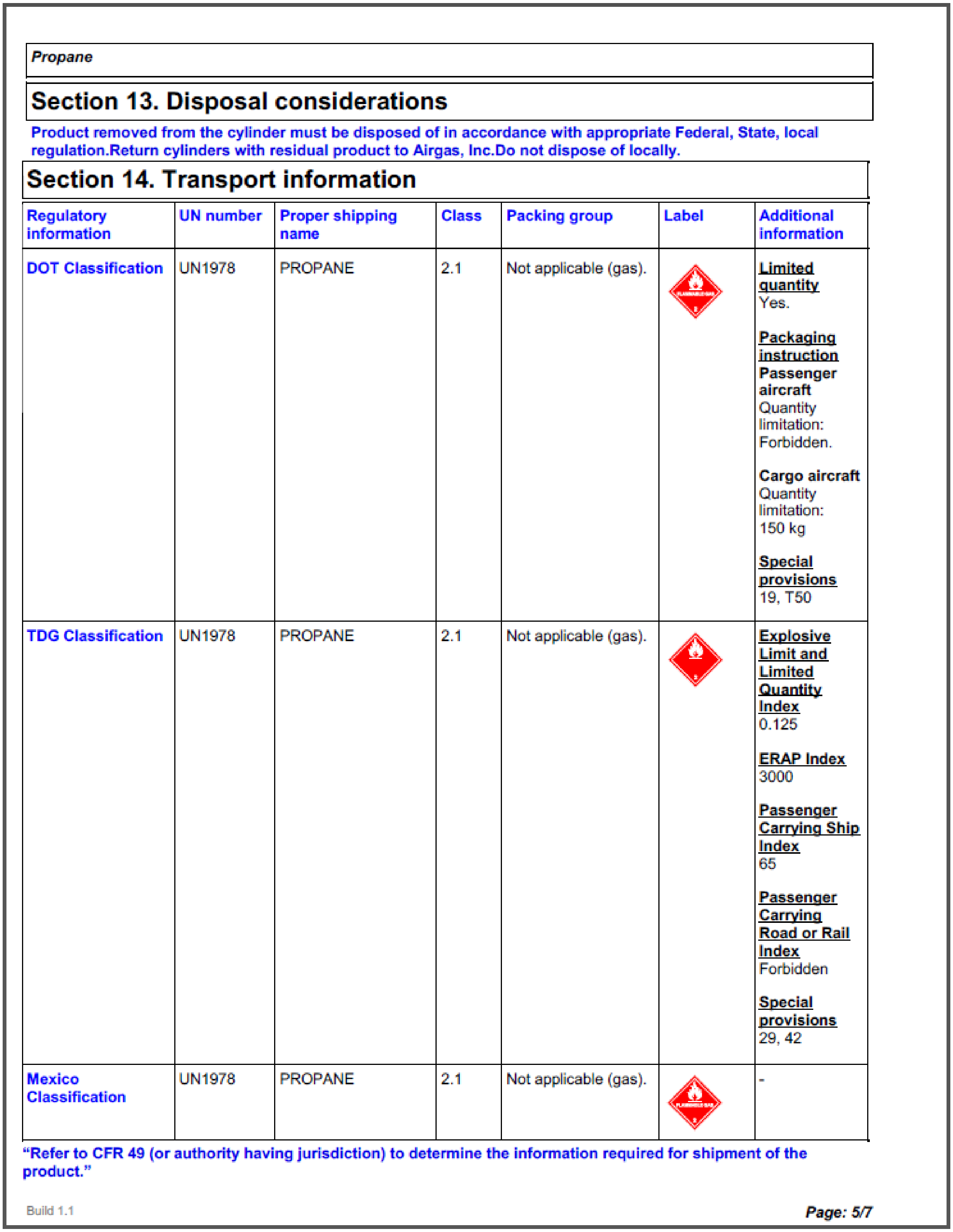
Carcinogenic effects	No known significant effects or critical hazards.
Mutagenic effects	No known significant effects or critical hazards.
Reproduction toxicity	No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Products of degradation	Products of degradation: carbon oxides (CO, CO_2) and water.
Environmental fate	Not available.
Environmental hazards	This product shows a low bioaccumulation potential.
Toxicity to the environment	Not available.



Propane

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1978	PROPANE	2.1	Not applicable (gas).		**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: Forbidden. **Cargo aircraft** Quantity limitation: 150 kg **Special provisions** 19, T50
TDG Classification	UN1978	PROPANE	2.1	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0.125 **ERAP Index** 3000 **Passenger Carrying Ship Index** 65 **Passenger Carrying Road or Rail Index** Forbidden **Special provisions** 29, 42
Mexico Classification	UN1978	PROPANE	2.1	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Build 1.1

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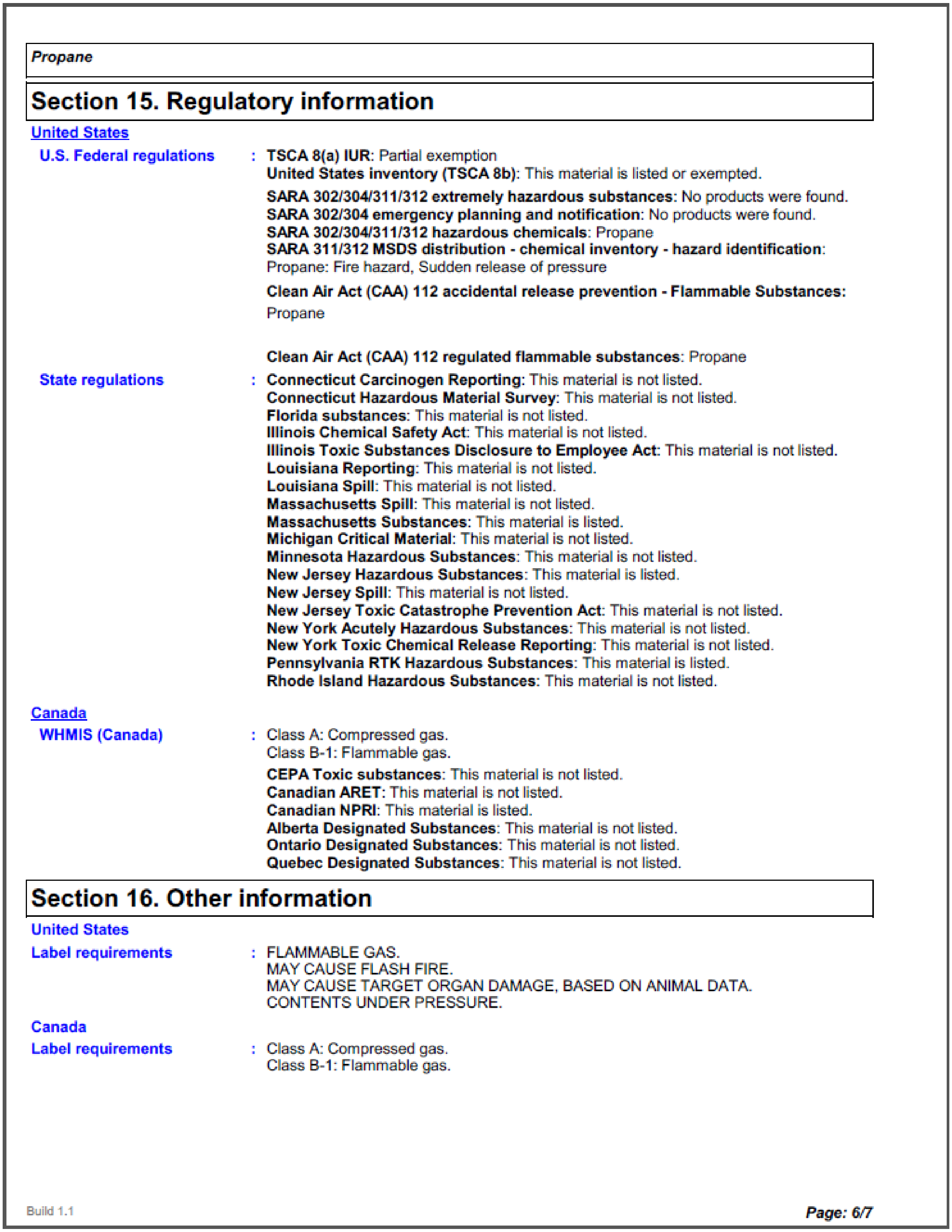


Propane

Section 15. Regulatory information

United States

U.S. Federal regulations : **TSCA 8(a) IUR**: Partial exemption
United States inventory (TSCA 8b): This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: Propane
SARA 311/312 MSDS distribution - chemical inventory - hazard identification:
Propane: Fire hazard, Sudden release of pressure

Clean Air Act (CAA) 112 accidental release prevention - Flammable Substances:
Propane

Clean Air Act (CAA) 112 regulated flammable substances: Propane

State regulations : **Connecticut Carcinogen Reporting**: This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class B-1: Flammable gas.

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

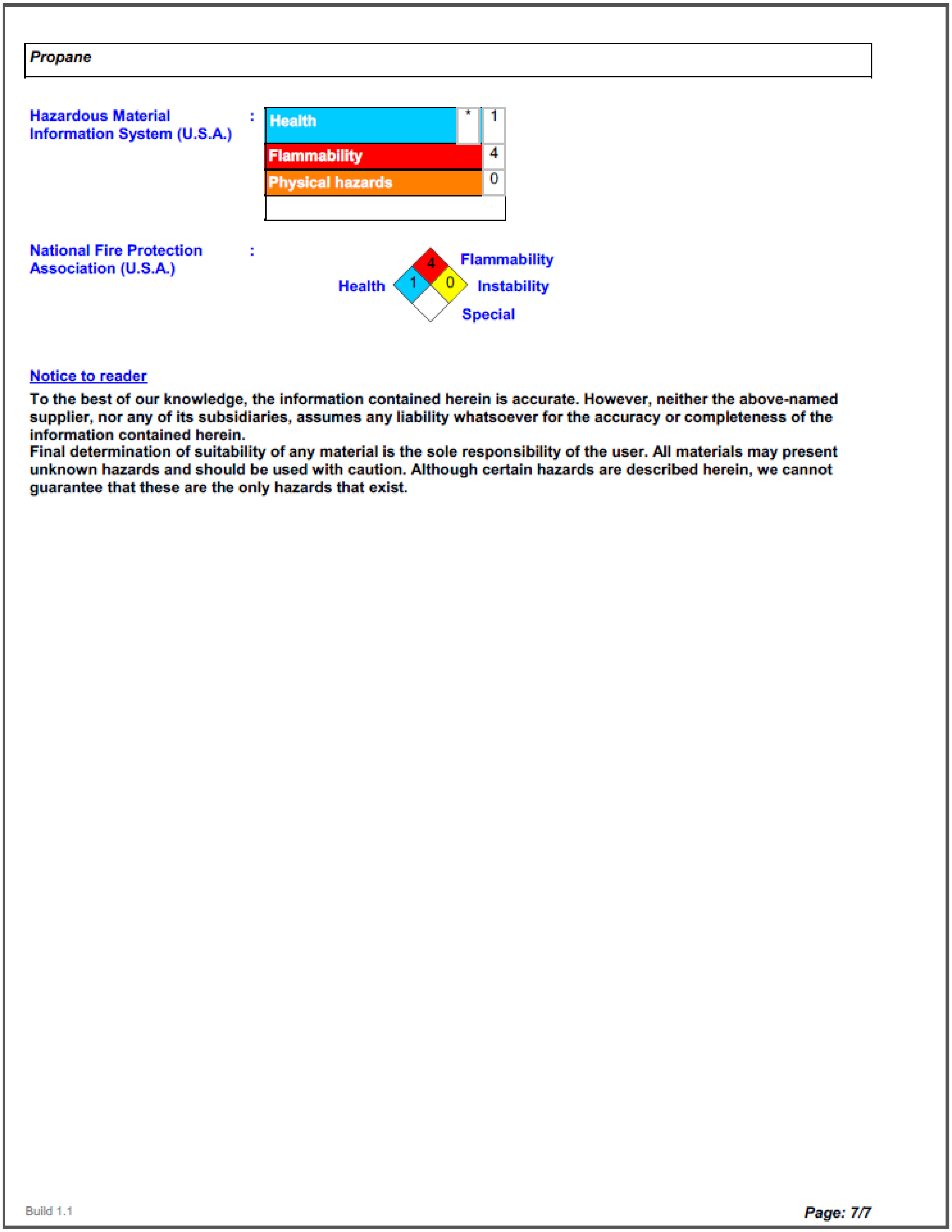
United States

Label requirements : FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.

Canada

Label requirements : Class A: Compressed gas.
Class B-1: Flammable gas.

Build 1.1 ***Page: 6/7***



Propane

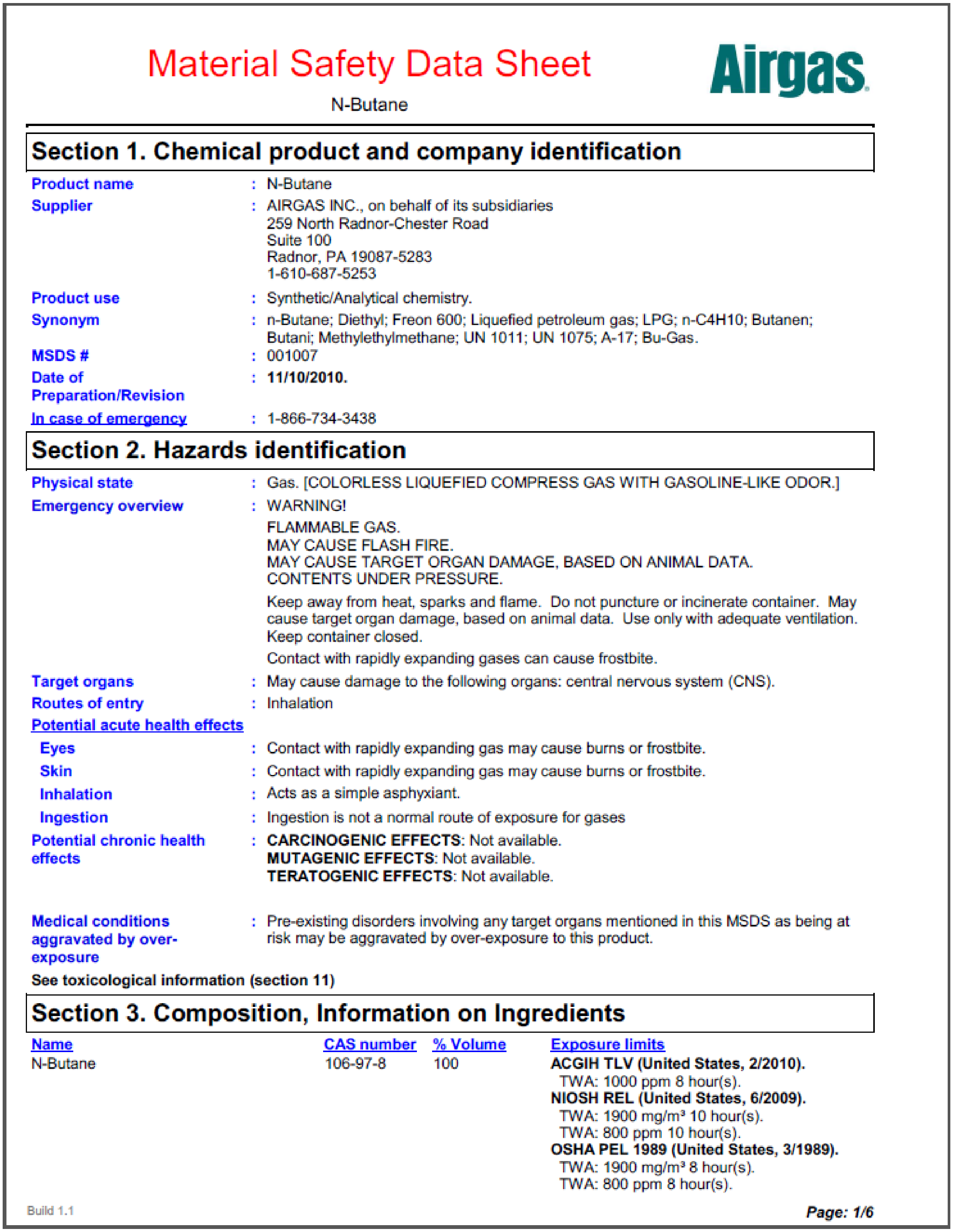
Hazardous Material Information System (U.S.A.) :

Health	*	1
Flammability		4
Physical hazards		0

National Fire Protection Association (U.S.A.) :

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.



Material Safety Data Sheet

Airgas

N-Butane

Section 1. Chemical product and company identification

Product name : N-Butane

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : n-Butane; Diethyl; Freon 600; Liquefied petroleum gas; LPG; n-C4H10; Butanen; Butani; Methylethylmethane; UN 1011; UN 1075; A-17; Bu-Gas.

MSDS # : 001007

Date of Preparation/Revision : **11/10/2010.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas. [COLORLESS LIQUEFIED COMPRESS GAS WITH GASOLINE-LIKE ODOR.]

Emergency overview : WARNING!

FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.

Keep away from heat, sparks and flame. Do not puncture or incinerate container. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container closed.

Contact with rapidly expanding gases can cause frostbite.

Target organs : May cause damage to the following organs: central nervous system (CNS).

Routes of entry : Inhalation

Potential acute health effects

Eyes : Contact with rapidly expanding gas may cause burns or frostbite.

Skin : Contact with rapidly expanding gas may cause burns or frostbite.

Inhalation : Acts as a simple asphyxiant.

Ingestion : Ingestion is not a normal route of exposure for gases

Potential chronic health effects : **CARCINOGENIC EFFECTS**: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.

Medical conditions aggravated by over-exposure : Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
N-Butane	106-97-8	100	**ACGIH TLV (United States, 2/2010).** TWA: 1000 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** TWA: 1900 mg/m³ 10 hour(s). TWA: 800 ppm 10 hour(s). **OSHA PEL 1989 (United States, 3/1989).** TWA: 1900 mg/m³ 8 hour(s). TWA: 800 ppm 8 hour(s).

Build 1.1

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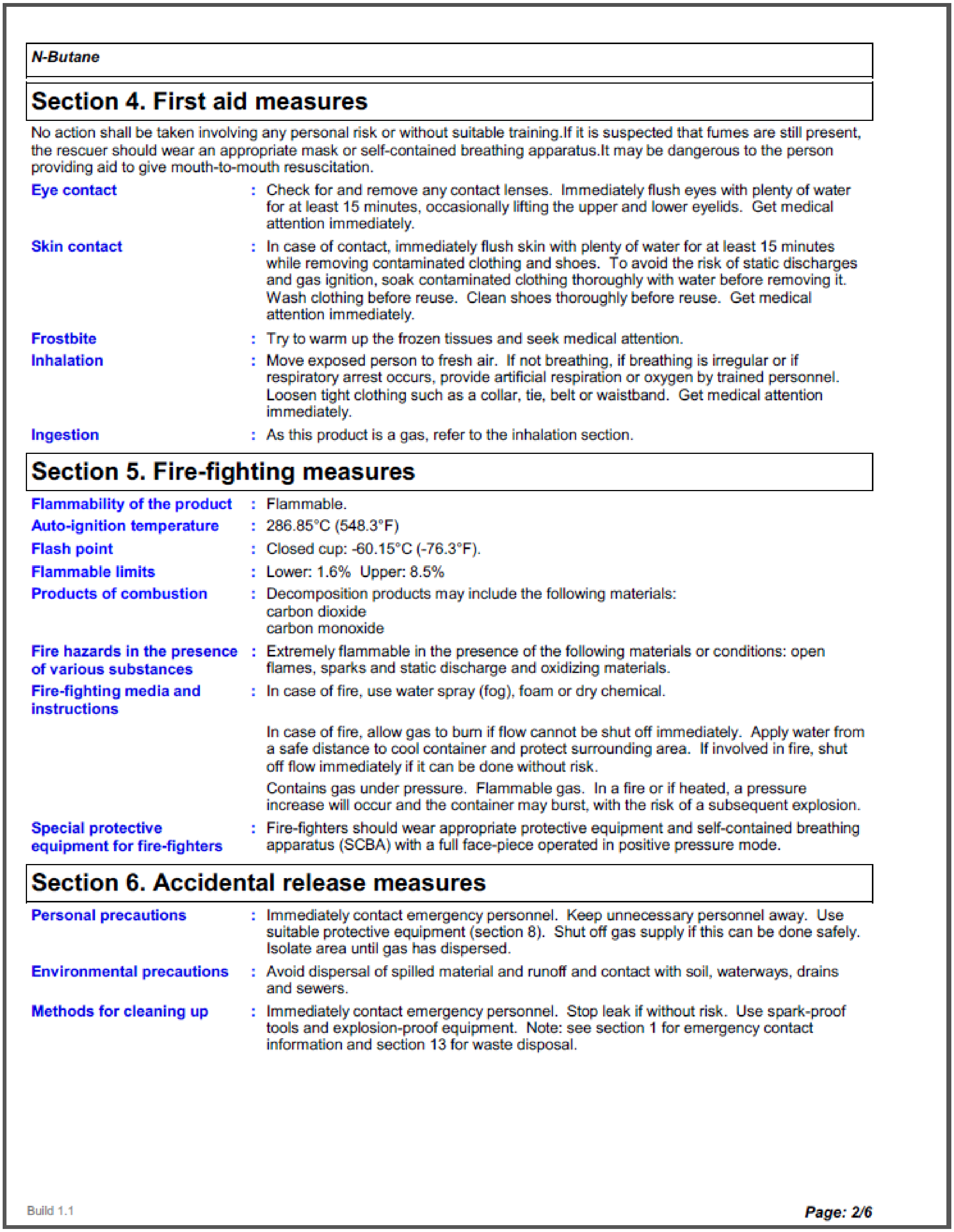


N-Butane

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 286.85°C (548.3°F)

Flash point : Closed cup: -60.15°C (-76.3°F).

Flammable limits : Lower: 1.6% Upper: 8.5%

Products of combustion : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Fire hazards in the presence of various substances : Extremely flammable in the presence of the following materials or conditions: open flames, sparks and static discharge and oxidizing materials.

Fire-fighting media and instructions : In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

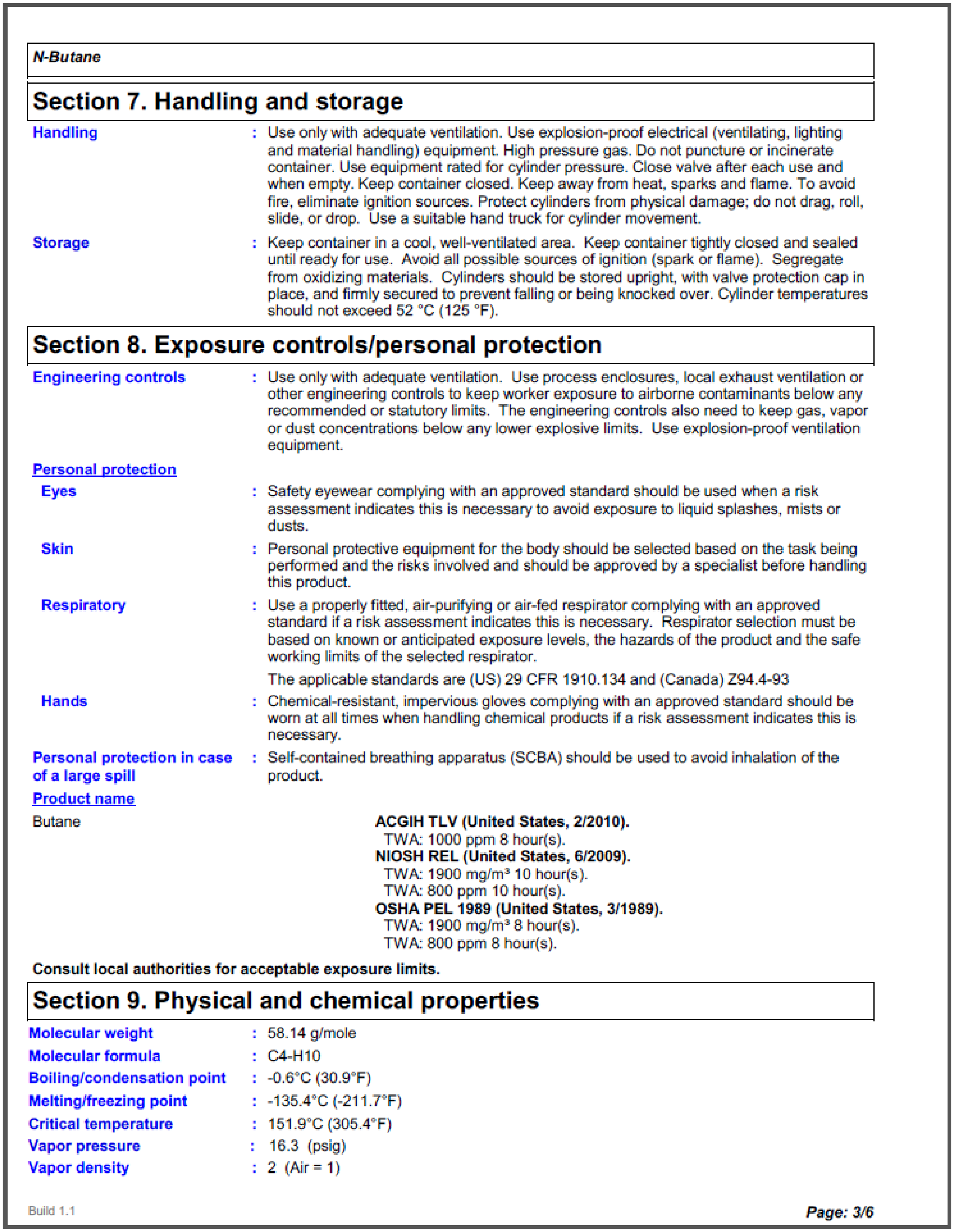
Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.



N-Butane

Section 7. Handling and storage

Handling	: Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.
Storage	: Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

Section 8. Exposure controls/personal protection

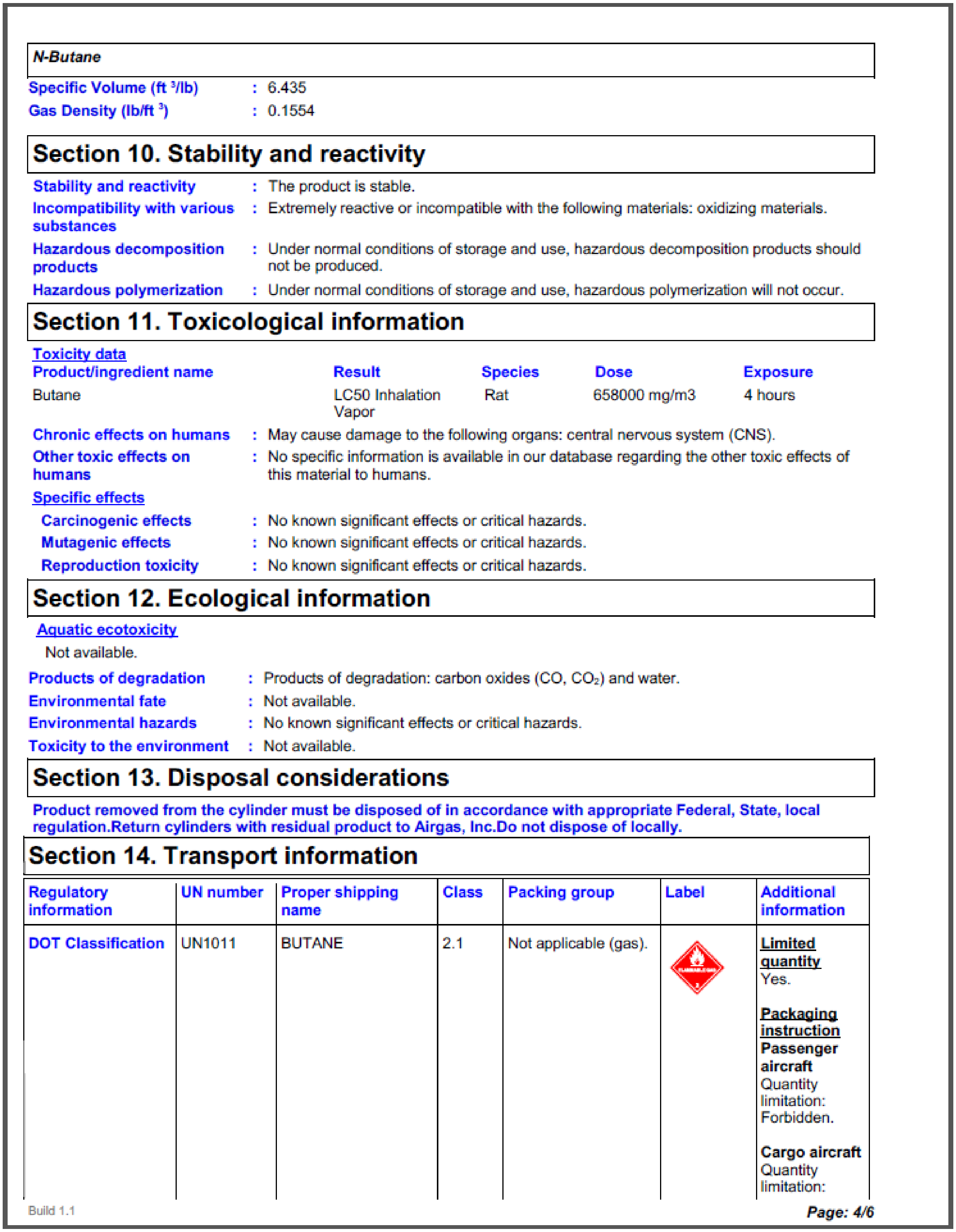
Engineering controls	: Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.
Personal protection	
Eyes	: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.
Skin	: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.
Respiratory	: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator. The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93
Hands	: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.
Personal protection in case of a large spill	: Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name	
Butane	**ACGIH TLV (United States, 2/2010).** TWA: 1000 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** TWA: 1900 mg/m³ 10 hour(s). TWA: 800 ppm 10 hour(s). **OSHA PEL 1989 (United States, 3/1989).** TWA: 1900 mg/m³ 8 hour(s). TWA: 800 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight	: 58.14 g/mole
Molecular formula	: C4-H10
Boiling/condensation point	: -0.6°C (30.9°F)
Melting/freezing point	: -135.4°C (-211.7°F)
Critical temperature	: 151.9°C (305.4°F)
Vapor pressure	: 16.3 (psig)
Vapor density	: 2 (Air = 1)



Specific Volume (ft ^{3}/lb) : 6.435
Gas Density (lb/ft ^{3}) : 0.1554

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.
Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Product/ingredient name	Result	Species	Dose	Exposure
Butane	LC50 Inhalation Vapor	Rat	658000 mg/m3	4 hours

Chronic effects on humans : May cause damage to the following organs: central nervous system (CNS).
Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.
Mutagenic effects : No known significant effects or critical hazards.
Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

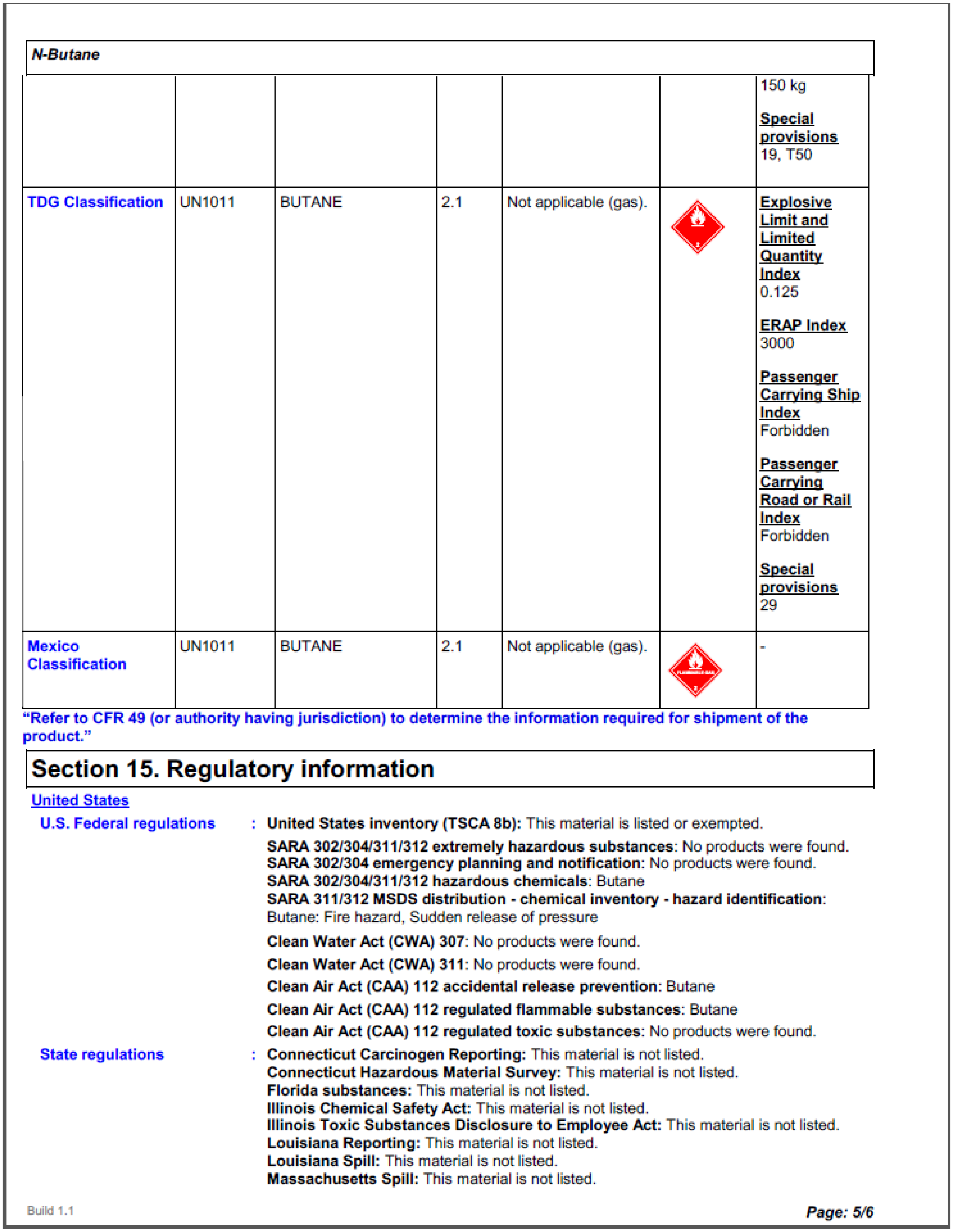
Products of degradation : Products of degradation: carbon oxides (CO, CO_2) and water.
Environmental fate : Not available.
Environmental hazards : No known significant effects or critical hazards.
Toxicity to the environment : Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1011	BUTANE	2.1	Not applicable (gas).	◆	**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: Forbidden. **Cargo aircraft** Quantity limitation:



						150 kg **Special provisions** 19, T50
TDG Classification	UN1011	BUTANE	2.1	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0.125 **ERAP Index** 3000 **Passenger Carrying Ship Index** Forbidden **Passenger Carrying Road or Rail Index** Forbidden **Special provisions** 29
Mexico Classification	UN1011	BUTANE	2.1	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

U.S. Federal regulations : **United States inventory (TSCA 8b):** This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: Butane
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Butane: Fire hazard, Sudden release of pressure

Clean Water Act (CWA) 307: No products were found.

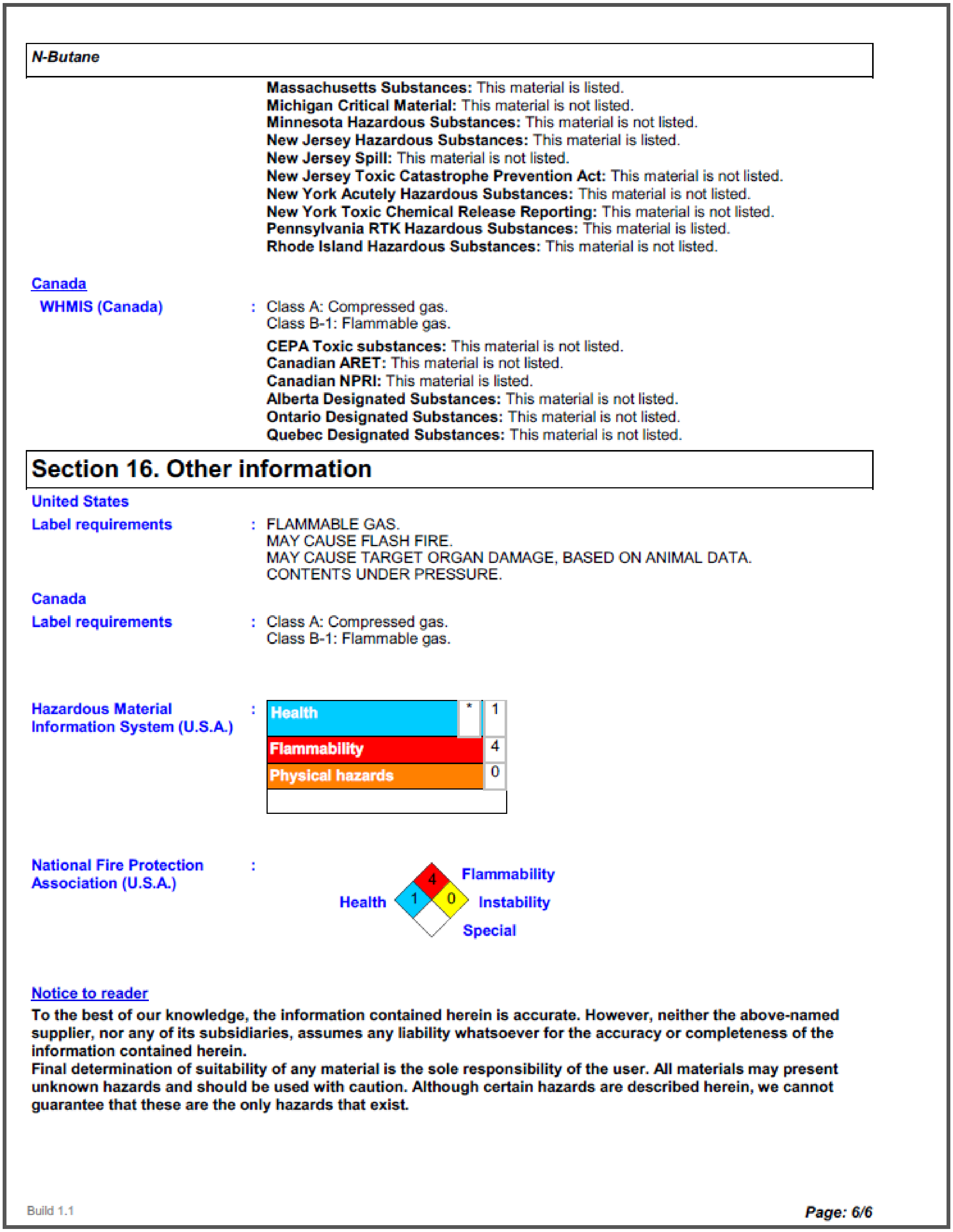
Clean Water Act (CWA) 311: No products were found.

Clean Air Act (CAA) 112 accidental release prevention: Butane

Clean Air Act (CAA) 112 regulated flammable substances: Butane

Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

State regulations : **Connecticut Carcinogen Reporting:** This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.



Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class B-1: Flammable gas.

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

United States

Label requirements : FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.

Canada

Label requirements : Class A: Compressed gas.
Class B-1: Flammable gas.

Hazardous Material Information System (U.S.A.) :

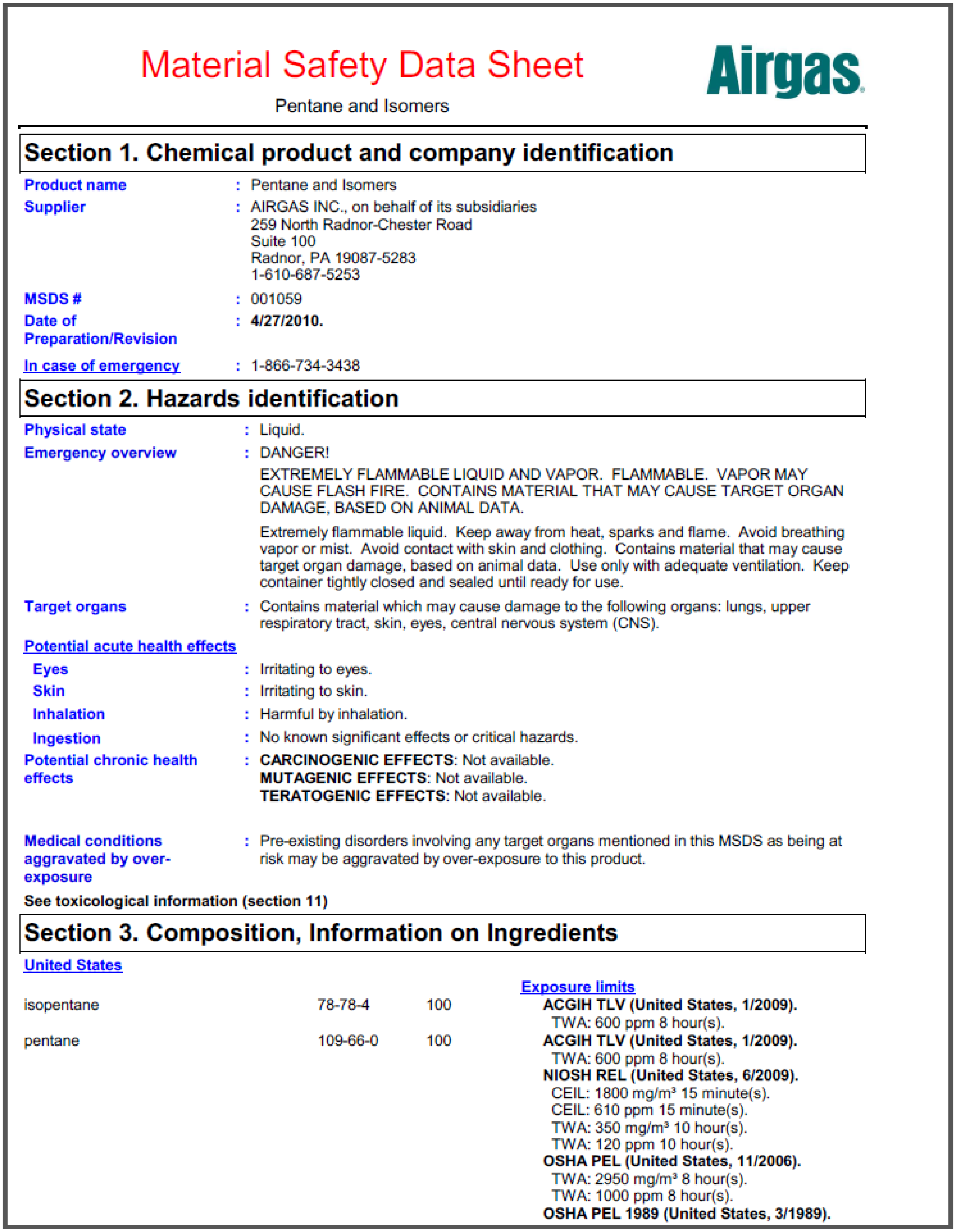
Health	*	1
Flammability		4
Physical hazards		0

National Fire Protection Association (U.S.A.) :

Flammability 4
Health 1
Instability 0
Special

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.



Material Safety Data Sheet

Pentane and Isomers

Airgas

Section 1. Chemical product and company identification

Product name : Pentane and Isomers

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

MSDS # : 001059

Date of Preparation/Revision : **4/27/2010.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Liquid.

Emergency overview : DANGER!

EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. CONTAINS MATERIAL THAT MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

Extremely flammable liquid. Keep away from heat, sparks and flame. Avoid breathing vapor or mist. Avoid contact with skin and clothing. Contains material that may cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container tightly closed and sealed until ready for use.

Target organs : Contains material which may cause damage to the following organs: lungs, upper respiratory tract, skin, eyes, central nervous system (CNS).

Potential acute health effects

- **Eyes** : Irritating to eyes.
- **Skin** : Irritating to skin.
- **Inhalation** : Harmful by inhalation.
- **Ingestion** : No known significant effects or critical hazards.

Potential chronic health effects : **CARCINOGENIC EFFECTS**: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.

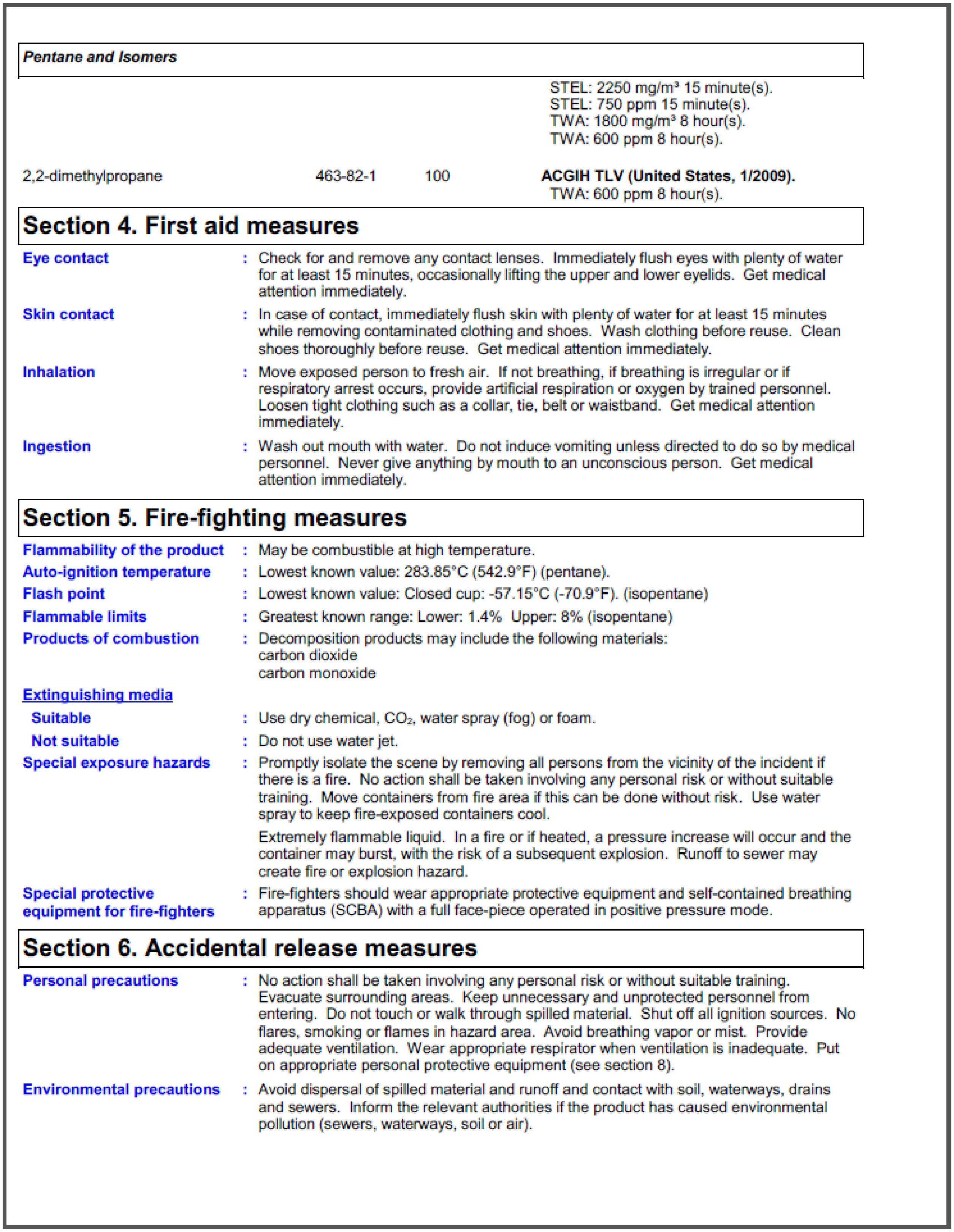
Medical conditions aggravated by over-exposure : Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

United States

			Exposure limits
isopentane	78-78-4	100	**ACGIH TLV (United States, 1/2009).** TWA: 600 ppm 8 hour(s).
pentane	109-66-0	100	**ACGIH TLV (United States, 1/2009).** TWA: 600 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** CEIL: 1800 mg/m^3 15 minute(s). CEIL: 610 ppm 15 minute(s). TWA: 350 mg/m^3 10 hour(s). TWA: 120 ppm 10 hour(s). **OSHA PEL (United States, 11/2006).** TWA: 2950 mg/m^3 8 hour(s). TWA: 1000 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).**



Pentane and Isomers

			STEL: 2250 mg/m³ 15 minute(s). STEL: 750 ppm 15 minute(s). TWA: 1800 mg/m³ 8 hour(s). TWA: 600 ppm 8 hour(s).
2,2-dimethylpropane	463-82-1	100	**ACGIH TLV (United States, 1/2009).** TWA: 600 ppm 8 hour(s).

Section 4. First aid measures

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : Wash out mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Get medical attention immediately.

Section 5. Fire-fighting measures

Flammability of the product : May be combustible at high temperature.

Auto-ignition temperature : Lowest known value: 283.85°C (542.9°F) (pentane).

Flash point : Lowest known value: Closed cup: -57.15°C (-70.9°F). (isopentane)

Flammable limits : Greatest known range: Lower: 1.4% Upper: 8% (isopentane)

Products of combustion : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Extinguishing media

Suitable : Use dry chemical, CO_2, water spray (fog) or foam.

Not suitable : Do not use water jet.

Special exposure hazards : Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool.

Extremely flammable liquid. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. Runoff to sewer may create fire or explosion hazard.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment (see section 8).

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

Pentane and Isomers

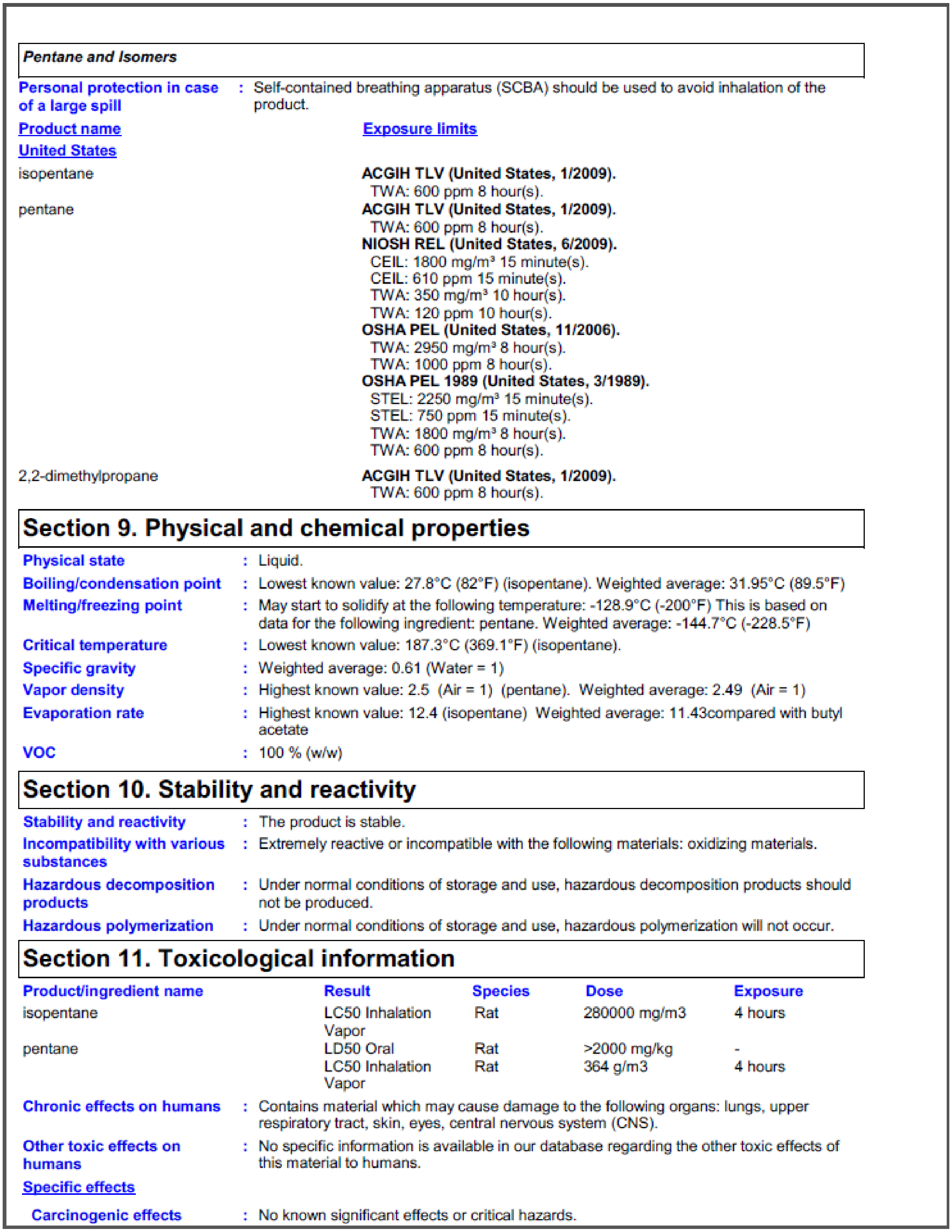
Methods for cleaning up	: Stop leak if without risk. Move containers from spill area. Approach release from upwind. Prevent entry into sewers, water courses, basements or confined areas. Wash spillages into an effluent treatment plant or proceed as follows. Contain and collect spillage with non-combustible, absorbent material e.g. sand, earth, vermiculite or diatomaceous earth and place in container for disposal according to local regulations (see section 13). Use spark-proof tools and explosion-proof equipment. Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilled product. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling	: Put on appropriate personal protective equipment (see section 8). Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use non-sparking tools. Take precautionary measures against electrostatic discharges. To avoid fire or explosion, dissipate static electricity during transfer by grounding and bonding containers and equipment before transferring material. Empty containers retain product residue and can be hazardous. Do not reuse container.
Storage	: Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabeled containers. Use appropriate containment to avoid environmental contamination.

Section 8. Exposure controls/personal protection

Recommended monitoring procedures	: If this product contains ingredients with exposure limits, personal, workplace atmosphere or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment.
Engineering measures	: Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.
Hygiene measures	: Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.
Personal protection	
Eyes	: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.
Skin	: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.
Respiratory	: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.
Hands	: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.



Pentane and Isomers

Personal protection in case of a large spill	: Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name	**Exposure limits**
United States	
isopentane	**ACGIH TLV (United States, 1/2009).** TWA: 600 ppm 8 hour(s).
pentane	**ACGIH TLV (United States, 1/2009).** TWA: 600 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** CEIL: 1800 mg/m³ 15 minute(s). CEIL: 610 ppm 15 minute(s). TWA: 350 mg/m³ 10 hour(s). TWA: 120 ppm 10 hour(s). **OSHA PEL (United States, 11/2006).** TWA: 2950 mg/m³ 8 hour(s). TWA: 1000 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** STEL: 2250 mg/m³ 15 minute(s). STEL: 750 ppm 15 minute(s). TWA: 1800 mg/m³ 8 hour(s). TWA: 600 ppm 8 hour(s).
2,2-dimethylpropane	**ACGIH TLV (United States, 1/2009).** TWA: 600 ppm 8 hour(s).

Section 9. Physical and chemical properties

Physical state	: Liquid.
Boiling/condensation point	: Lowest known value: 27.8°C (82°F) (isopentane). Weighted average: 31.95°C (89.5°F)
Melting/freezing point	: May start to solidify at the following temperature: -128.9°C (-200°F) This is based on data for the following ingredient: pentane. Weighted average: -144.7°C (-228.5°F)
Critical temperature	: Lowest known value: 187.3°C (369.1°F) (isopentane).
Specific gravity	: Weighted average: 0.61 (Water = 1)
Vapor density	: Highest known value: 2.5 (Air = 1) (pentane). Weighted average: 2.49 (Air = 1)
Evaporation rate	: Highest known value: 12.4 (isopentane) Weighted average: 11.43compared with butyl acetate
VOC	: 100 % (w/w)

Section 10. Stability and reactivity

Stability and reactivity	: The product is stable.
Incompatibility with various substances	: Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products	: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization	: Under normal conditions of storage and use, hazardous polymerization will not occur.

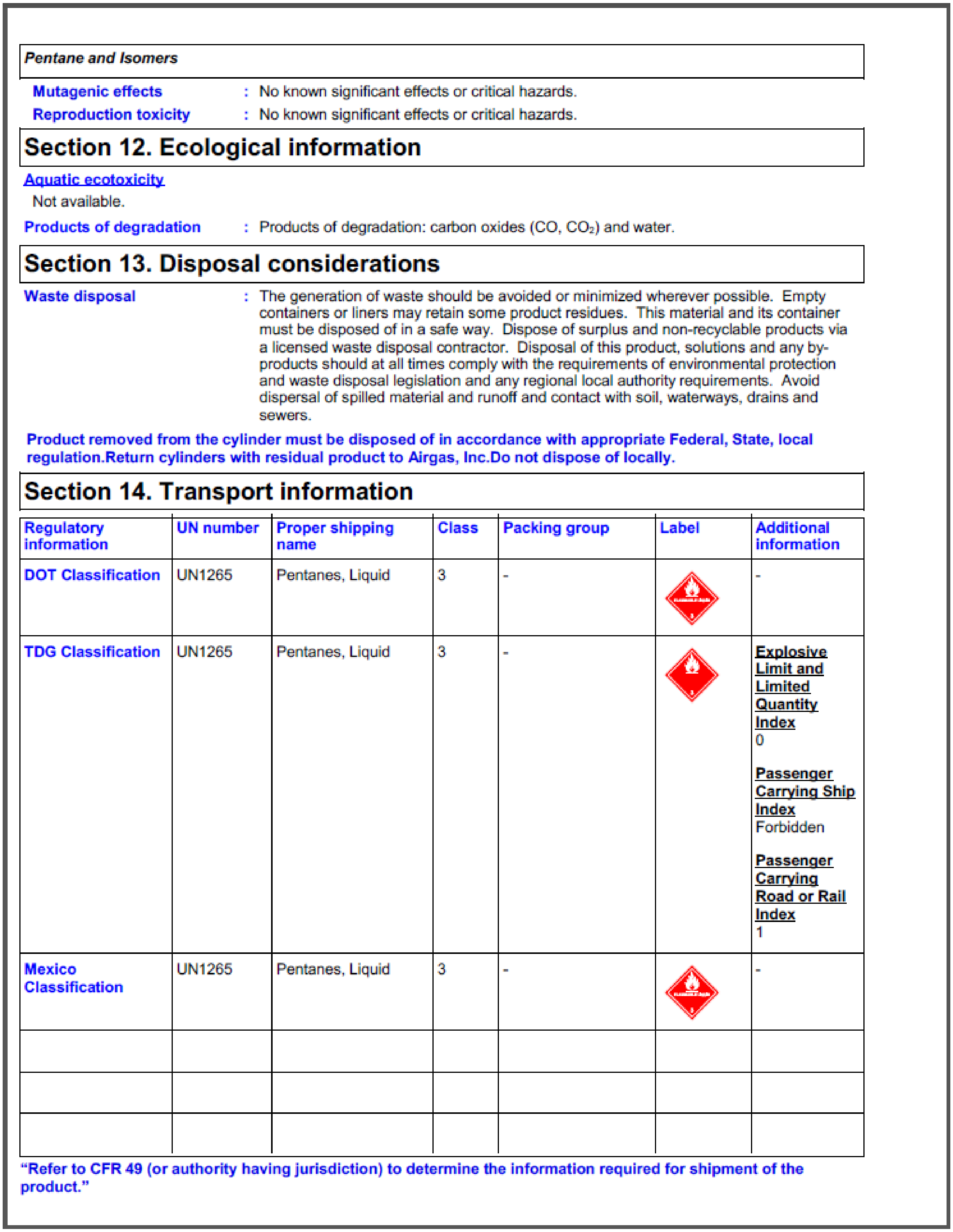
Section 11. Toxicological information

Product/ingredient name	**Result**	**Species**	**Dose**	**Exposure**
isopentane	LC50 Inhalation Vapor	Rat	280000 mg/m3	4 hours
pentane	LD50 Oral	Rat	>2000 mg/kg	-
	LC50 Inhalation Vapor	Rat	364 g/m3	4 hours

Chronic effects on humans	: Contains material which may cause damage to the following organs: lungs, upper respiratory tract, skin, eyes, central nervous system (CNS).
Other toxic effects on humans	: No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects	: No known significant effects or critical hazards.



Pentane and Isomers

Mutagenic effects : No known significant effects or critical hazards.

Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Products of degradation : Products of degradation: carbon oxides (CO, CO_2) and water.

Section 13. Disposal considerations

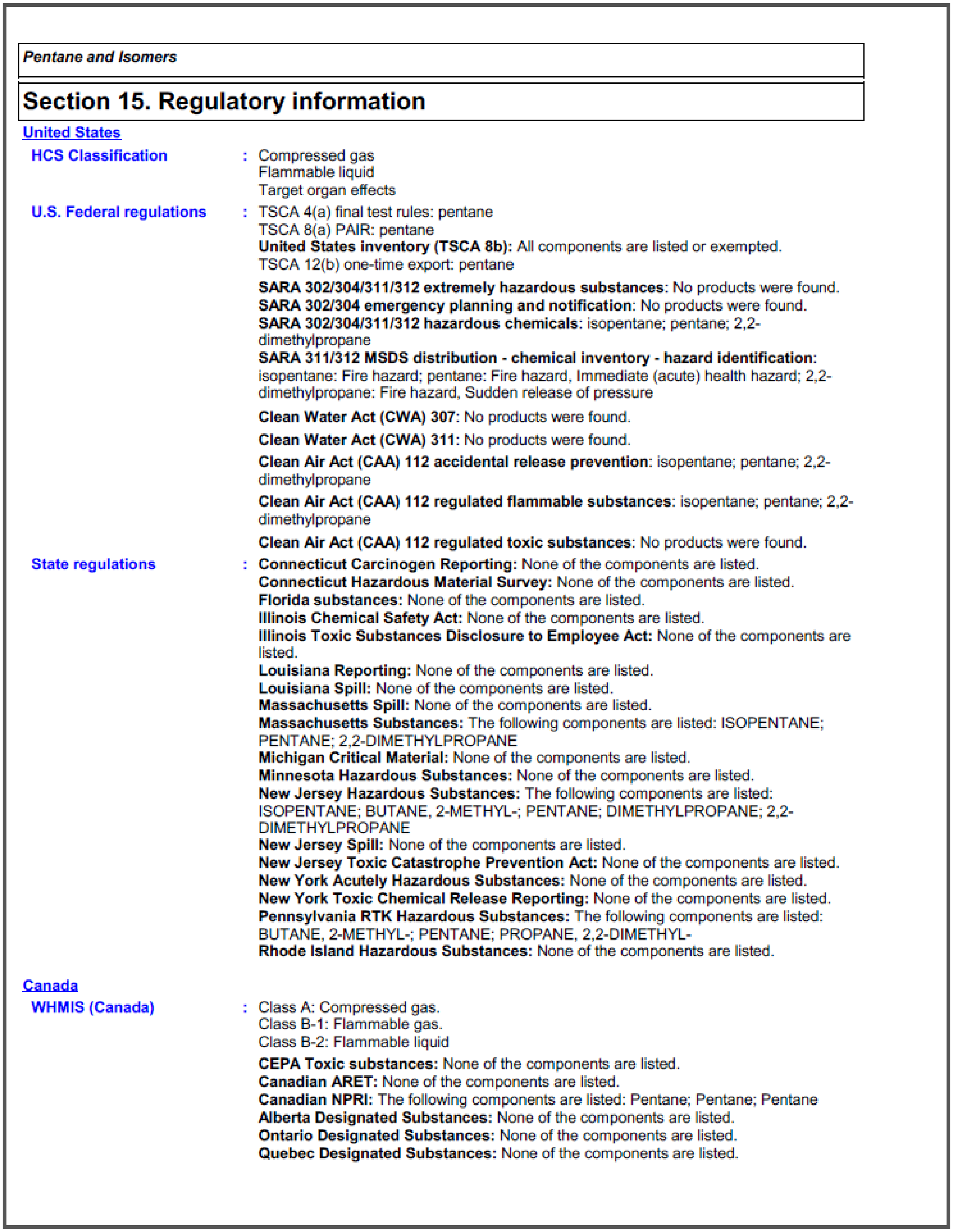
Waste disposal : The generation of waste should be avoided or minimized wherever possible. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe way. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1265	Pentanes, Liquid	3	-		-
TDG Classification	UN1265	Pentanes, Liquid	3	-		**Explosive Limit and Limited Quantity Index** 0 **Passenger Carrying Ship Index** Forbidden **Passenger Carrying Road or Rail Index** 1
Mexico Classification	UN1265	Pentanes, Liquid	3	-		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."



Pentane and Isomers

Section 15. Regulatory information

United States

HCS Classification : Compressed gas
Flammable liquid
Target organ effects

U.S. Federal regulations : TSCA 4(a) final test rules: pentane
TSCA 8(a) PAIR: pentane
United States inventory (TSCA 8b): All components are listed or exempted.
TSCA 12(b) one-time export: pentane

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: isopentane; pentane; 2,2-dimethylpropane
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: isopentane: Fire hazard; pentane: Fire hazard, Immediate (acute) health hazard; 2,2-dimethylpropane: Fire hazard, Sudden release of pressure

Clean Water Act (CWA) 307: No products were found.

Clean Water Act (CWA) 311: No products were found.

Clean Air Act (CAA) 112 accidental release prevention: isopentane; pentane; 2,2-dimethylpropane

Clean Air Act (CAA) 112 regulated flammable substances: isopentane; pentane; 2,2-dimethylpropane

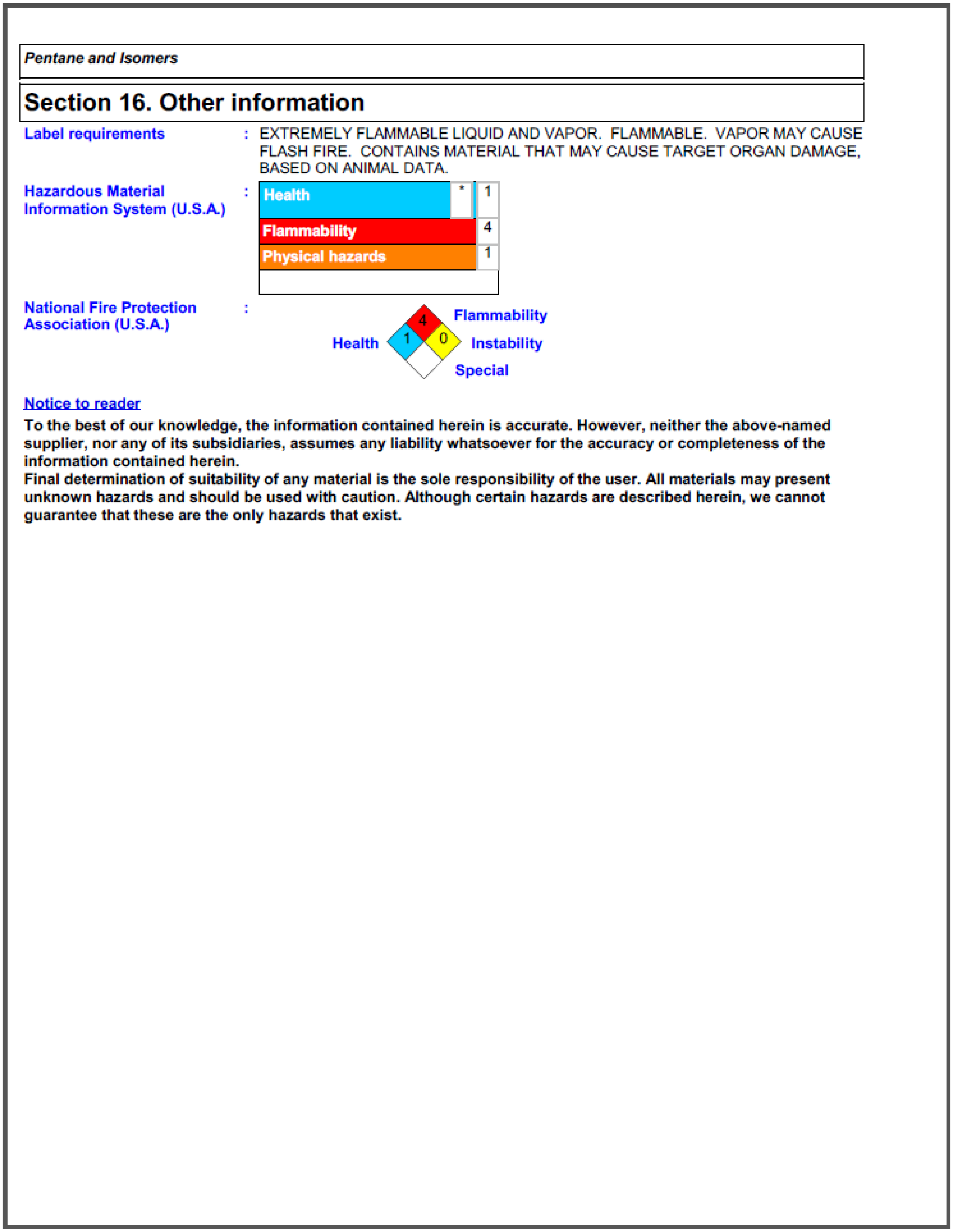
Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

State regulations : **Connecticut Carcinogen Reporting:** None of the components are listed.
Connecticut Hazardous Material Survey: None of the components are listed.
Florida substances: None of the components are listed.
Illinois Chemical Safety Act: None of the components are listed.
Illinois Toxic Substances Disclosure to Employee Act: None of the components are listed.
Louisiana Reporting: None of the components are listed.
Louisiana Spill: None of the components are listed.
Massachusetts Spill: None of the components are listed.
Massachusetts Substances: The following components are listed: ISOPENTANE; PENTANE; 2,2-DIMETHYLPROPANE
Michigan Critical Material: None of the components are listed.
Minnesota Hazardous Substances: None of the components are listed.
New Jersey Hazardous Substances: The following components are listed: ISOPENTANE; BUTANE, 2-METHYL-; PENTANE; DIMETHYLPROPANE; 2,2-DIMETHYLPROPANE
New Jersey Spill: None of the components are listed.
New Jersey Toxic Catastrophe Prevention Act: None of the components are listed.
New York Acutely Hazardous Substances: None of the components are listed.
New York Toxic Chemical Release Reporting: None of the components are listed.
Pennsylvania RTK Hazardous Substances: The following components are listed: BUTANE, 2-METHYL-; PENTANE; PROPANE, 2,2-DIMETHYL-
Rhode Island Hazardous Substances: None of the components are listed.

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class B-1: Flammable gas.
Class B-2: Flammable liquid

CEPA Toxic substances: None of the components are listed.
Canadian ARET: None of the components are listed.
Canadian NPRI: The following components are listed: Pentane; Pentane; Pentane
Alberta Designated Substances: None of the components are listed.
Ontario Designated Substances: None of the components are listed.
Quebec Designated Substances: None of the components are listed.



Pentane and Isomers

Section 16. Other information

Label requirements : EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. CONTAINS MATERIAL THAT MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

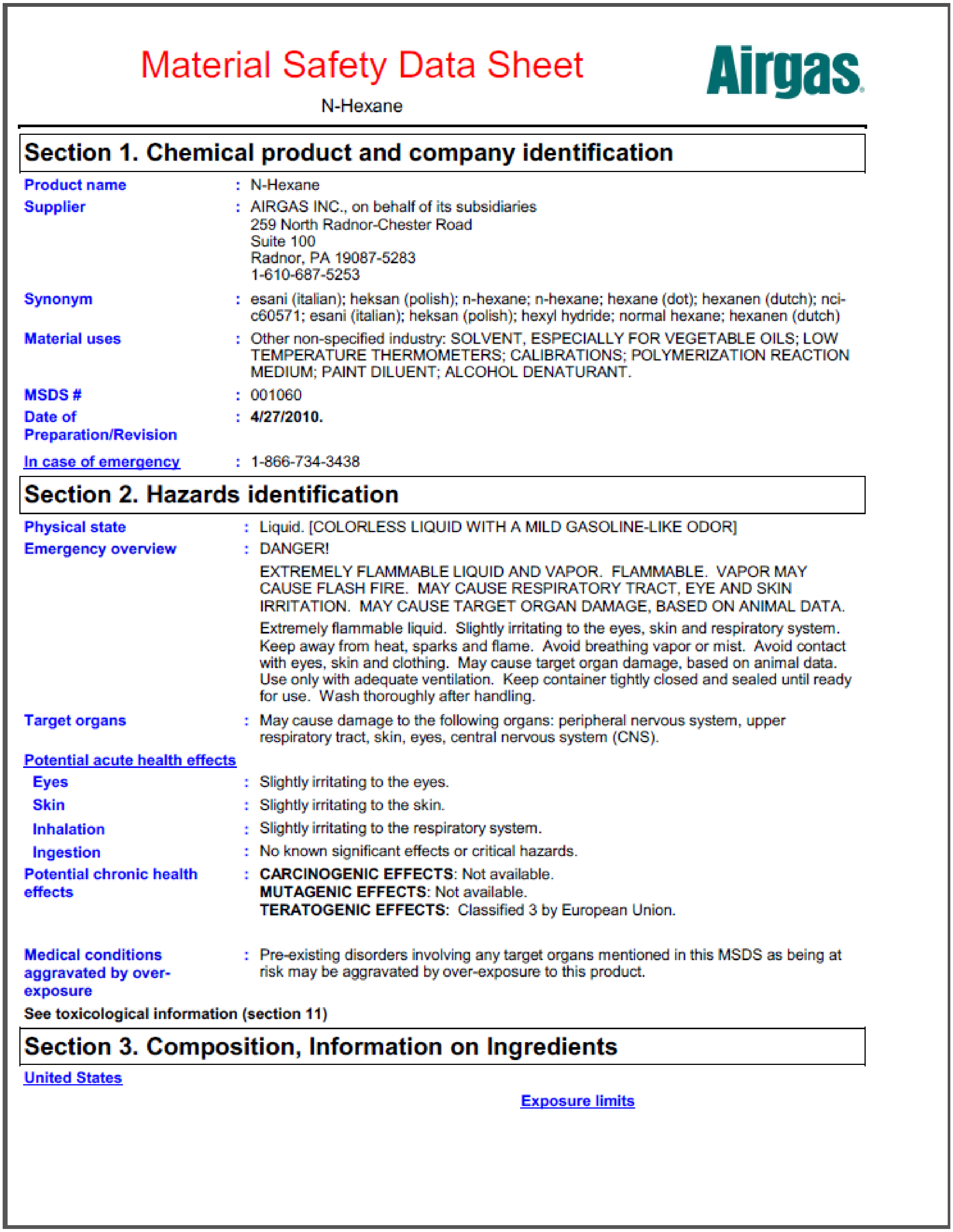
Hazardous Material Information System (U.S.A.) :

Health	*	1
Flammability		4
Physical hazards		1

National Fire Protection Association (U.S.A.) :

Flammability 4
Health 1
Instability 0
Special

Notice to reader



Material Safety Data Sheet

Airgas

N-Hexane

Section 1. Chemical product and company identification

Product name : N-Hexane

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Synonym : esani (italian); heksan (polish); n-hexane; n-hexane; hexane (dot); hexanen (dutch); nci-c60571; esani (italian); heksan (polish); hexyl hydride; normal hexane; hexanen (dutch)

Material uses : Other non-specified industry: SOLVENT, ESPECIALLY FOR VEGETABLE OILS; LOW TEMPERATURE THERMOMETERS; CALIBRATIONS; POLYMERIZATION REACTION MEDIUM; PAINT DILUENT; ALCOHOL DENATURANT.

MSDS # : 001060

Date of Preparation/Revision : **4/27/2010.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Liquid. [COLORLESS LIQUID WITH A MILD GASOLINE-LIKE ODOR]

Emergency overview : DANGER!

EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. MAY CAUSE RESPIRATORY TRACT, EYE AND SKIN IRRITATION. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

Extremely flammable liquid. Slightly irritating to the eyes, skin and respiratory system. Keep away from heat, sparks and flame. Avoid breathing vapor or mist. Avoid contact with eyes, skin and clothing. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container tightly closed and sealed until ready for use. Wash thoroughly after handling.

Target organs : May cause damage to the following organs: peripheral nervous system, upper respiratory tract, skin, eyes, central nervous system (CNS).

Potential acute health effects

Eyes : Slightly irritating to the eyes.

Skin : Slightly irritating to the skin.

Inhalation : Slightly irritating to the respiratory system.

Ingestion : No known significant effects or critical hazards.

Potential chronic health effects : **CARCINOGENIC EFFECTS**: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Classified 3 by European Union.

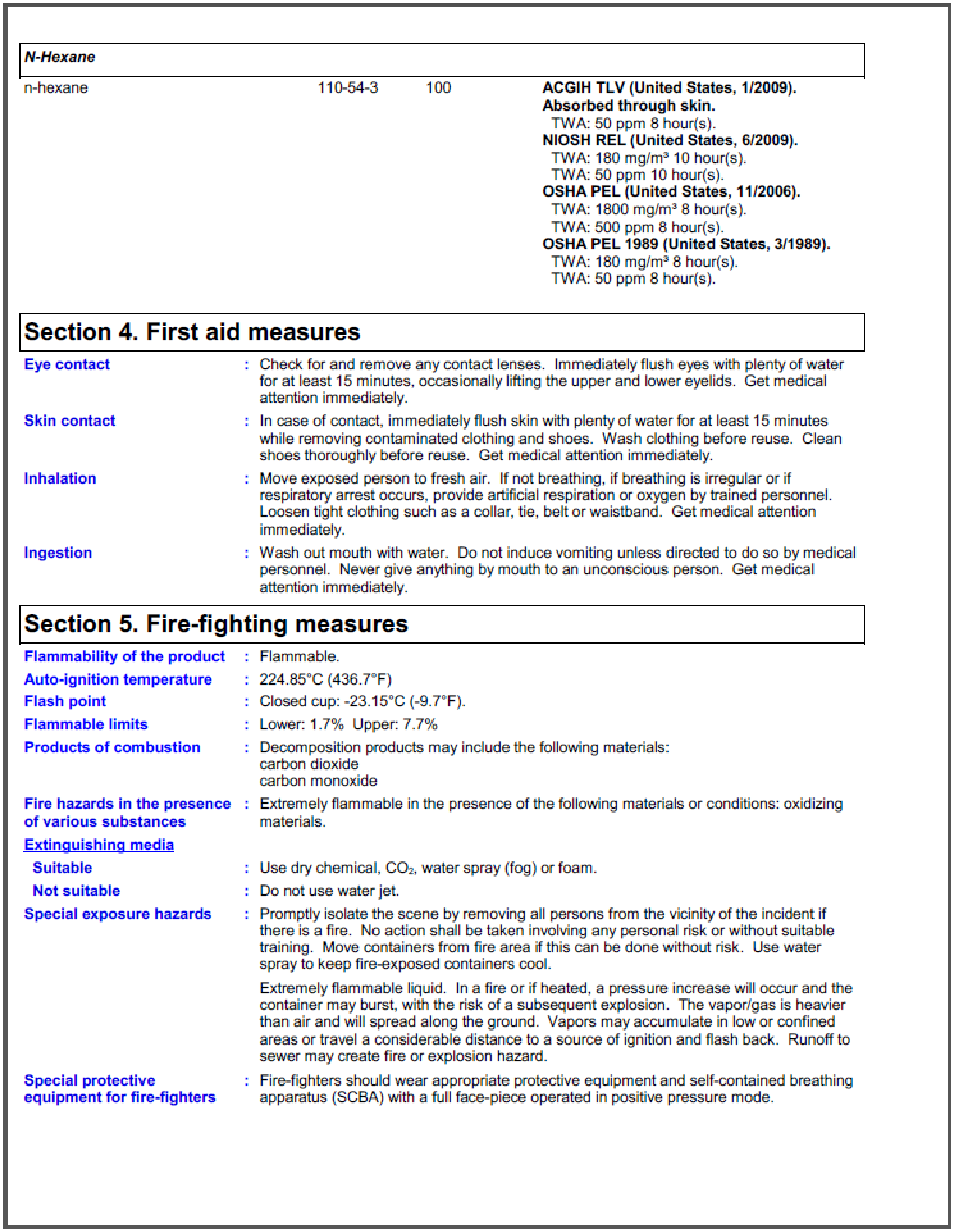
Medical conditions aggravated by over-exposure : Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

United States

Exposure limits



N-Hexane

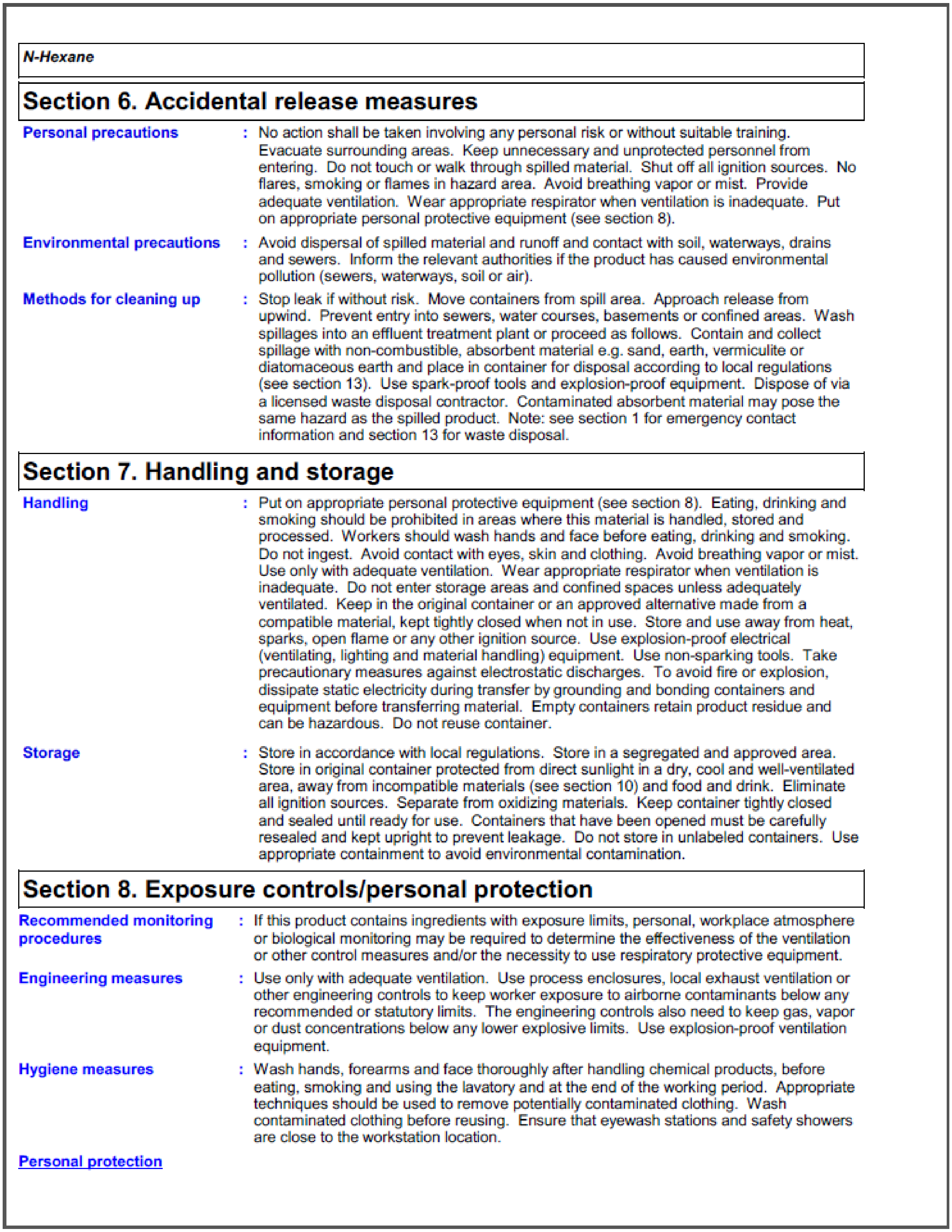
n-hexane	110-54-3	100	**ACGIH TLV (United States, 1/2009).** **Absorbed through skin.** TWA: 50 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** TWA: 180 mg/m³ 10 hour(s). TWA: 50 ppm 10 hour(s). **OSHA PEL (United States, 11/2006).** TWA: 1800 mg/m³ 8 hour(s). TWA: 500 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** TWA: 180 mg/m³ 8 hour(s). TWA: 50 ppm 8 hour(s).

Section 4. First aid measures

Eye contact	: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.
Skin contact	: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.
Inhalation	: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.
Ingestion	: Wash out mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Get medical attention immediately.

Section 5. Fire-fighting measures

Flammability of the product	: Flammable.
Auto-ignition temperature	: 224.85°C (436.7°F)
Flash point	: Closed cup: -23.15°C (-9.7°F).
Flammable limits	: Lower: 1.7% Upper: 7.7%
Products of combustion	: Decomposition products may include the following materials: carbon dioxide carbon monoxide
Fire hazards in the presence of various substances	: Extremely flammable in the presence of the following materials or conditions: oxidizing materials.
Extinguishing media	
Suitable	: Use dry chemical, CO_2, water spray (fog) or foam.
Not suitable	: Do not use water jet.
Special exposure hazards	: Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool. Extremely flammable liquid. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. The vapor/gas is heavier than air and will spread along the ground. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back. Runoff to sewer may create fire or explosion hazard.
Special protective equipment for fire-fighters	: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.



N-Hexane

Section 6. Accidental release measures

Personal precautions : No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment (see section 8).

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

Methods for cleaning up : Stop leak if without risk. Move containers from spill area. Approach release from upwind. Prevent entry into sewers, water courses, basements or confined areas. Wash spillages into an effluent treatment plant or proceed as follows. Contain and collect spillage with non-combustible, absorbent material e.g. sand, earth, vermiculite or diatomaceous earth and place in container for disposal according to local regulations (see section 13). Use spark-proof tools and explosion-proof equipment. Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilled product. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : Put on appropriate personal protective equipment (see section 8). Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use non-sparking tools. Take precautionary measures against electrostatic discharges. To avoid fire or explosion, dissipate static electricity during transfer by grounding and bonding containers and equipment before transferring material. Empty containers retain product residue and can be hazardous. Do not reuse container.

Storage : Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabeled containers. Use appropriate containment to avoid environmental contamination.

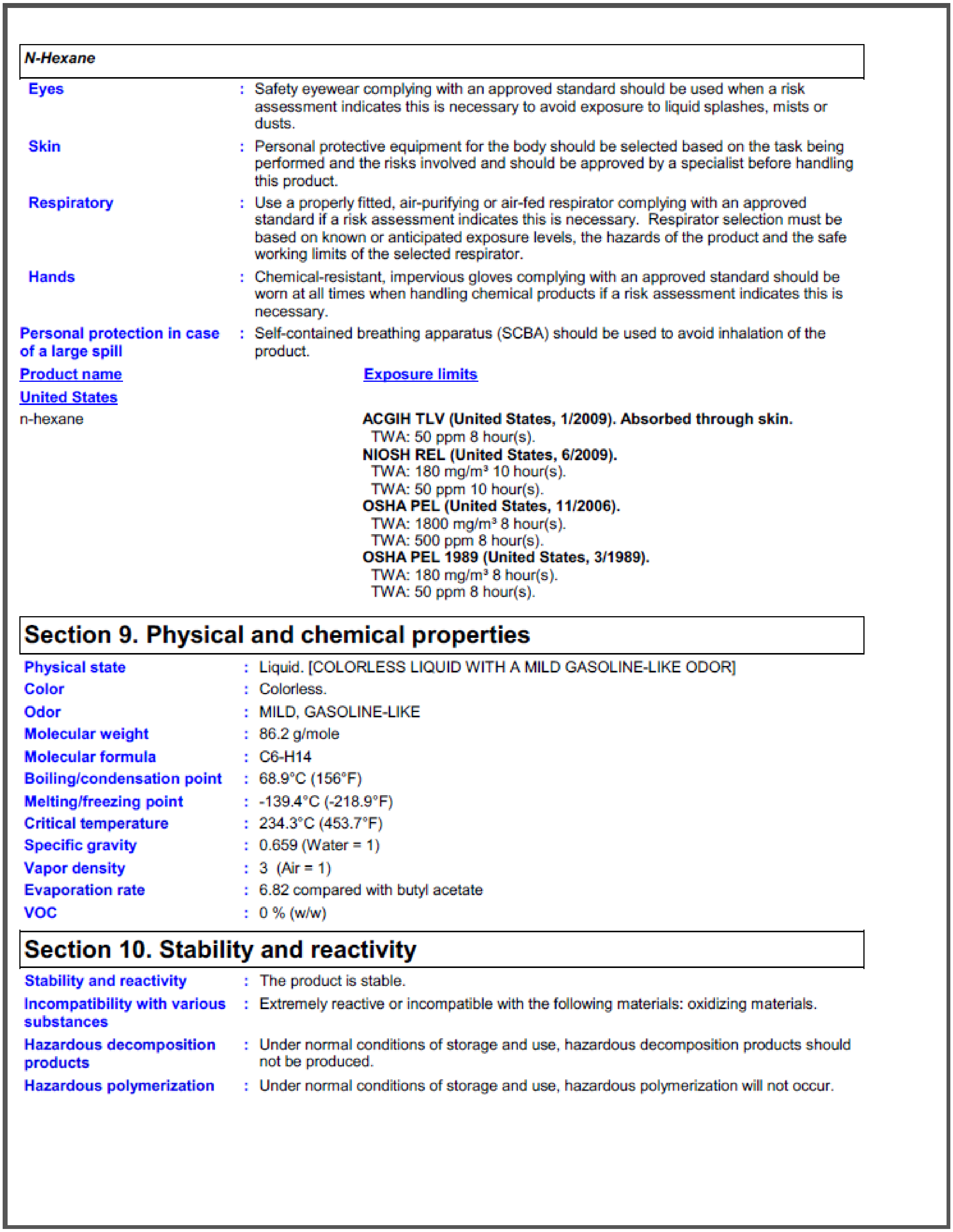
Section 8. Exposure controls/personal protection

Recommended monitoring procedures : If this product contains ingredients with exposure limits, personal, workplace atmosphere or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment.

Engineering measures : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Hygiene measures : Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal protection



N-Hexane

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name	**Exposure limits**
United States	
n-hexane	**ACGIH TLV (United States, 1/2009). Absorbed through skin.** TWA: 50 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** TWA: 180 mg/m³ 10 hour(s). TWA: 50 ppm 10 hour(s). **OSHA PEL (United States, 11/2006).** TWA: 1800 mg/m³ 8 hour(s). TWA: 500 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** TWA: 180 mg/m³ 8 hour(s). TWA: 50 ppm 8 hour(s).

Section 9. Physical and chemical properties

Physical state : Liquid. [COLORLESS LIQUID WITH A MILD GASOLINE-LIKE ODOR]

Color : Colorless.

Odor : MILD, GASOLINE-LIKE

Molecular weight : 86.2 g/mole

Molecular formula : C6-H14

Boiling/condensation point : 68.9°C (156°F)

Melting/freezing point : -139.4°C (-218.9°F)

Critical temperature : 234.3°C (453.7°F)

Specific gravity : 0.659 (Water = 1)

Vapor density : 3 (Air = 1)

Evaporation rate : 6.82 compared with butyl acetate

VOC : 0 % (w/w)

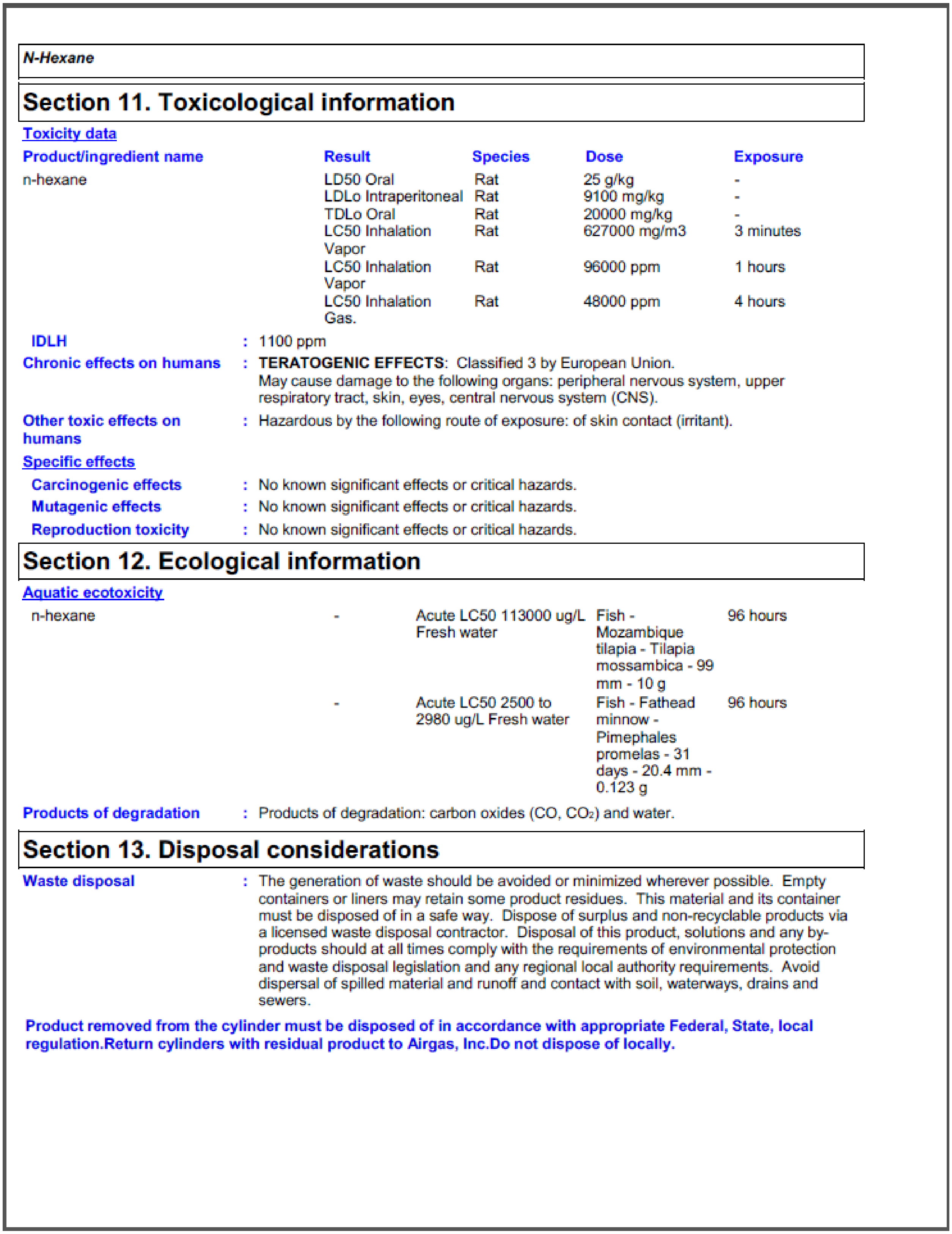
Section 10. Stability and reactivity

Stability and reactivity : The product is stable.

Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.

Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.



N-Hexane

Section 11. Toxicological information

Toxicity data

Product/ingredient name	Result	Species	Dose	Exposure
n-hexane	LD50 Oral	Rat	25 g/kg	-
	LDLo Intraperitoneal	Rat	9100 mg/kg	-
	TDLo Oral	Rat	20000 mg/kg	-
	LC50 Inhalation Vapor	Rat	627000 mg/m3	3 minutes
	LC50 Inhalation Vapor	Rat	96000 ppm	1 hours
	LC50 Inhalation Gas.	Rat	48000 ppm	4 hours

IDLH : 1100 ppm

Chronic effects on humans : **TERATOGENIC EFFECTS**: Classified 3 by European Union. May cause damage to the following organs: peripheral nervous system, upper respiratory tract, skin, eyes, central nervous system (CNS).

Other toxic effects on humans : Hazardous by the following route of exposure: of skin contact (irritant).

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.

Mutagenic effects : No known significant effects or critical hazards.

Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

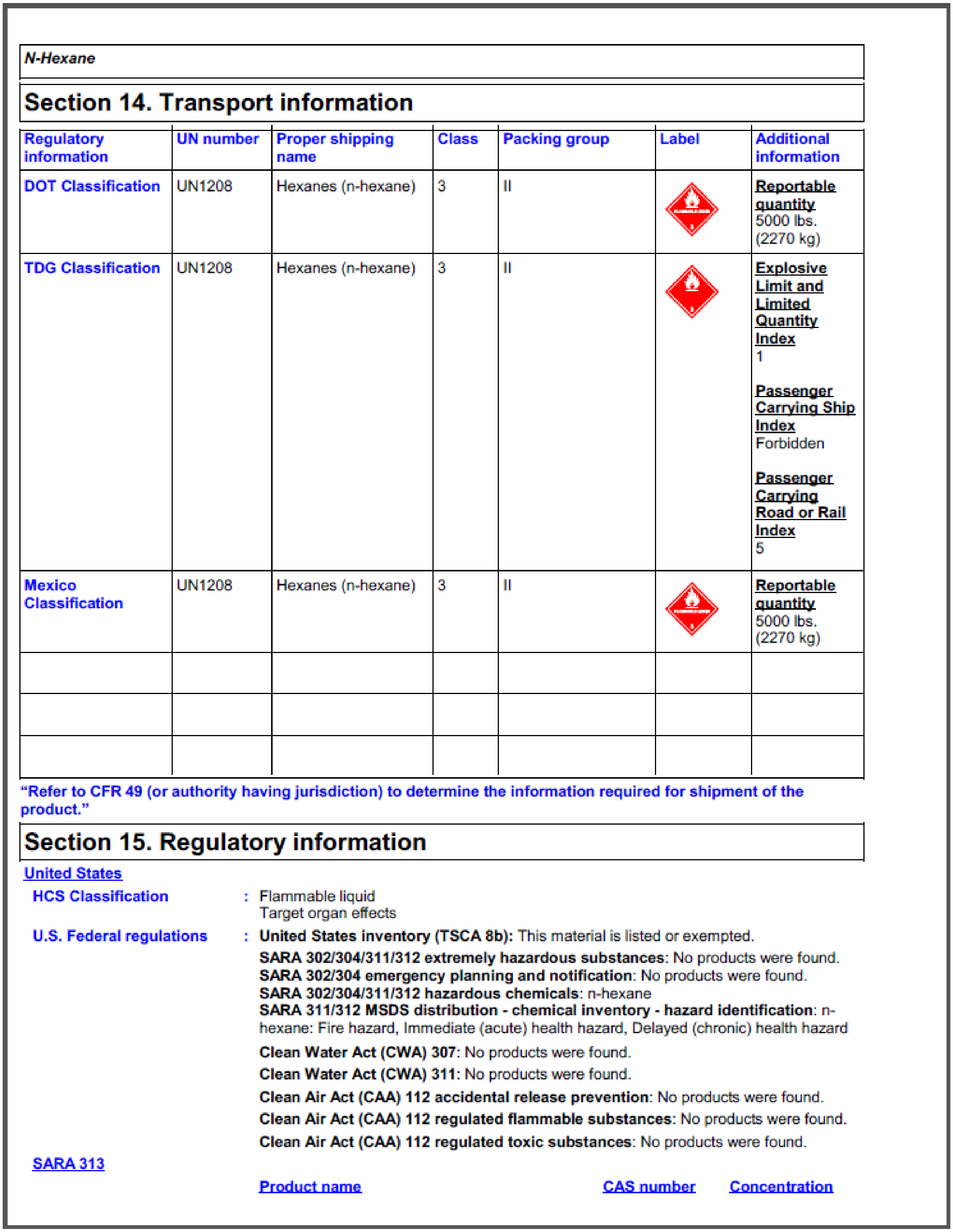
n-hexane	-	Acute LC50 113000 ug/L Fresh water	Fish - Mozambique tilapia - Tilapia mossambica - 99 mm - 10 g	96 hours
	-	Acute LC50 2500 to 2980 ug/L Fresh water	Fish - Fathead minnow - Pimephales promelas - 31 days - 20.4 mm - 0.123 g	96 hours

Products of degradation : Products of degradation: carbon oxides (CO, CO_2) and water.

Section 13. Disposal considerations

Waste disposal : The generation of waste should be avoided or minimized wherever possible. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe way. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.



N-Hexane

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1208	Hexanes (n-hexane)	3	II	◆	**Reportable quantity** 5000 lbs. (2270 kg)
TDG Classification	UN1208	Hexanes (n-hexane)	3	II	◆	**Explosive Limit and Limited Quantity Index** 1 **Passenger Carrying Ship Index** Forbidden **Passenger Carrying Road or Rail Index** 5
Mexico Classification	UN1208	Hexanes (n-hexane)	3	II	◆	**Reportable quantity** 5000 lbs. (2270 kg)

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

HCS Classification : Flammable liquid
Target organ effects

U.S. Federal regulations : **United States inventory (TSCA 8b):** This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: n-hexane
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: n-hexane: Fire hazard, Immediate (acute) health hazard, Delayed (chronic) health hazard

Clean Water Act (CWA) 307: No products were found.

Clean Water Act (CWA) 311: No products were found.

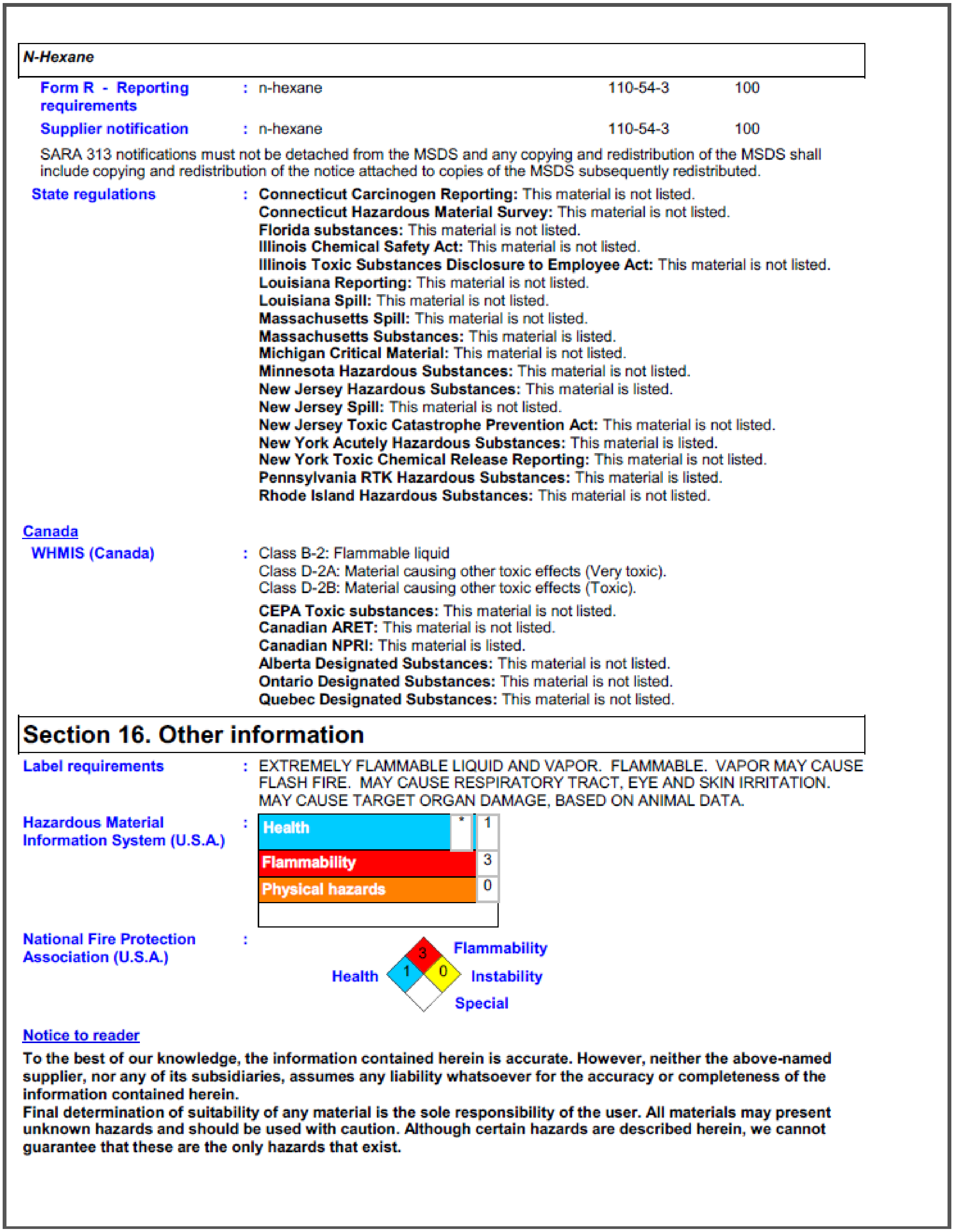
Clean Air Act (CAA) 112 accidental release prevention: No products were found.

Clean Air Act (CAA) 112 regulated flammable substances: No products were found.

Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

SARA 313

Product name	CAS number	Concentration



N-Hexane

Form R - Reporting requirements	:	n-hexane	110-54-3	100
Supplier notification	:	n-hexane	110-54-3	100

SARA 313 notifications must not be detached from the MSDS and any copying and redistribution of the MSDS shall include copying and redistribution of the notice attached to copies of the MSDS subsequently redistributed.

State regulations :
Connecticut Carcinogen Reporting: This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) :
Class B-2: Flammable liquid
Class D-2A: Material causing other toxic effects (Very toxic).
Class D-2B: Material causing other toxic effects (Toxic).

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

Label requirements : EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. MAY CAUSE RESPIRATORY TRACT, EYE AND SKIN IRRITATION. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

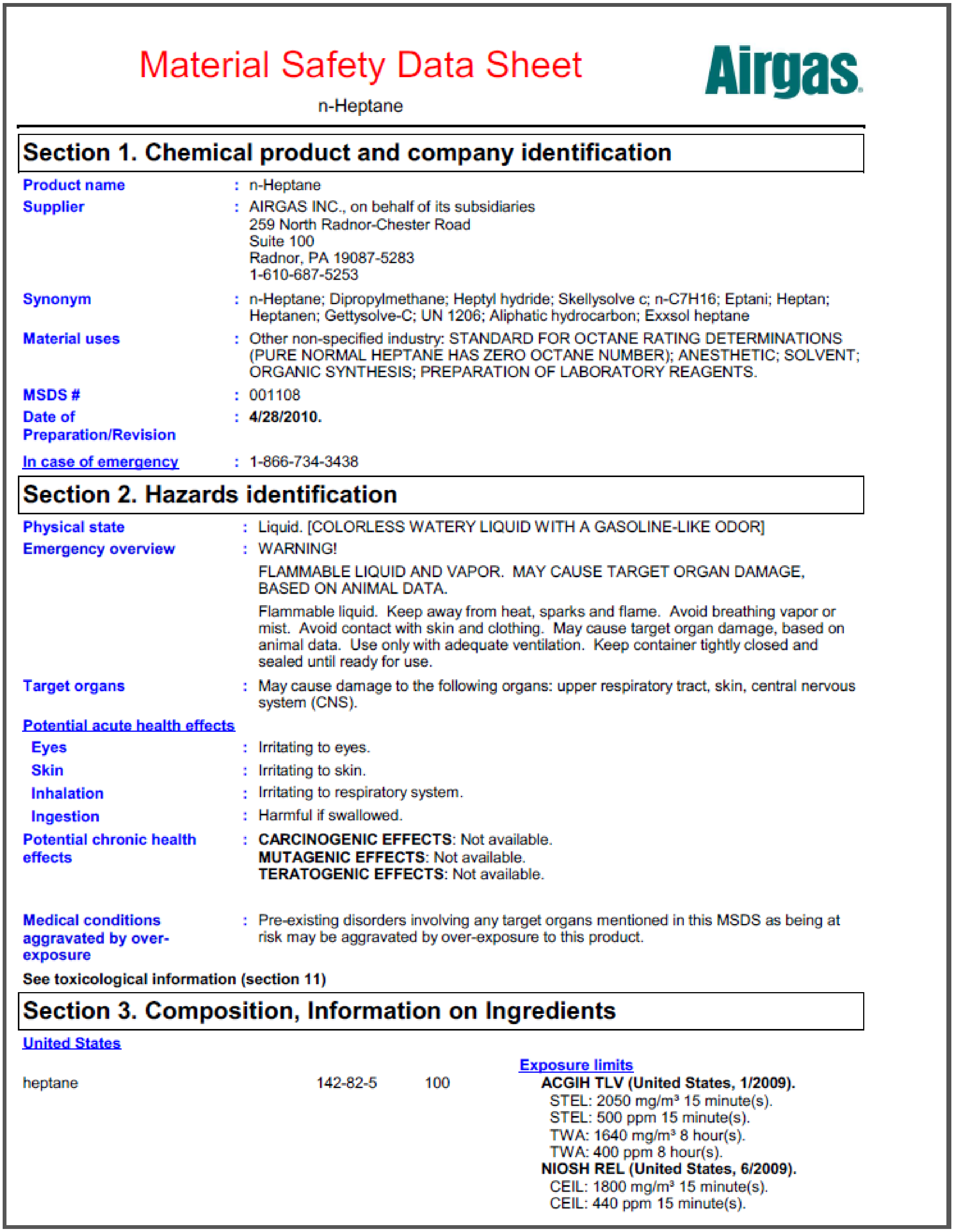
Hazardous Material Information System (U.S.A.) :

Health	*	1
Flammability		3
Physical hazards		0

National Fire Protection Association (U.S.A.) :

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.



Material Safety Data Sheet

Airgas

n-Heptane

Section 1. Chemical product and company identification

Product name : n-Heptane

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Synonym : n-Heptane; Dipropylmethane; Heptyl hydride; Skellysolve c; n-C7H16; Eptani; Heptan; Heptanen; Gettysolve-C; UN 1206; Aliphatic hydrocarbon; Exxsol heptane

Material uses : Other non-specified industry: STANDARD FOR OCTANE RATING DETERMINATIONS (PURE NORMAL HEPTANE HAS ZERO OCTANE NUMBER); ANESTHETIC; SOLVENT; ORGANIC SYNTHESIS; PREPARATION OF LABORATORY REAGENTS.

MSDS # : 001108

Date of Preparation/Revision : **4/28/2010.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Liquid. [COLORLESS WATERY LIQUID WITH A GASOLINE-LIKE ODOR]

Emergency overview : WARNING!

FLAMMABLE LIQUID AND VAPOR. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

Flammable liquid. Keep away from heat, sparks and flame. Avoid breathing vapor or mist. Avoid contact with skin and clothing. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container tightly closed and sealed until ready for use.

Target organs : May cause damage to the following organs: upper respiratory tract, skin, central nervous system (CNS).

Potential acute health effects

- **Eyes** : Irritating to eyes.
- **Skin** : Irritating to skin.
- **Inhalation** : Irritating to respiratory system.
- **Ingestion** : Harmful if swallowed.

Potential chronic health effects : **CARCINOGENIC EFFECTS**: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.

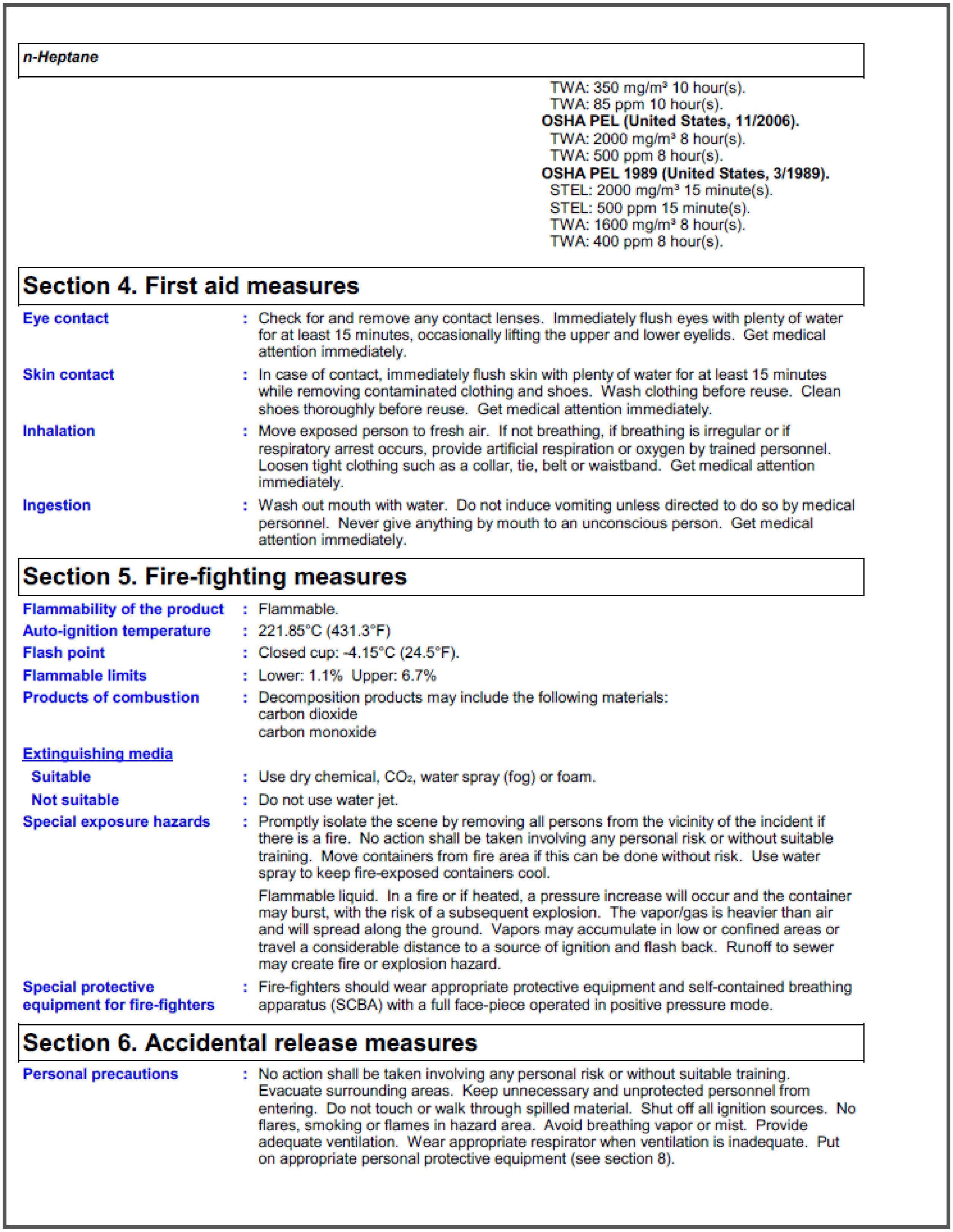
Medical conditions aggravated by over-exposure : Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

United States

			Exposure limits
heptane	142-82-5	100	**ACGIH TLV (United States, 1/2009).** STEL: 2050 mg/m^3 15 minute(s). STEL: 500 ppm 15 minute(s). TWA: 1640 mg/m^3 8 hour(s). TWA: 400 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** CEIL: 1800 mg/m^3 15 minute(s). CEIL: 440 ppm 15 minute(s).



n-Heptane

TWA: 350 mg/m^3 10 hour(s).
TWA: 85 ppm 10 hour(s).
OSHA PEL (United States, 11/2006).
TWA: 2000 mg/m^3 8 hour(s).
TWA: 500 ppm 8 hour(s).
OSHA PEL 1989 (United States, 3/1989).
STEL: 2000 mg/m^3 15 minute(s).
STEL: 500 ppm 15 minute(s).
TWA: 1600 mg/m^3 8 hour(s).
TWA: 400 ppm 8 hour(s).

Section 4. First aid measures

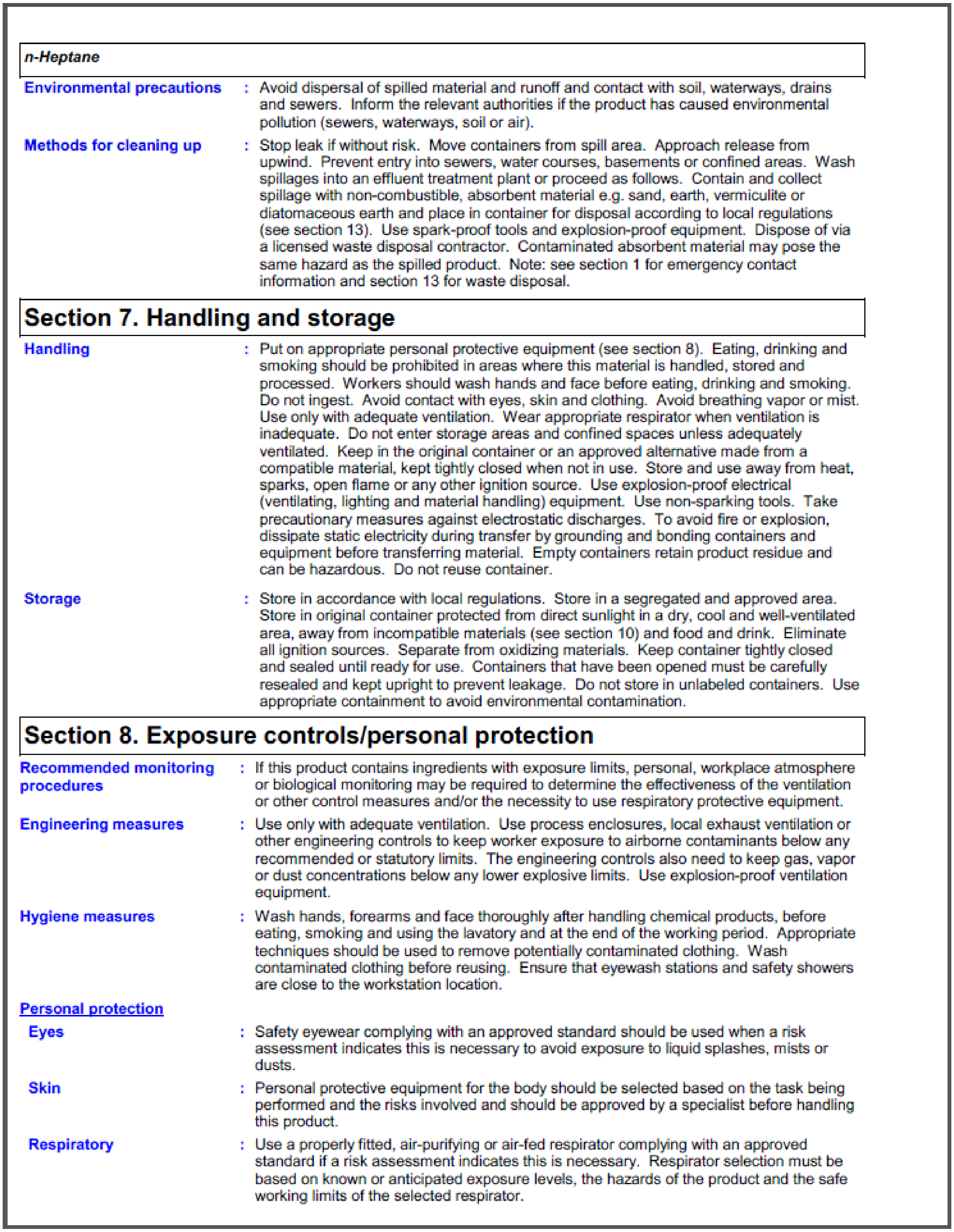
Eye contact	:	Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.
Skin contact	:	In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.
Inhalation	:	Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.
Ingestion	:	Wash out mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Get medical attention immediately.

Section 5. Fire-fighting measures

Flammability of the product	:	Flammable.
Auto-ignition temperature	:	221.85°C (431.3°F)
Flash point	:	Closed cup: -4.15°C (24.5°F).
Flammable limits	:	Lower: 1.1% Upper: 6.7%
Products of combustion	:	Decomposition products may include the following materials: carbon dioxide carbon monoxide
Extinguishing media		
Suitable	:	Use dry chemical, CO_2, water spray (fog) or foam.
Not suitable	:	Do not use water jet.
Special exposure hazards	:	Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool. Flammable liquid. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. The vapor/gas is heavier than air and will spread along the ground. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back. Runoff to sewer may create fire or explosion hazard.
Special protective equipment for fire-fighters	:	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions	:	No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment (see section 8).



n-Heptane

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

Methods for cleaning up : Stop leak if without risk. Move containers from spill area. Approach release from upwind. Prevent entry into sewers, water courses, basements or confined areas. Wash spillages into an effluent treatment plant or proceed as follows. Contain and collect spillage with non-combustible, absorbent material e.g. sand, earth, vermiculite or diatomaceous earth and place in container for disposal according to local regulations (see section 13). Use spark-proof tools and explosion-proof equipment. Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilled product. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : Put on appropriate personal protective equipment (see section 8). Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use non-sparking tools. Take precautionary measures against electrostatic discharges. To avoid fire or explosion, dissipate static electricity during transfer by grounding and bonding containers and equipment before transferring material. Empty containers retain product residue and can be hazardous. Do not reuse container.

Storage : Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabeled containers. Use appropriate containment to avoid environmental contamination.

Section 8. Exposure controls/personal protection

Recommended monitoring procedures : If this product contains ingredients with exposure limits, personal, workplace atmosphere or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment.

Engineering measures : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

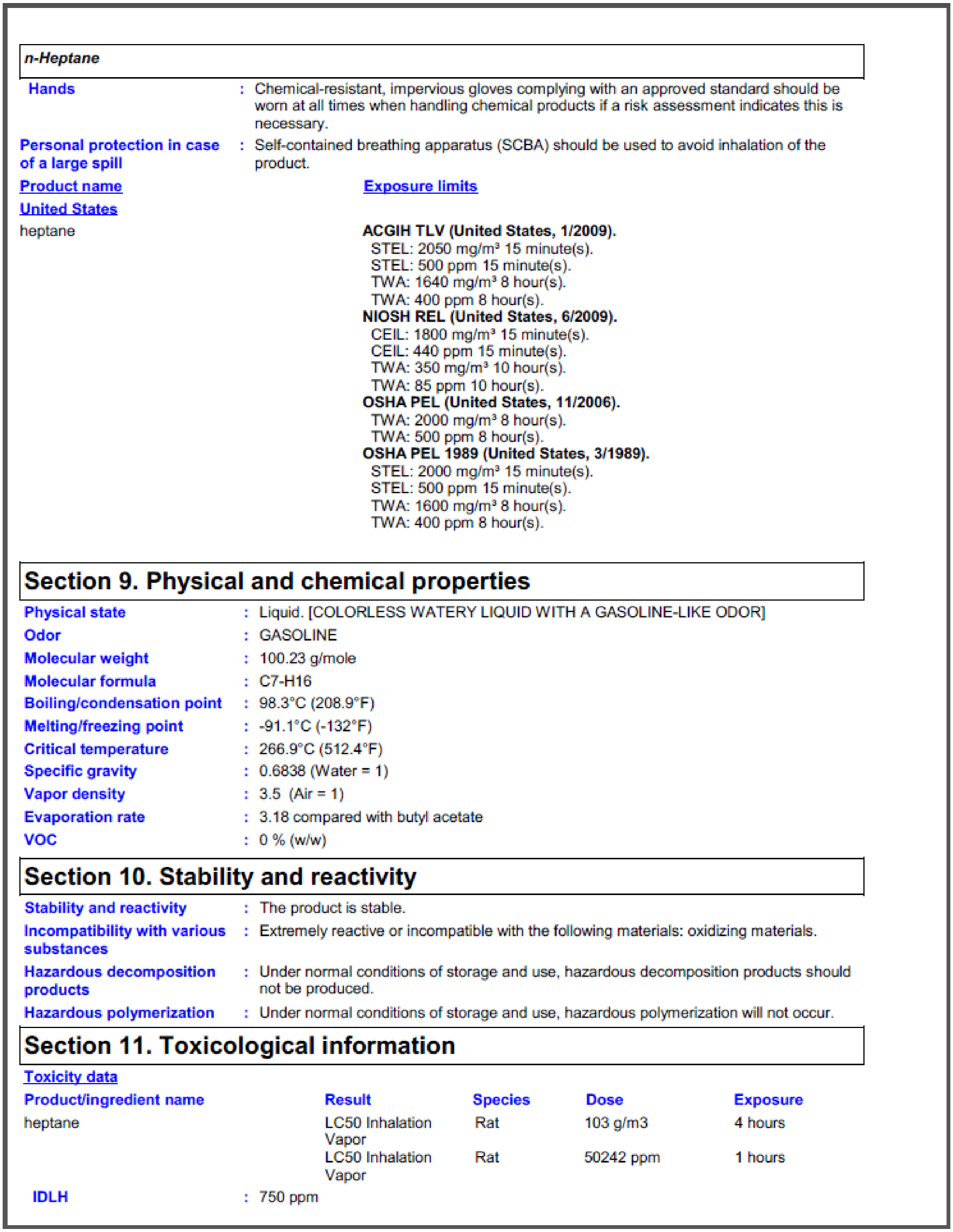
Hygiene measures : Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.



n-Heptane

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name	**Exposure limits**
United States	
heptane	**ACGIH TLV (United States, 1/2009).** STEL: 2050 mg/m³ 15 minute(s). STEL: 500 ppm 15 minute(s). TWA: 1640 mg/m³ 8 hour(s). TWA: 400 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** CEIL: 1800 mg/m³ 15 minute(s). CEIL: 440 ppm 15 minute(s). TWA: 350 mg/m³ 10 hour(s). TWA: 85 ppm 10 hour(s). **OSHA PEL (United States, 11/2006).** TWA: 2000 mg/m³ 8 hour(s). TWA: 500 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** STEL: 2000 mg/m³ 15 minute(s). STEL: 500 ppm 15 minute(s). TWA: 1600 mg/m³ 8 hour(s). TWA: 400 ppm 8 hour(s).

Section 9. Physical and chemical properties

Physical state : Liquid. [COLORLESS WATERY LIQUID WITH A GASOLINE-LIKE ODOR]
Odor : GASOLINE
Molecular weight : 100.23 g/mole
Molecular formula : C7-H16
Boiling/condensation point : 98.3°C (208.9°F)
Melting/freezing point : -91.1°C (-132°F)
Critical temperature : 266.9°C (512.4°F)
Specific gravity : 0.6838 (Water = 1)
Vapor density : 3.5 (Air = 1)
Evaporation rate : 3.18 compared with butyl acetate
VOC : 0 % (w/w)

Section 10. Stability and reactivity

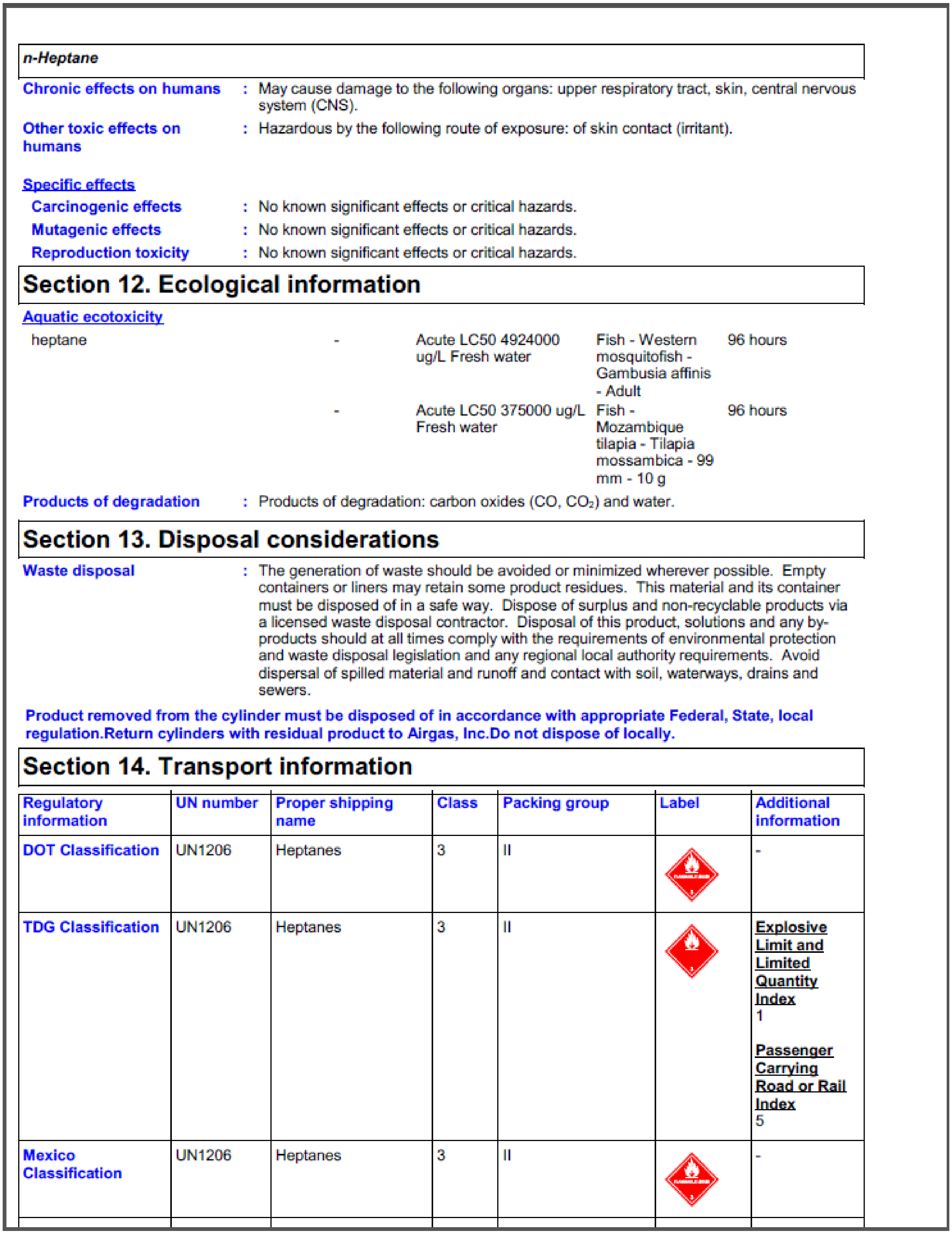
Stability and reactivity : The product is stable.
Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Product/ingredient name	**Result**	**Species**	**Dose**	**Exposure**
heptane	LC50 Inhalation Vapor	Rat	103 g/m3	4 hours
	LC50 Inhalation Vapor	Rat	50242 ppm	1 hours

IDLH : 750 ppm



n-Heptane

Chronic effects on humans : May cause damage to the following organs: upper respiratory tract, skin, central nervous system (CNS).

Other toxic effects on humans : Hazardous by the following route of exposure: of skin contact (irritant).

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.

Mutagenic effects : No known significant effects or critical hazards.

Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

heptane	-	Acute LC50 4924000 ug/L Fresh water	Fish - Western mosquitofish - Gambusia affinis - Adult	96 hours
	-	Acute LC50 375000 ug/L Fresh water	Fish - Mozambique tilapia - Tilapia mossambica - 99 mm - 10 g	96 hours

Products of degradation : Products of degradation: carbon oxides (CO, CO_2) and water.

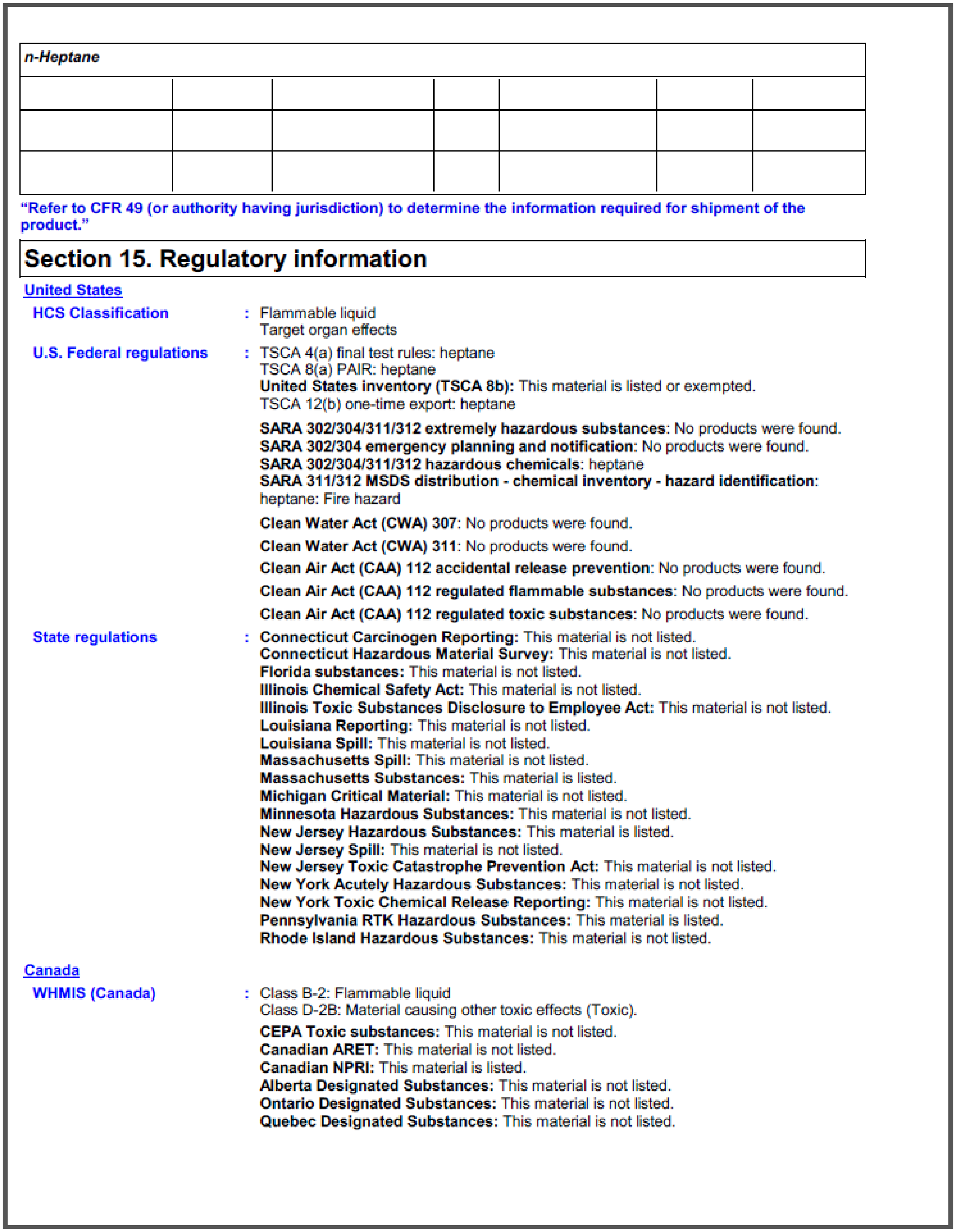
Section 13. Disposal considerations

Waste disposal : The generation of waste should be avoided or minimized wherever possible. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe way. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1206	Heptanes	3	II		-
TDG Classification	UN1206	Heptanes	3	II		**Explosive Limit and Limited Quantity Index** 1 **Passenger Carrying Road or Rail Index** 5
Mexico Classification	UN1206	Heptanes	3	II		-



n-Heptane

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

HCS Classification : Flammable liquid
Target organ effects

U.S. Federal regulations : TSCA 4(a) final test rules: heptane
TSCA 8(a) PAIR: heptane
United States inventory (TSCA 8b): This material is listed or exempted.
TSCA 12(b) one-time export: heptane

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: heptane
SARA 311/312 MSDS distribution - chemical inventory - hazard identification:
heptane: Fire hazard

Clean Water Act (CWA) 307: No products were found.

Clean Water Act (CWA) 311: No products were found.

Clean Air Act (CAA) 112 accidental release prevention: No products were found.

Clean Air Act (CAA) 112 regulated flammable substances: No products were found.

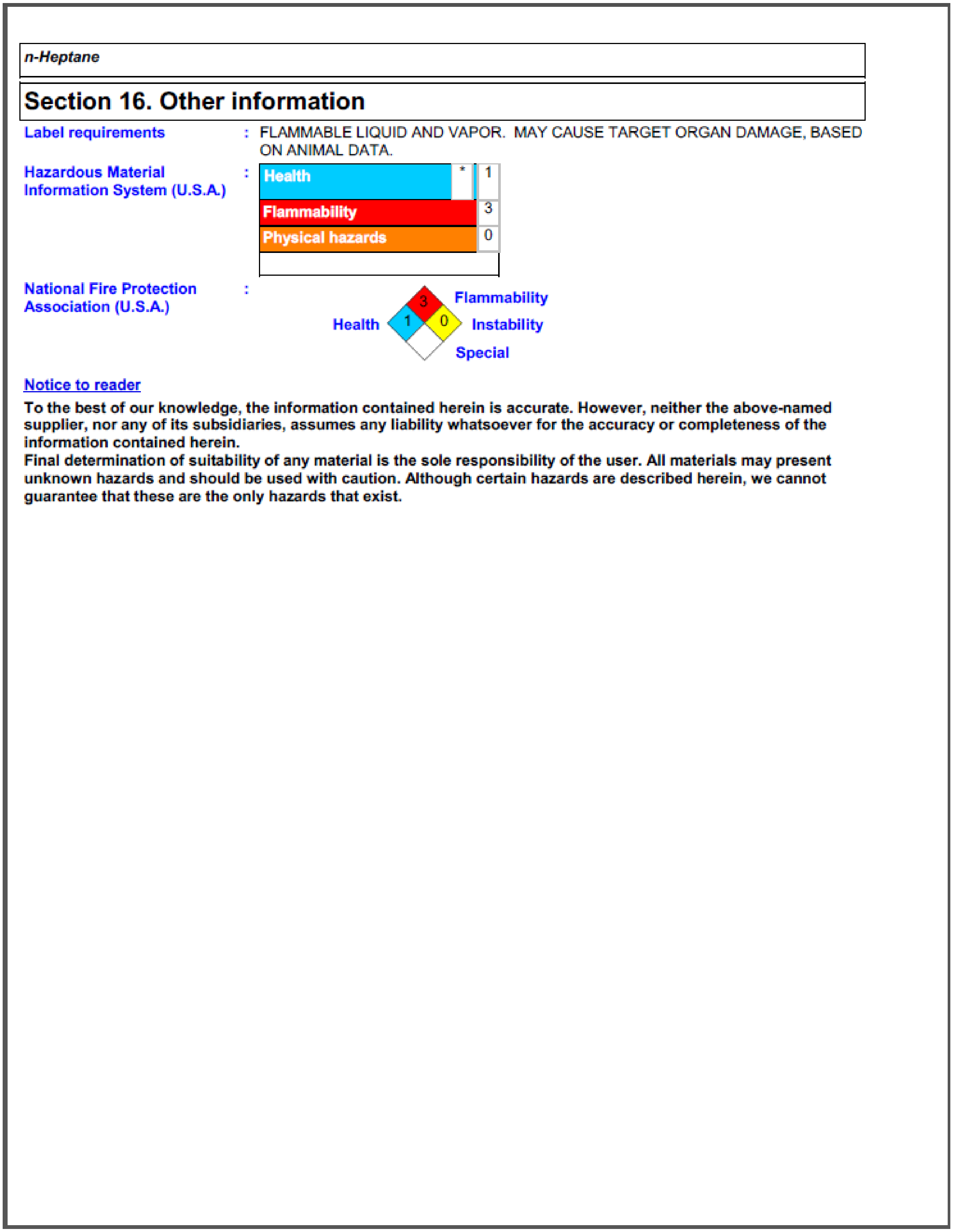
Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

State regulations : **Connecticut Carcinogen Reporting:** This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class B-2: Flammable liquid
Class D-2B: Material causing other toxic effects (Toxic).

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.



n-Heptane

Section 16. Other information

Label requirements : FLAMMABLE LIQUID AND VAPOR. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

Hazardous Material Information System (U.S.A.) :

Health	*	1
Flammability		3
Physical hazards		0

National Fire Protection Association (U.S.A.) :

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
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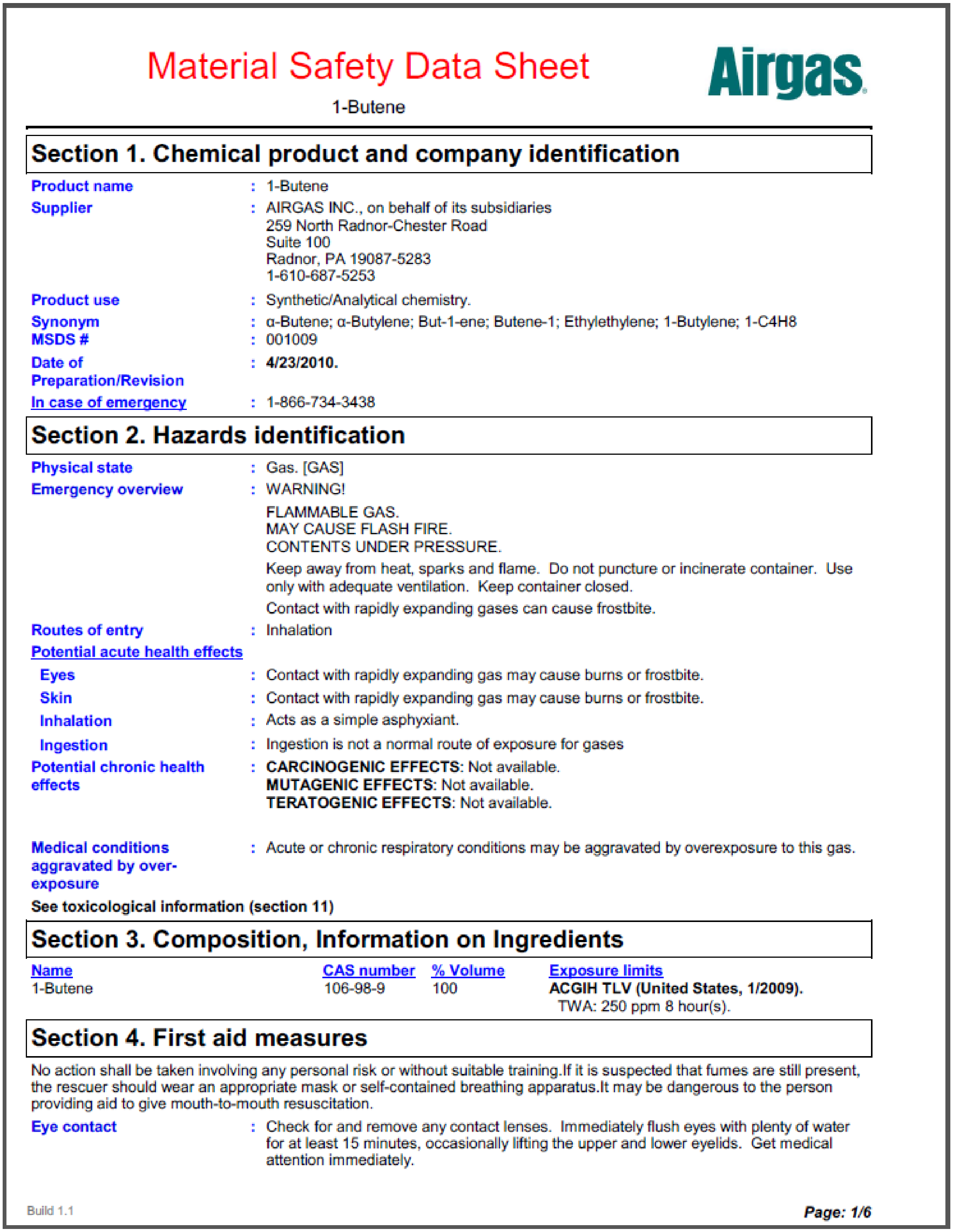

Material Safety Data Sheet

1-Butene

Airgas

Section 1. Chemical product and company identification

Product name : 1-Butene

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : α-Butene; α-Butylene; But-1-ene; Butene-1; Ethylethylene; 1-Butylene; 1-C4H8

MSDS # : 001009

Date of Preparation/Revision : **4/23/2010.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas. [GAS]

Emergency overview : WARNING!

FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
CONTENTS UNDER PRESSURE.

Keep away from heat, sparks and flame. Do not puncture or incinerate container. Use only with adequate ventilation. Keep container closed.

Contact with rapidly expanding gases can cause frostbite.

Routes of entry : Inhalation

Potential acute health effects

Eyes : Contact with rapidly expanding gas may cause burns or frostbite.

Skin : Contact with rapidly expanding gas may cause burns or frostbite.

Inhalation : Acts as a simple asphyxiant.

Ingestion : Ingestion is not a normal route of exposure for gases

Potential chronic health effects : **CARCINOGENIC EFFECTS**: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.

Medical conditions aggravated by over-exposure : Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
1-Butene	106-98-9	100	**ACGIH TLV (United States, 1/2009).** TWA: 250 ppm 8 hour(s).

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Build 1.1

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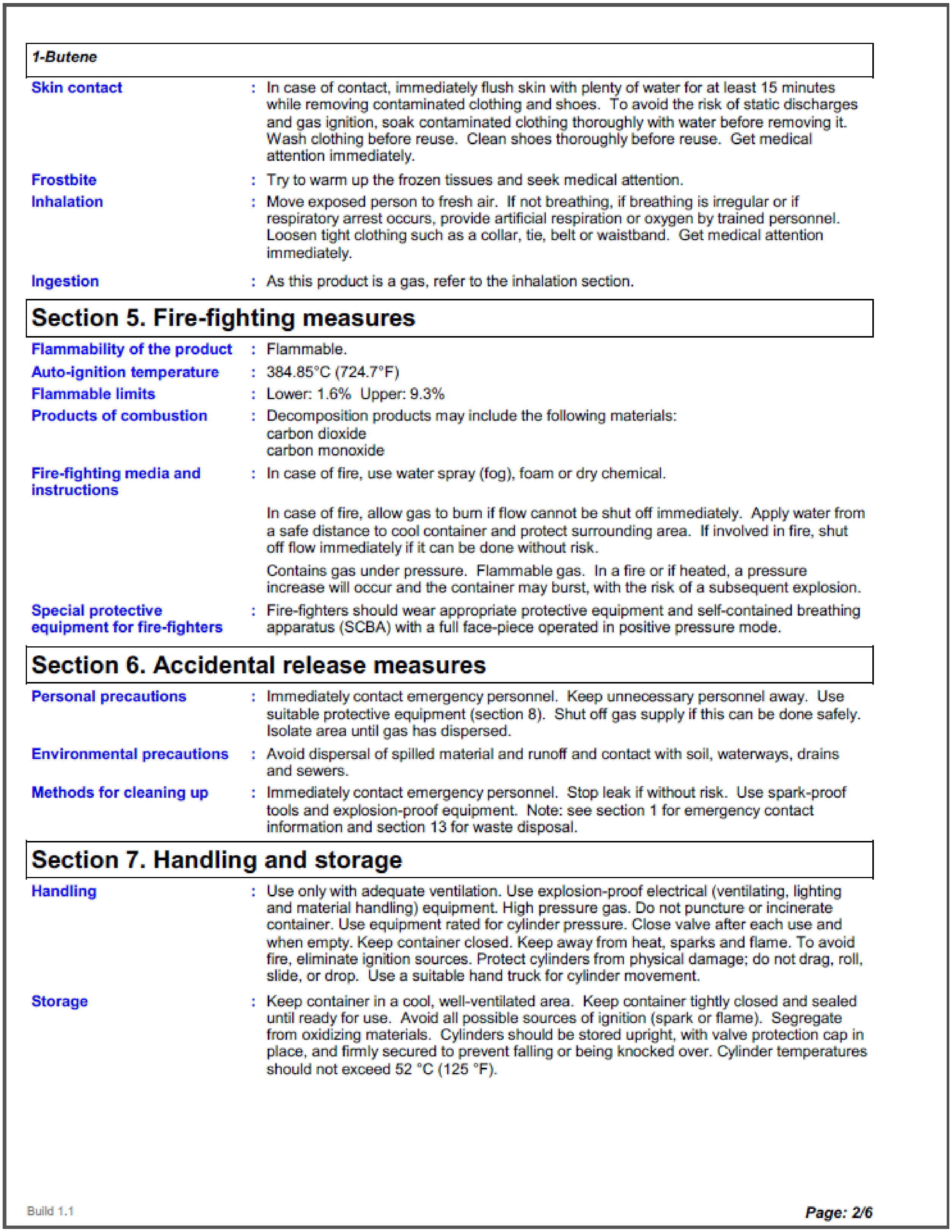


1-Butene

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 384.85°C (724.7°F)

Flammable limits : Lower: 1.6% Upper: 9.3%

Products of combustion : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Fire-fighting media and instructions : In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

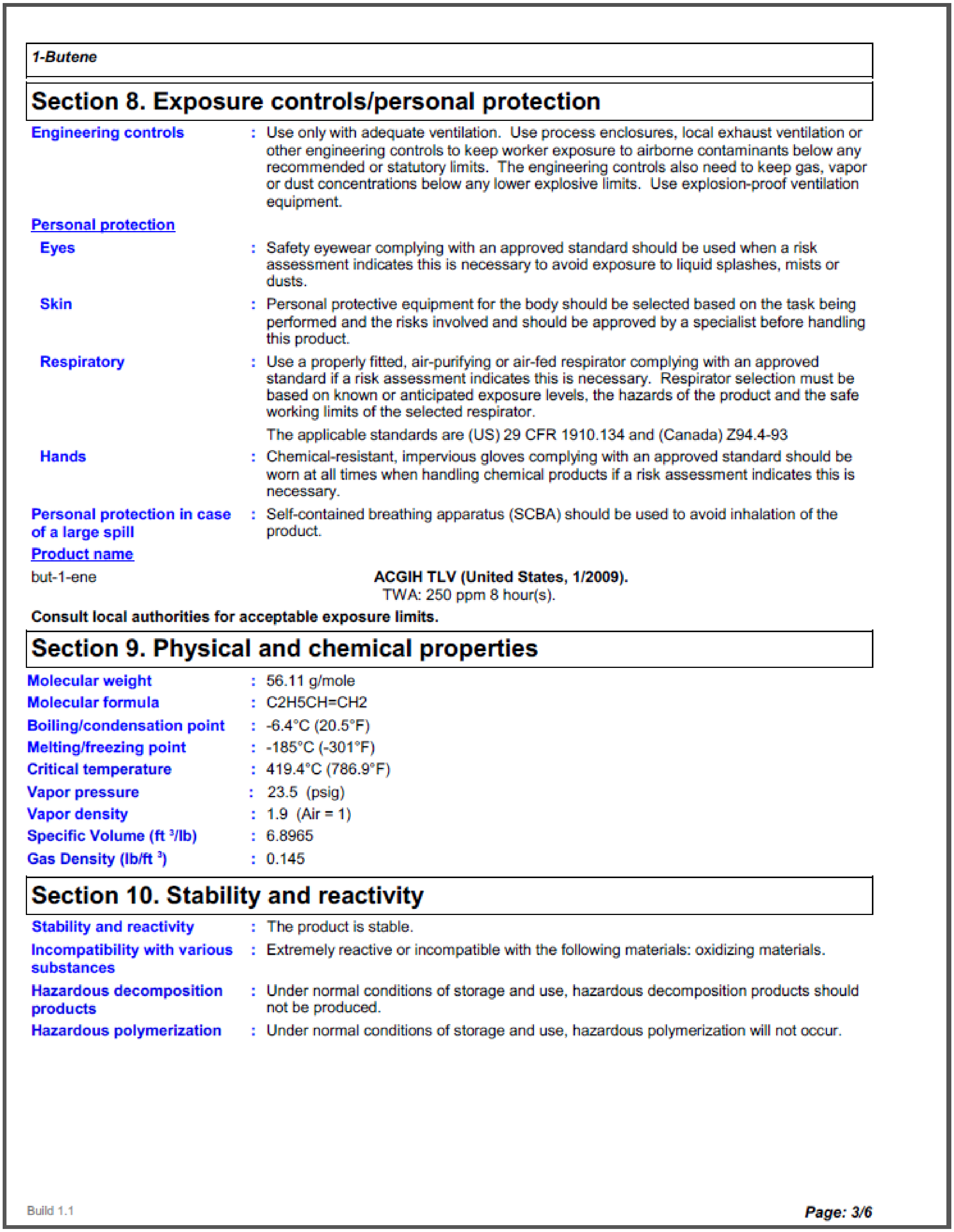
Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Storage : Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).



1-Butene

Section 8. Exposure controls/personal protection

Engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name	
but-1-ene	**ACGIH TLV (United States, 1/2009).** TWA: 250 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight : 56.11 g/mole

Molecular formula : C2H5CH=CH2

Boiling/condensation point : -6.4°C (20.5°F)

Melting/freezing point : -185°C (-301°F)

Critical temperature : 419.4°C (786.9°F)

Vapor pressure : 23.5 (psig)

Vapor density : 1.9 (Air = 1)

Specific Volume (ft ^{3}/lb) : 6.8965

Gas Density (lb/ft ^{3}) : 0.145

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.

Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.

Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Build 1.1

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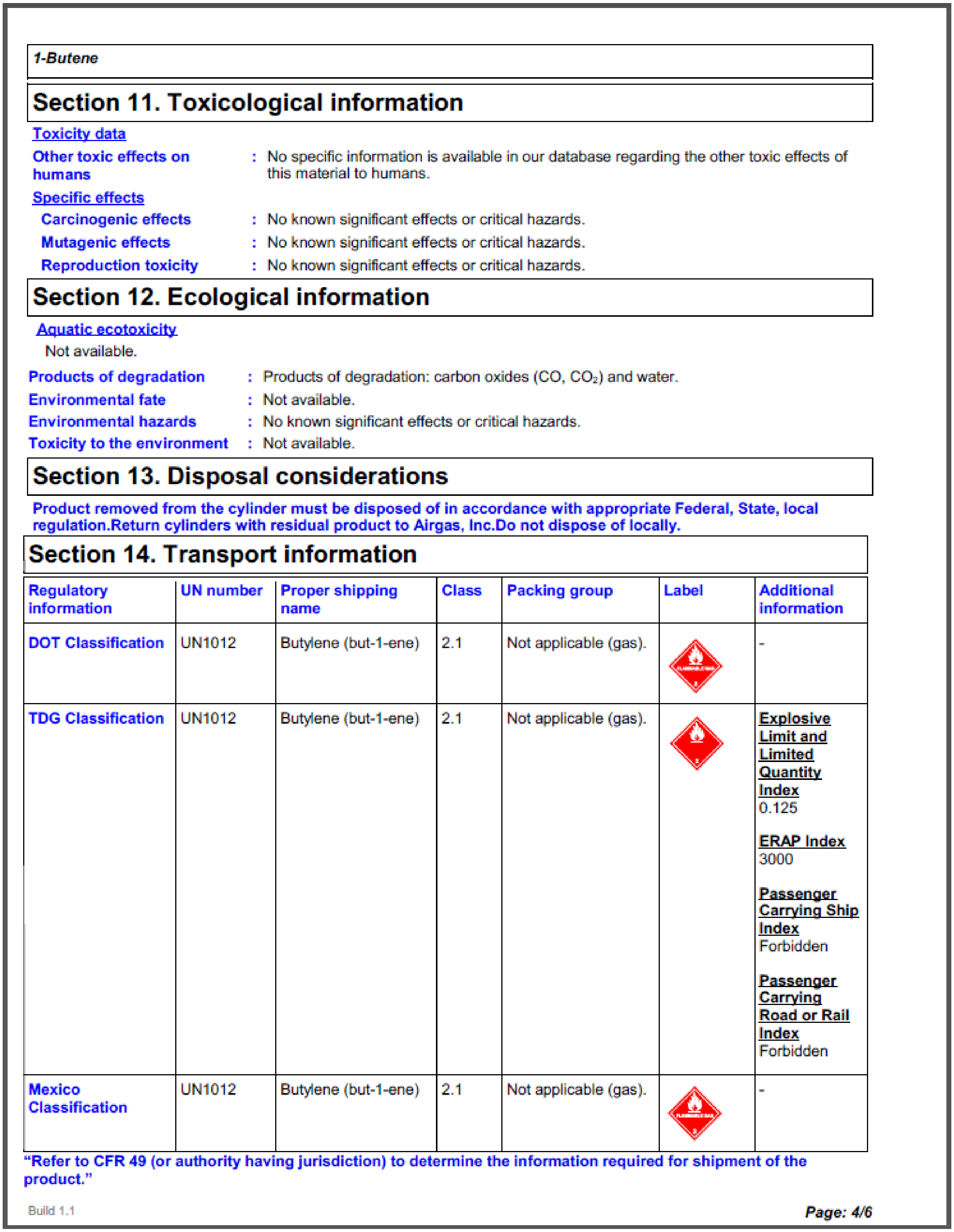


1-Butene

Section 11. Toxicological information

Toxicity data

Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.

Mutagenic effects : No known significant effects or critical hazards.

Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Products of degradation : Products of degradation: carbon oxides (CO, CO_2) and water.

Environmental fate : Not available.

Environmental hazards : No known significant effects or critical hazards.

Toxicity to the environment : Not available.

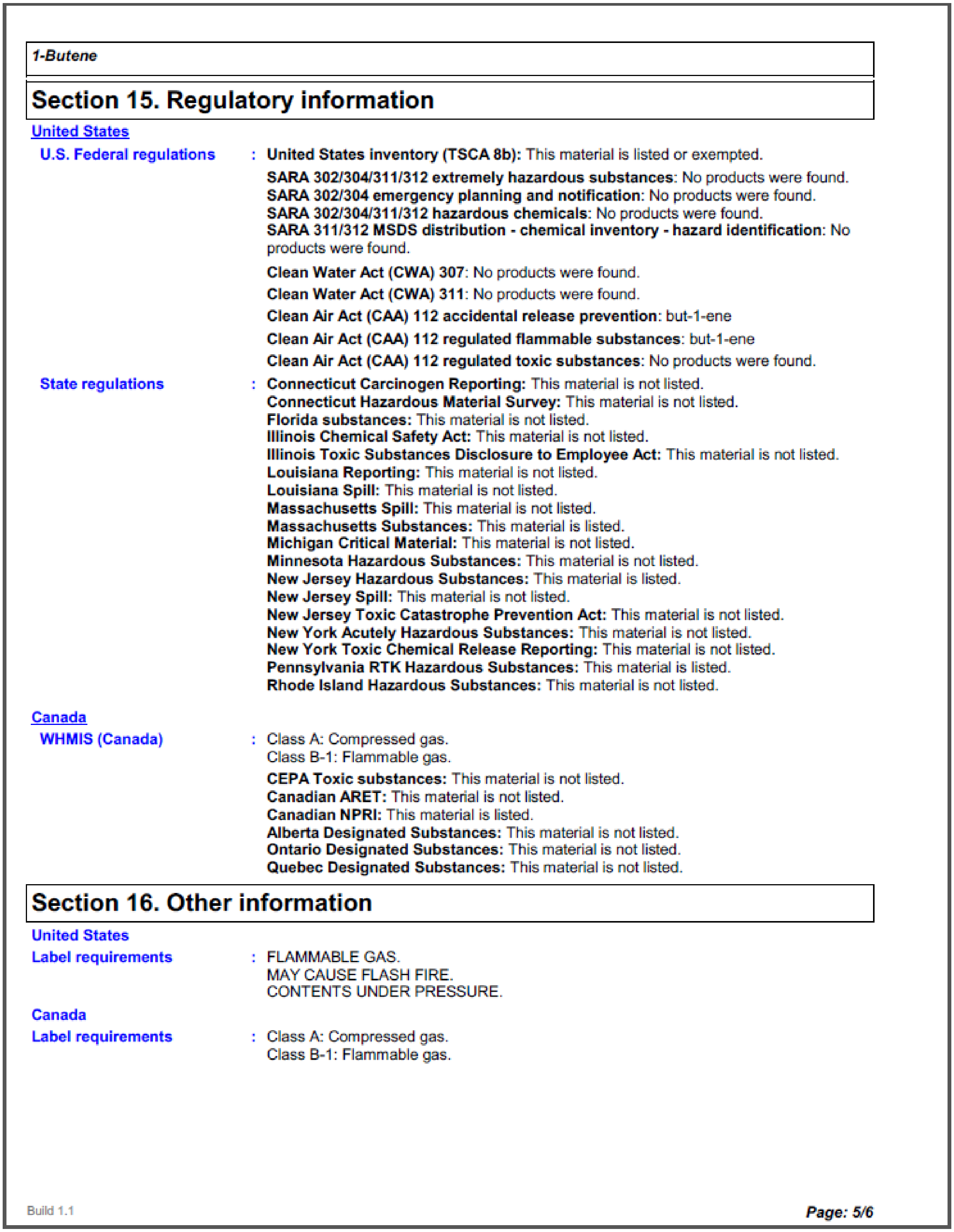
Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1012	Butylene (but-1-ene)	2.1	Not applicable (gas).		-
TDG Classification	UN1012	Butylene (but-1-ene)	2.1	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0.125 **ERAP Index** 3000 **Passenger Carrying Ship Index** Forbidden **Passenger Carrying Road or Rail Index** Forbidden
Mexico Classification	UN1012	Butylene (but-1-ene)	2.1	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."



1-Butene

Section 15. Regulatory information

United States

U.S. Federal regulations : **United States inventory (TSCA 8b):** This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: No products were found.
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: No products were found.

Clean Water Act (CWA) 307: No products were found.

Clean Water Act (CWA) 311: No products were found.

Clean Air Act (CAA) 112 accidental release prevention: but-1-ene

Clean Air Act (CAA) 112 regulated flammable substances: but-1-ene

Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

State regulations : **Connecticut Carcinogen Reporting:** This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class B-1: Flammable gas.

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

United States

Label requirements : FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
CONTENTS UNDER PRESSURE.

Canada

Label requirements : Class A: Compressed gas.
Class B-1: Flammable gas.

Build 1.1

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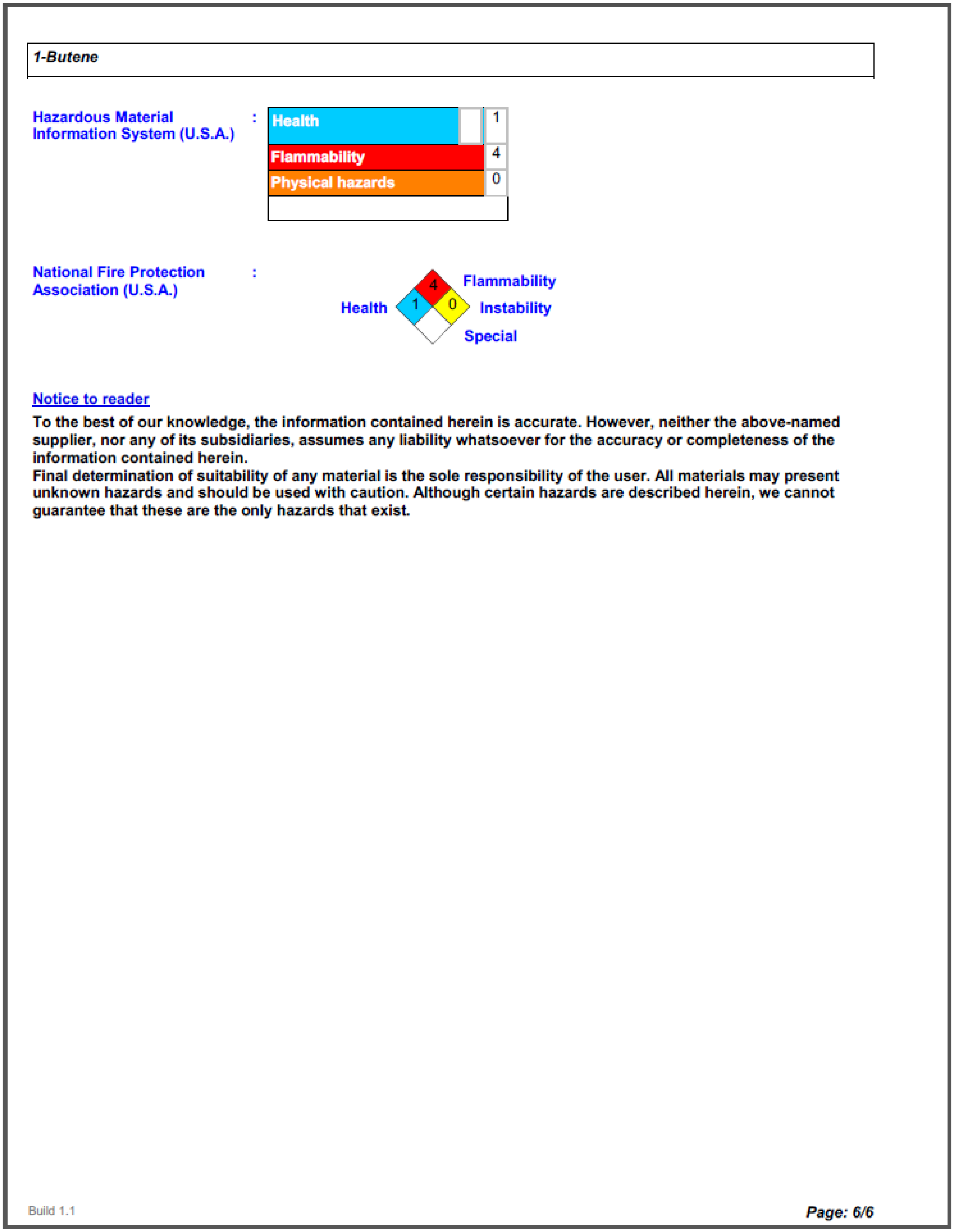

1-Butene

Hazardous Material Information System (U.S.A.) :

Health	1
Flammability	4
Physical hazards	0

National Fire Protection Association (U.S.A.) :

Flammability 4
Health 1
Instability 0
Special

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

Build 1.1

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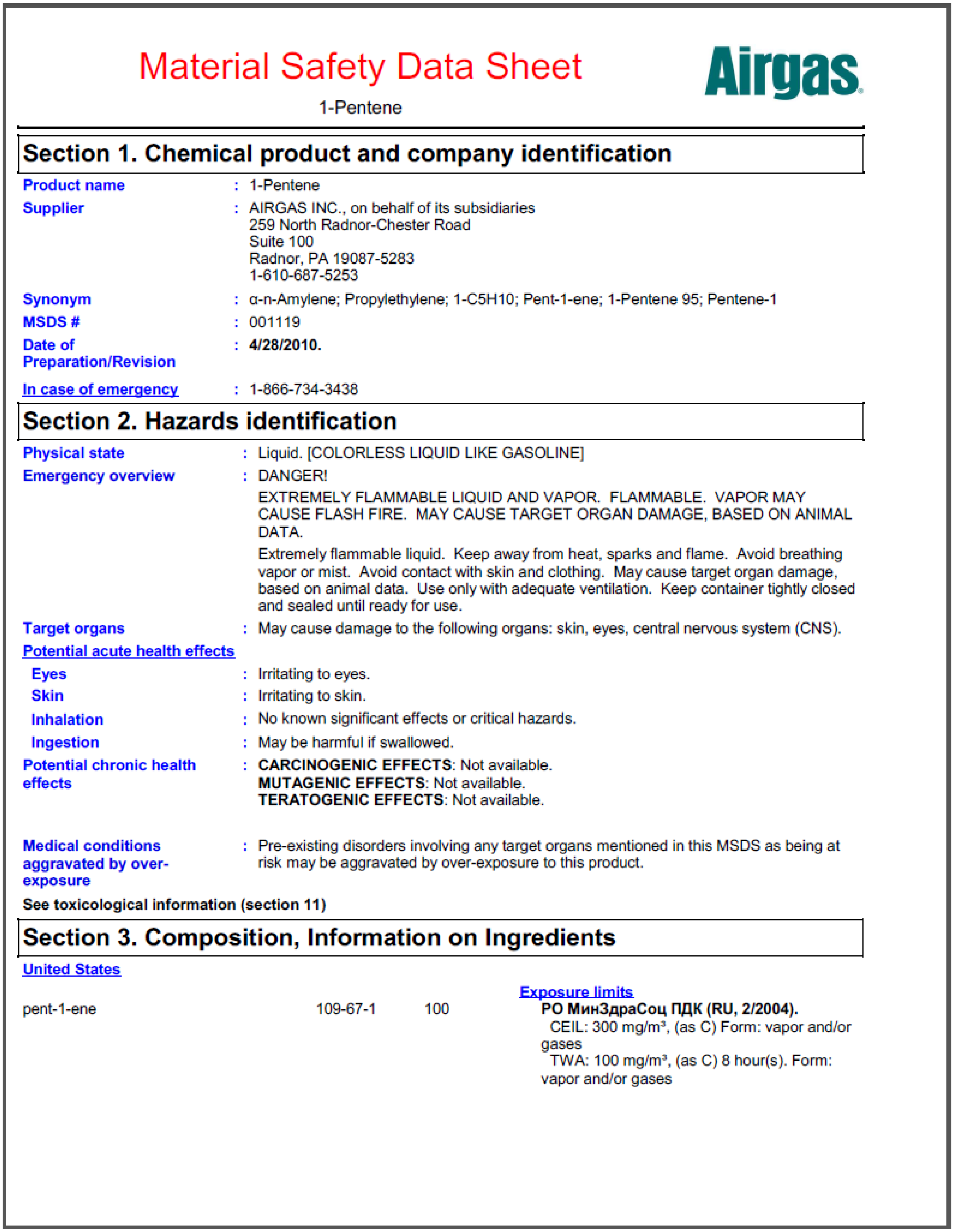


Material Safety Data Sheet

Airgas

1-Pentene

Section 1. Chemical product and company identification

Product name	: 1-Pentene
Supplier	: AIRGAS INC., on behalf of its subsidiaries 259 North Radnor-Chester Road Suite 100 Radnor, PA 19087-5283 1-610-687-5253
Synonym	: α-n-Amylene; Propylethylene; 1-C5H10; Pent-1-ene; 1-Pentene 95; Pentene-1
MSDS #	: 001119
Date of Preparation/Revision	: **4/28/2010.**
In case of emergency	: 1-866-734-3438

Section 2. Hazards identification

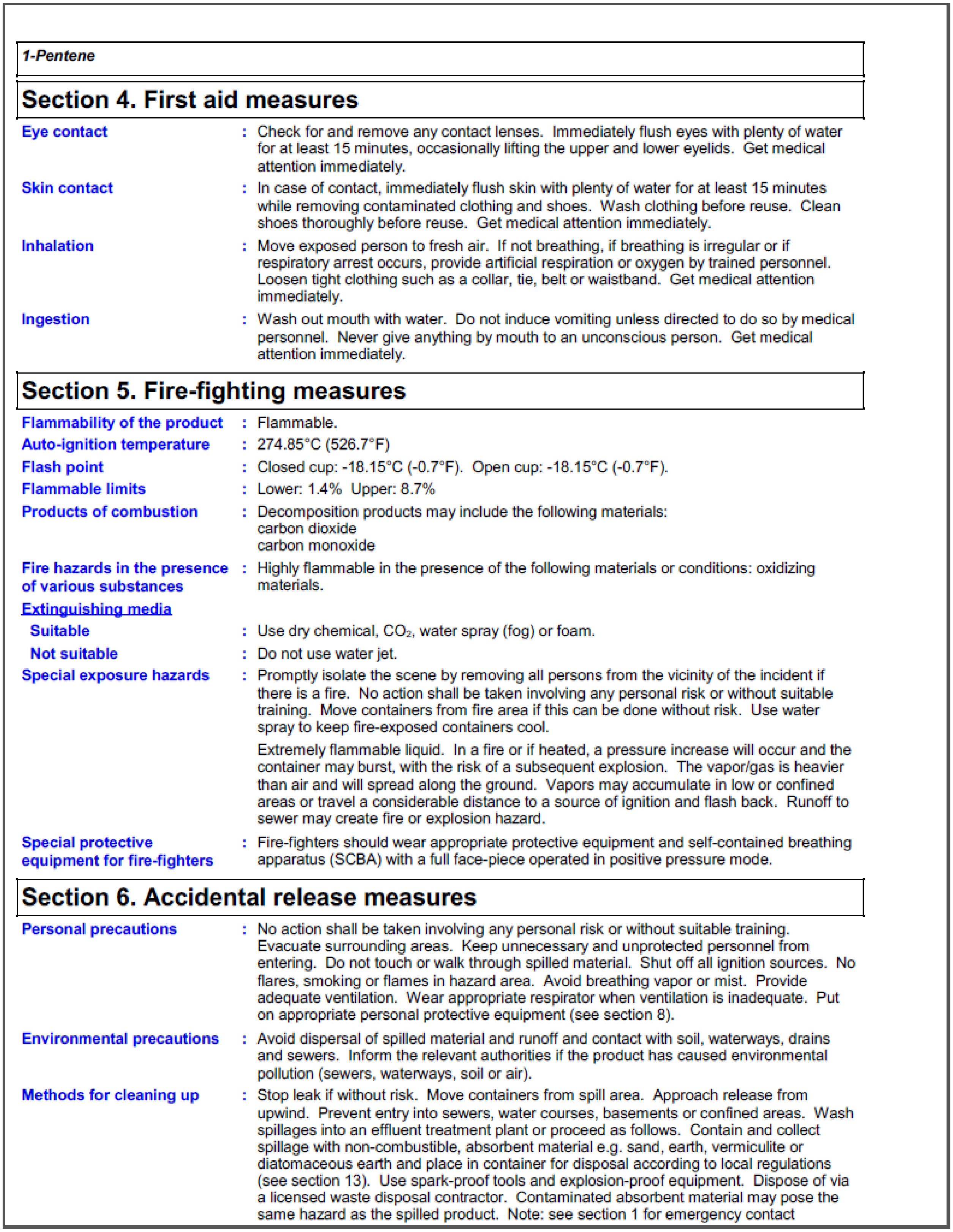
Physical state	: Liquid. [COLORLESS LIQUID LIKE GASOLINE]
Emergency overview	: DANGER! EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA. Extremely flammable liquid. Keep away from heat, sparks and flame. Avoid breathing vapor or mist. Avoid contact with skin and clothing. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container tightly closed and sealed until ready for use.
Target organs	: May cause damage to the following organs: skin, eyes, central nervous system (CNS).
Potential acute health effects	
Eyes	: Irritating to eyes.
Skin	: Irritating to skin.
Inhalation	: No known significant effects or critical hazards.
Ingestion	: May be harmful if swallowed.
Potential chronic health effects	: **CARCINOGENIC EFFECTS**: Not available. **MUTAGENIC EFFECTS**: Not available. **TERATOGENIC EFFECTS**: Not available.
Medical conditions aggravated by over-exposure	: Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

United States

			Exposure limits
pent-1-ene	109-67-1	100	**РО МинЗдраСоц ПДК (RU, 2/2004).** CEIL: 300 mg/m³, (as C) Form: vapor and/or gases TWA: 100 mg/m³, (as C) 8 hour(s). Form: vapor and/or gases



1-Pentene

Section 4. First aid measures

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : Wash out mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Get medical attention immediately.

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 274.85°C (526.7°F)

Flash point : Closed cup: -18.15°C (-0.7°F). Open cup: -18.15°C (-0.7°F).

Flammable limits : Lower: 1.4% Upper: 8.7%

Products of combustion : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Fire hazards in the presence of various substances : Highly flammable in the presence of the following materials or conditions: oxidizing materials.

Extinguishing media

Suitable : Use dry chemical, CO_2, water spray (fog) or foam.

Not suitable : Do not use water jet.

Special exposure hazards : Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool.

Extremely flammable liquid. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. The vapor/gas is heavier than air and will spread along the ground. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back. Runoff to sewer may create fire or explosion hazard.

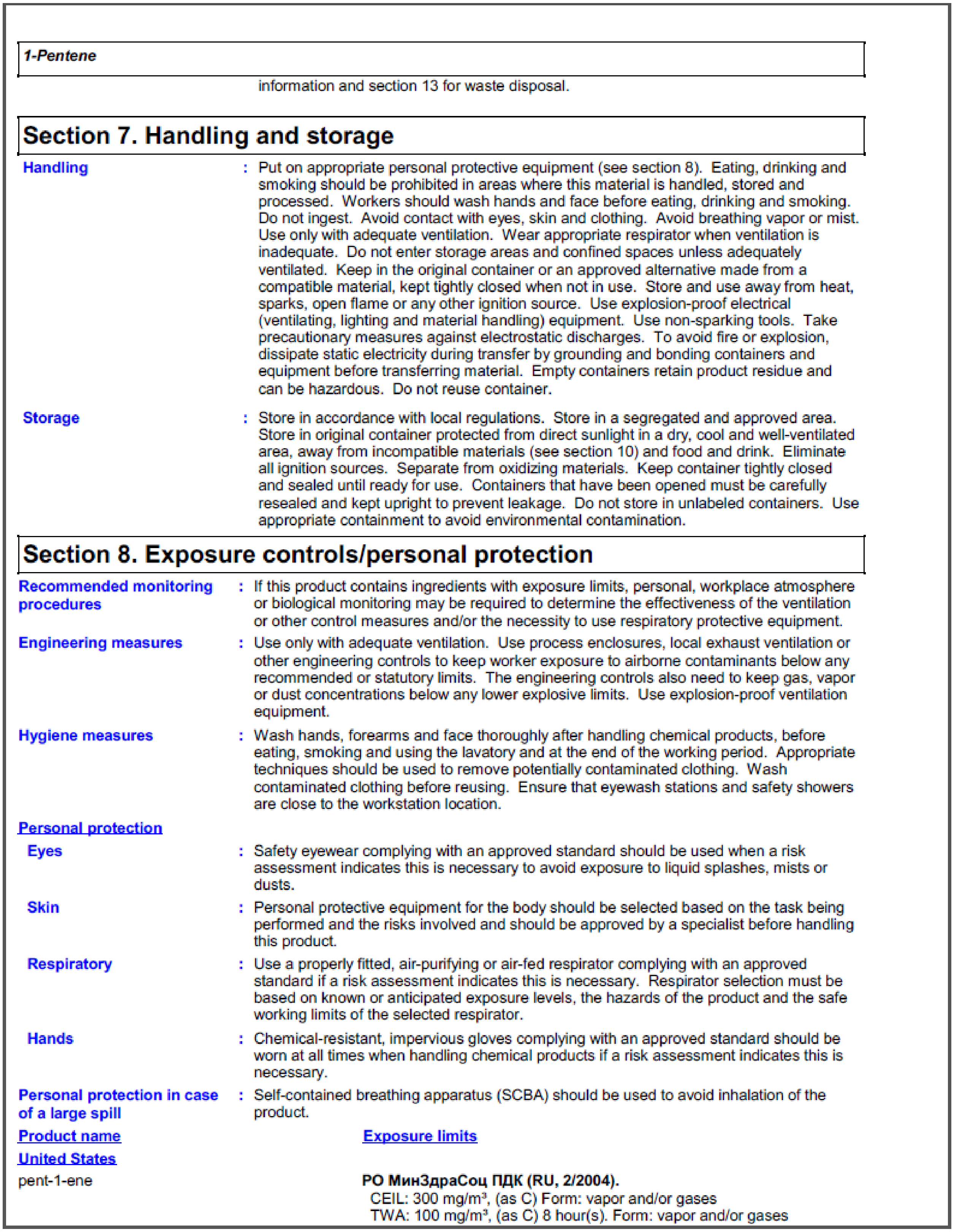
Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment (see section 8).

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

Methods for cleaning up : Stop leak if without risk. Move containers from spill area. Approach release from upwind. Prevent entry into sewers, water courses, basements or confined areas. Wash spillages into an effluent treatment plant or proceed as follows. Contain and collect spillage with non-combustible, absorbent material e.g. sand, earth, vermiculite or diatomaceous earth and place in container for disposal according to local regulations (see section 13). Use spark-proof tools and explosion-proof equipment. Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilled product. Note: see section 1 for emergency contact



1-Pentene

information and section 13 for waste disposal.

Section 7. Handling and storage

Handling	Put on appropriate personal protective equipment (see section 8). Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use non-sparking tools. Take precautionary measures against electrostatic discharges. To avoid fire or explosion, dissipate static electricity during transfer by grounding and bonding containers and equipment before transferring material. Empty containers retain product residue and can be hazardous. Do not reuse container.
Storage	Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabeled containers. Use appropriate containment to avoid environmental contamination.

Section 8. Exposure controls/personal protection

Recommended monitoring procedures	If this product contains ingredients with exposure limits, personal, workplace atmosphere or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment.
Engineering measures	Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.
Hygiene measures	Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.
Personal protection	
Eyes	Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.
Skin	Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.
Respiratory	Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.
Hands	Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.
Personal protection in case of a large spill	Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name	**Exposure limits**
United States	
pent-1-ene	**РО МинЗдраСоц ПДК (RU, 2/2004).** CEIL: 300 mg/m^3, (as C) Form: vapor and/or gases TWA: 100 mg/m^3, (as C) 8 hour(s). Form: vapor and/or gases

1-Pentene

Section 9. Physical and chemical properties

Physical state : Liquid. [COLORLESS LIQUID LIKE GASOLINE]
Color : COLORLESS
Molecular weight : 70.13 g/mole
Molecular formula : C5-H10
Boiling/condensation point : 30°C (86°F)
Melting/freezing point : -165.2°C (-265.4°F)
Critical temperature : 191.7°C (377.1°F)
Specific gravity : 0.641 (Water = 1)
Vapor density : 2.4 (Air = 1)
VOC : 0 % (w/w)

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.
Incompatibility with various substances : Highly reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Product/ingredient name	**Result**	**Species**	**Dose**	**Exposure**
pent-1-ene	LC50 Inhalation Vapor	Rat	175000 mg/m3	4 hours

Chronic effects on humans : May cause damage to the following organs: skin, eyes, central nervous system (CNS).
Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.
Mutagenic effects : No known significant effects or critical hazards.
Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

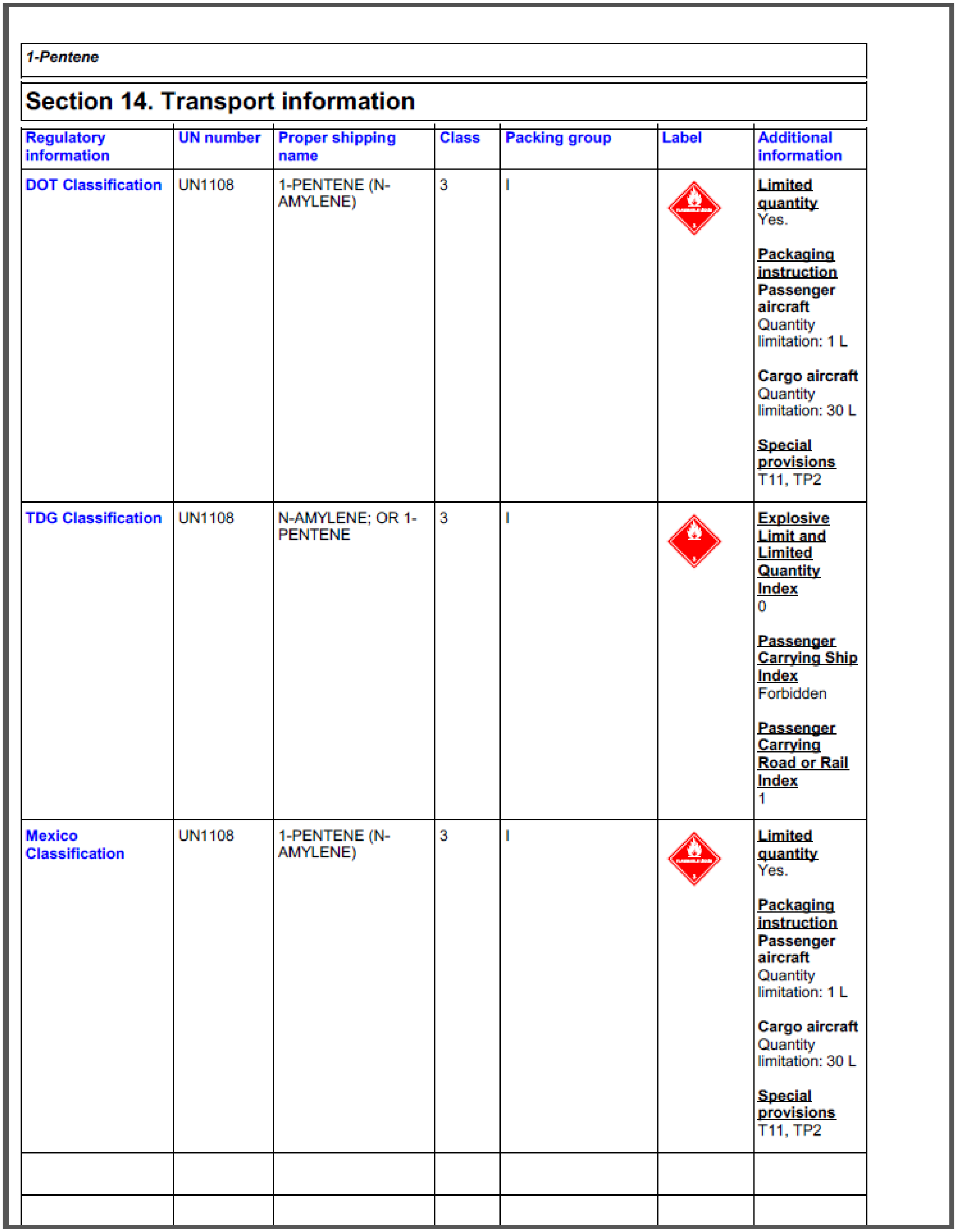
Not available.

Products of degradation : Products of degradation: carbon oxides (CO, CO_2) and water.

Section 13. Disposal considerations

Waste disposal : The generation of waste should be avoided or minimized wherever possible. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe way. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

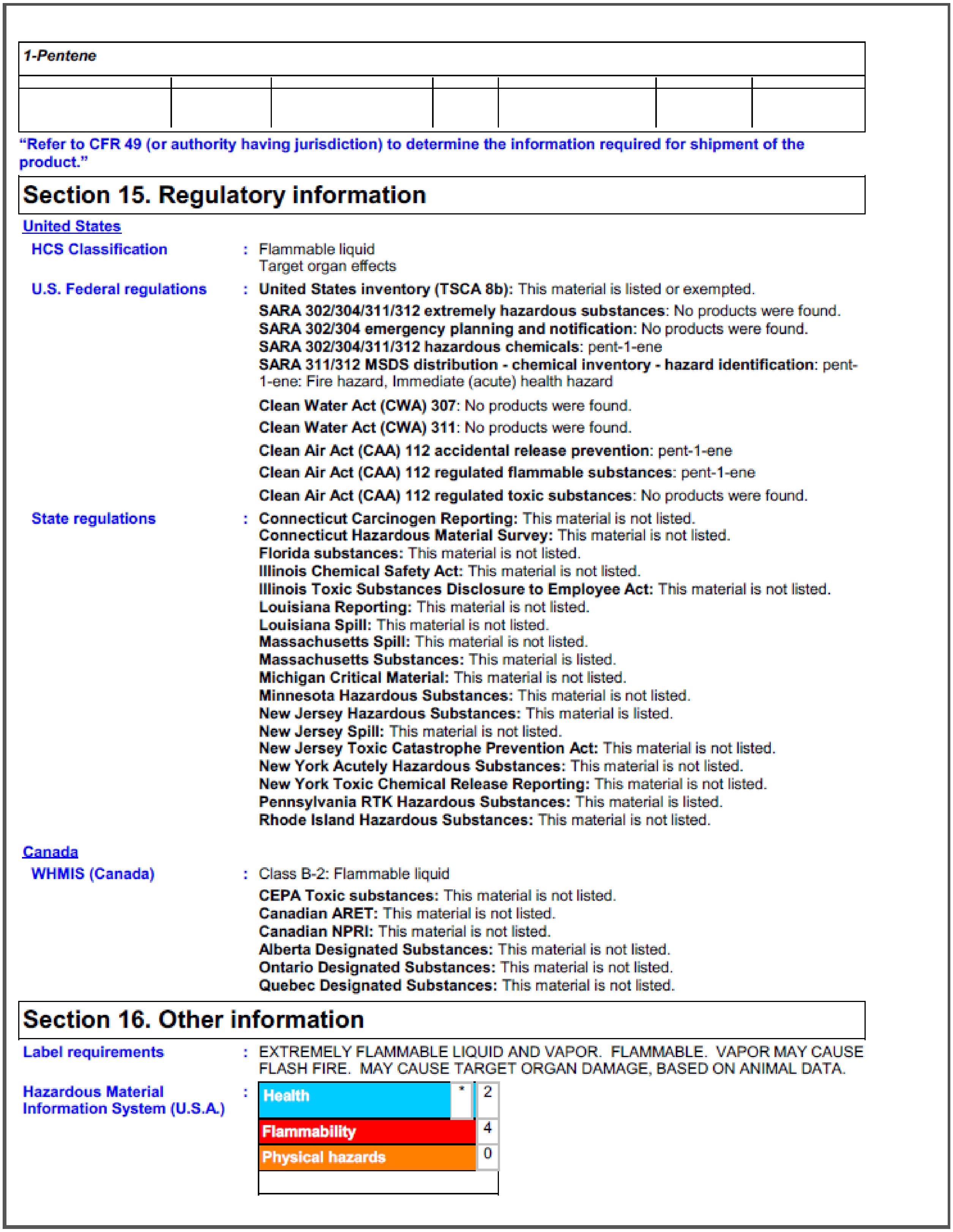
Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.



1-Pentene

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1108	1-PENTENE (N-AMYLENE)	3	I	◆	**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: 1 L **Cargo aircraft** Quantity limitation: 30 L **Special provisions** T11, TP2
TDG Classification	UN1108	N-AMYLENE; OR 1-PENTENE	3	I	◆	**Explosive Limit and Limited Quantity Index** 0 **Passenger Carrying Ship Index** Forbidden **Passenger Carrying Road or Rail Index** 1
Mexico Classification	UN1108	1-PENTENE (N-AMYLENE)	3	I	◆	**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: 1 L **Cargo aircraft** Quantity limitation: 30 L **Special provisions** T11, TP2



1-Pentene

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

HCS Classification : Flammable liquid
Target organ effects

U.S. Federal regulations : **United States inventory (TSCA 8b):** This material is listed or exempted.
SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: pent-1-ene
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: pent-1-ene: Fire hazard, Immediate (acute) health hazard

Clean Water Act (CWA) 307: No products were found.

Clean Water Act (CWA) 311: No products were found.

Clean Air Act (CAA) 112 accidental release prevention: pent-1-ene

Clean Air Act (CAA) 112 regulated flammable substances: pent-1-ene

Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

State regulations : **Connecticut Carcinogen Reporting:** This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class B-2: Flammable liquid

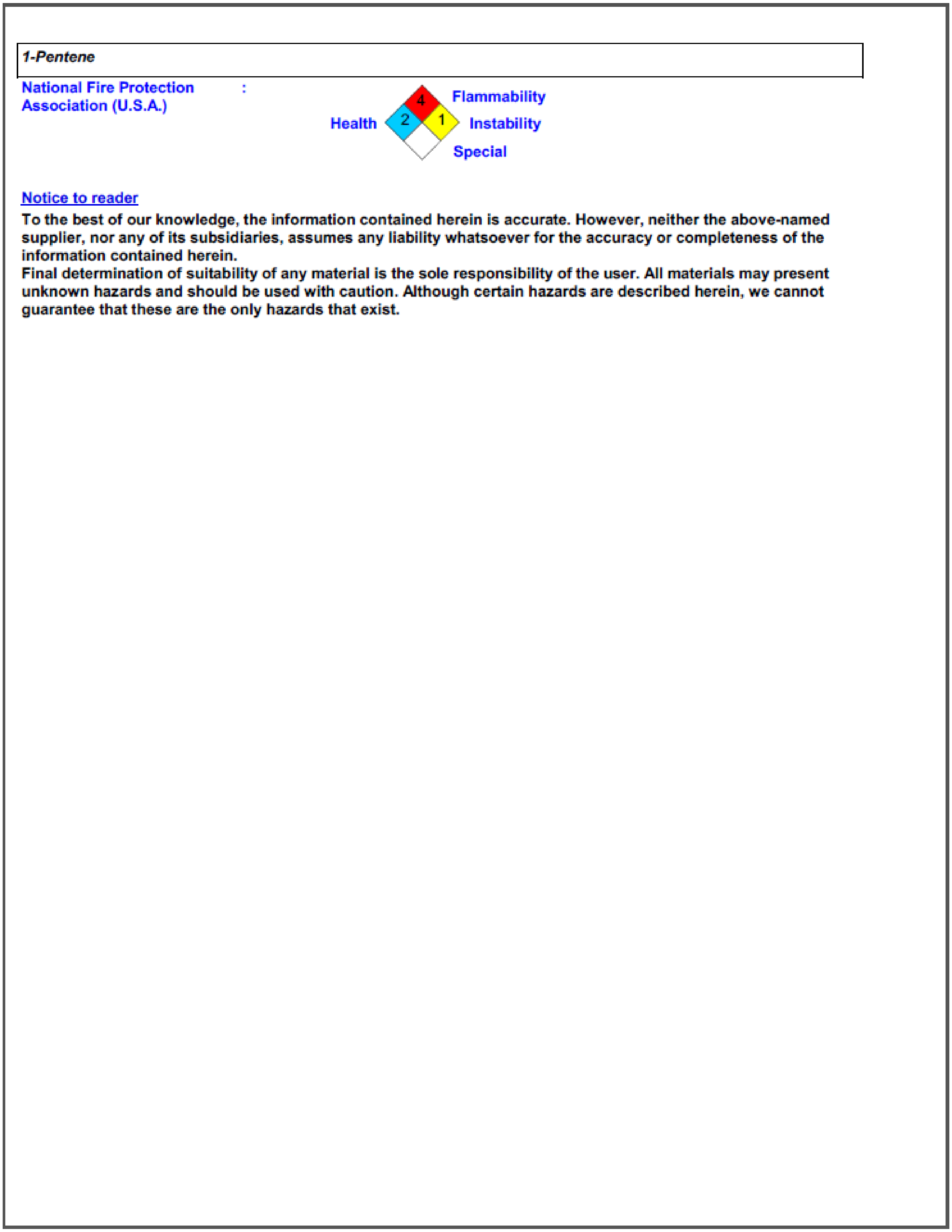
CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is not listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

Label requirements : EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

Hazardous Material Information System (U.S.A.) :

Health	*	2
Flammability		4
Physical hazards		0

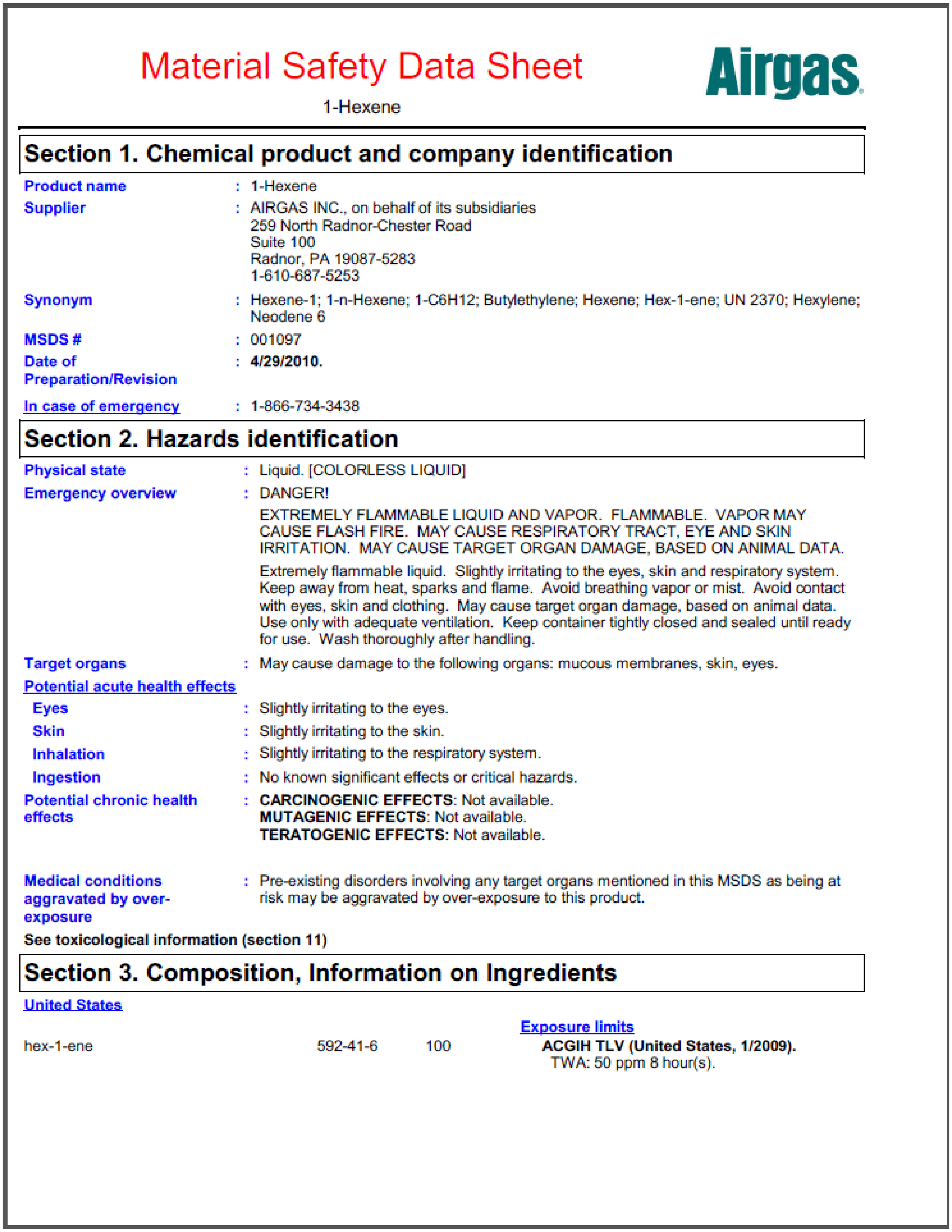


1-Pentene

National Fire Protection Association (U.S.A.) :

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.



Material Safety Data Sheet

Airgas

1-Hexene

Section 1. Chemical product and company identification

Product name : 1-Hexene

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Synonym : Hexene-1; 1-n-Hexene; 1-C6H12; Butylethylene; Hexene; Hex-1-ene; UN 2370; Hexylene; Neodene 6

MSDS # : 001097

Date of Preparation/Revision : **4/29/2010.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Liquid. [COLORLESS LIQUID]

Emergency overview : DANGER!

EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. MAY CAUSE RESPIRATORY TRACT, EYE AND SKIN IRRITATION. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

Extremely flammable liquid. Slightly irritating to the eyes, skin and respiratory system. Keep away from heat, sparks and flame. Avoid breathing vapor or mist. Avoid contact with eyes, skin and clothing. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container tightly closed and sealed until ready for use. Wash thoroughly after handling.

Target organs : May cause damage to the following organs: mucous membranes, skin, eyes.

Potential acute health effects

Eyes : Slightly irritating to the eyes.

Skin : Slightly irritating to the skin.

Inhalation : Slightly irritating to the respiratory system.

Ingestion : No known significant effects or critical hazards.

Potential chronic health effects : **CARCINOGENIC EFFECTS**: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.

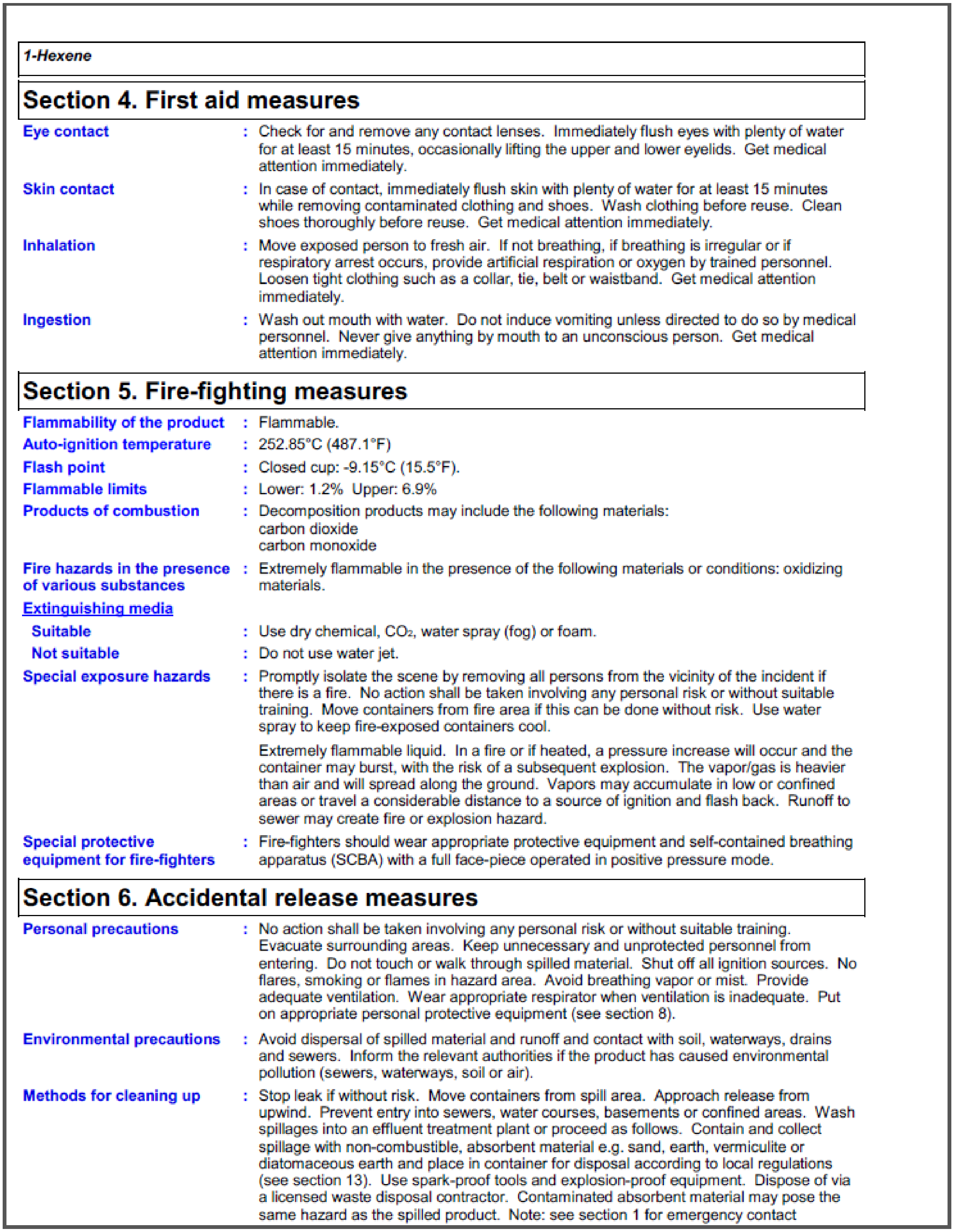
Medical conditions aggravated by over-exposure : Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

United States

			Exposure limits
hex-1-ene	592-41-6	100	**ACGIH TLV (United States, 1/2009).** TWA: 50 ppm 8 hour(s).



1-Hexene

Section 4. First aid measures

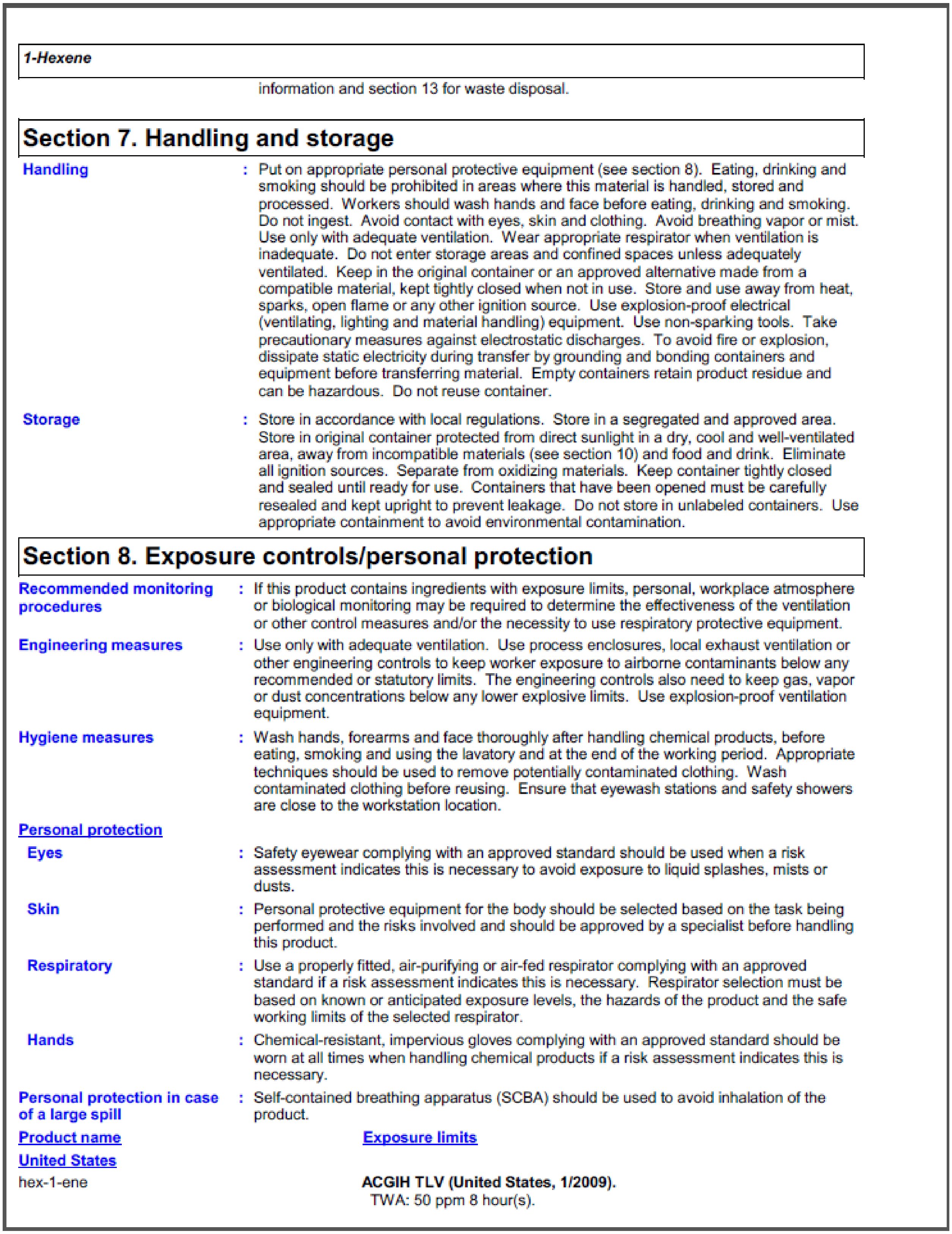
Eye contact	Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.
Skin contact	In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.
Inhalation	Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.
Ingestion	Wash out mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Get medical attention immediately.

Section 5. Fire-fighting measures

Flammability of the product	Flammable.
Auto-ignition temperature	252.85°C (487.1°F)
Flash point	Closed cup: -9.15°C (15.5°F).
Flammable limits	Lower: 1.2% Upper: 6.9%
Products of combustion	Decomposition products may include the following materials: carbon dioxide carbon monoxide
Fire hazards in the presence of various substances	Extremely flammable in the presence of the following materials or conditions: oxidizing materials.
Extinguishing media	
Suitable	Use dry chemical, CO_2, water spray (fog) or foam.
Not suitable	Do not use water jet.
Special exposure hazards	Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool. Extremely flammable liquid. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. The vapor/gas is heavier than air and will spread along the ground. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back. Runoff to sewer may create fire or explosion hazard.
Special protective equipment for fire-fighters	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions	No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment (see section 8).
Environmental precautions	Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).
Methods for cleaning up	Stop leak if without risk. Move containers from spill area. Approach release from upwind. Prevent entry into sewers, water courses, basements or confined areas. Wash spillages into an effluent treatment plant or proceed as follows. Contain and collect spillage with non-combustible, absorbent material e.g. sand, earth, vermiculite or diatomaceous earth and place in container for disposal according to local regulations (see section 13). Use spark-proof tools and explosion-proof equipment. Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilled product. Note: see section 1 for emergency contact



1-Hexene

information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : Put on appropriate personal protective equipment (see section 8). Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use non-sparking tools. Take precautionary measures against electrostatic discharges. To avoid fire or explosion, dissipate static electricity during transfer by grounding and bonding containers and equipment before transferring material. Empty containers retain product residue and can be hazardous. Do not reuse container.

Storage : Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabeled containers. Use appropriate containment to avoid environmental contamination.

Section 8. Exposure controls/personal protection

Recommended monitoring procedures : If this product contains ingredients with exposure limits, personal, workplace atmosphere or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment.

Engineering measures : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Hygiene measures : Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

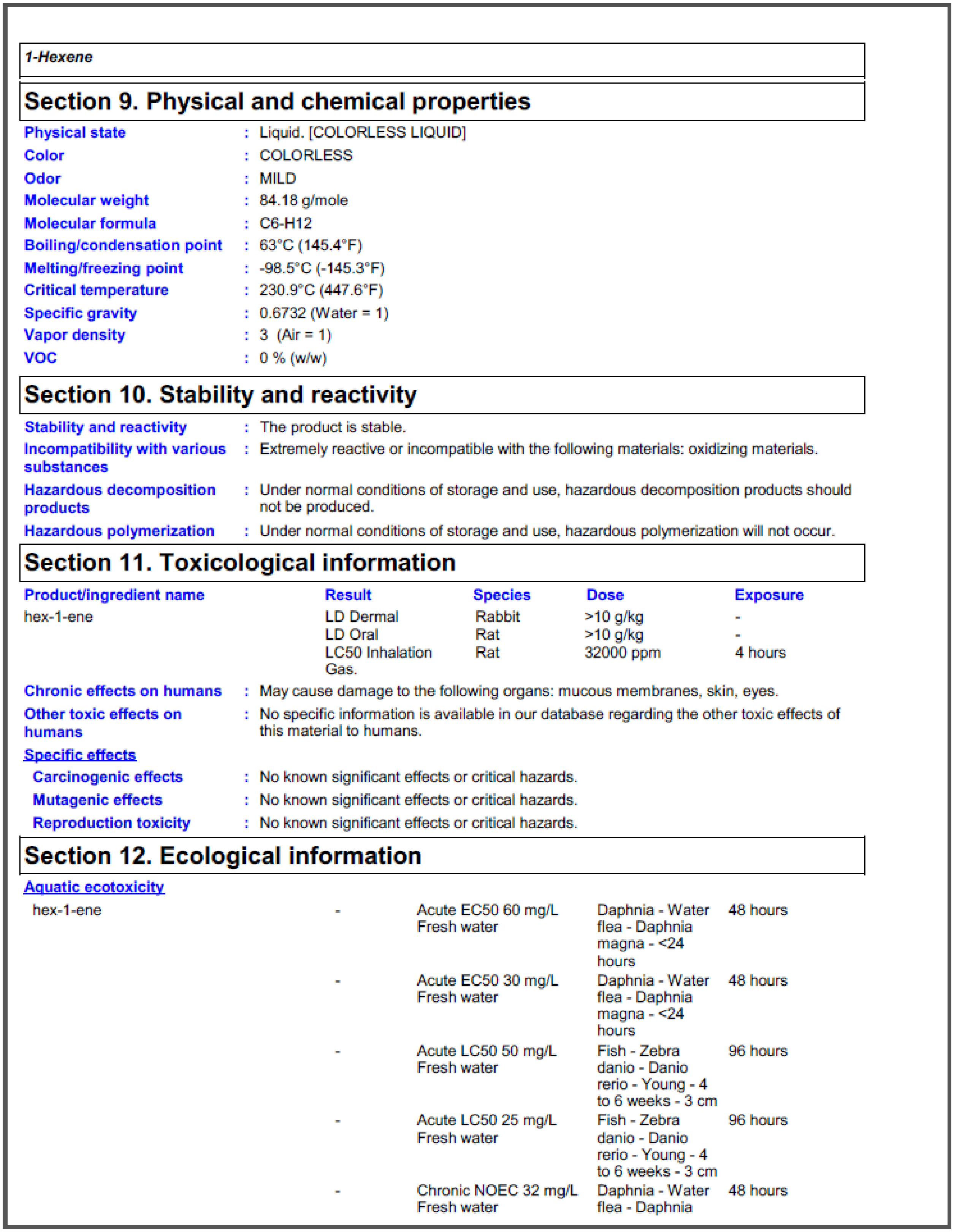
Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name	Exposure limits
United States	
hex-1-ene	**ACGIH TLV (United States, 1/2009).** TWA: 50 ppm 8 hour(s).



1-Hexene

Section 9. Physical and chemical properties

Physical state : Liquid. [COLORLESS LIQUID]
Color : COLORLESS
Odor : MILD
Molecular weight : 84.18 g/mole
Molecular formula : C6-H12
Boiling/condensation point : 63°C (145.4°F)
Melting/freezing point : -98.5°C (-145.3°F)
Critical temperature : 230.9°C (447.6°F)
Specific gravity : 0.6732 (Water = 1)
Vapor density : 3 (Air = 1)
VOC : 0 % (w/w)

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.
Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Product/ingredient name	Result	Species	Dose	Exposure
hex-1-ene	LD Dermal	Rabbit	>10 g/kg	-
	LD Oral	Rat	>10 g/kg	-
	LC50 Inhalation Gas.	Rat	32000 ppm	4 hours

Chronic effects on humans : May cause damage to the following organs: mucous membranes, skin, eyes.
Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.
Mutagenic effects : No known significant effects or critical hazards.
Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

hex-1-ene	-	Acute EC50 60 mg/L Fresh water	Daphnia - Water flea - Daphnia magna - <24 hours	48 hours
	-	Acute EC50 30 mg/L Fresh water	Daphnia - Water flea - Daphnia magna - <24 hours	48 hours
	-	Acute LC50 50 mg/L Fresh water	Fish - Zebra danio - Danio rerio - Young - 4 to 6 weeks - 3 cm	96 hours
	-	Acute LC50 25 mg/L Fresh water	Fish - Zebra danio - Danio rerio - Young - 4 to 6 weeks - 3 cm	96 hours
	-	Chronic NOEC 32 mg/L Fresh water	Daphnia - Water flea - Daphnia	48 hours

1-Hexene

			magna - <24 hours	
	-	Chronic NOEC 10 mg/L Fresh water	Fish - Zebra danio - Danio rerio - Young - 4 to 6 weeks - 3 cm	96 hours
	-	Chronic NOEC 10 mg/L Fresh water	Daphnia - Water flea - Daphnia magna - <24 hours	48 hours

Products of degradation : Products of degradation: carbon oxides (CO, CO_2) and water.

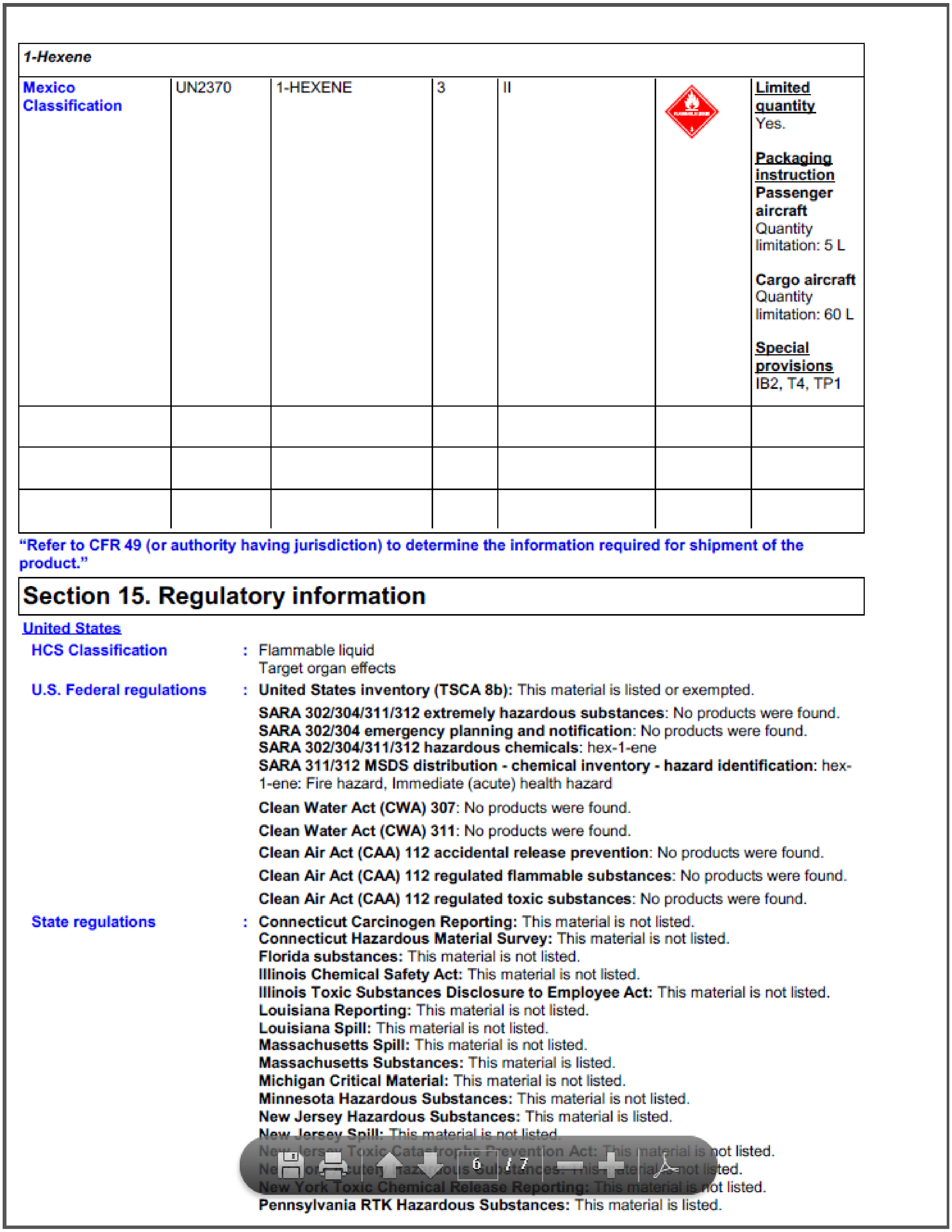
Section 13. Disposal considerations

Waste disposal : The generation of waste should be avoided or minimized wherever possible. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe way. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN2370	1-HEXENE	3	II		**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: 5 L **Cargo aircraft** Quantity limitation: 60 L **Special provisions** IB2, T4, TP1
TDG Classification	UN2370	1-HEXENE	3	II		**Passenger Carrying Ship Index** Forbidden **Passenger Carrying Road or Rail Index** 5



1-Hexene						
Mexico Classification	UN2370	1-HEXENE	3	II		**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: 5 L **Cargo aircraft** Quantity limitation: 60 L **Special provisions** IB2, T4, TP1

“Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product.”

Section 15. Regulatory information

United States

HCS Classification : Flammable liquid
Target organ effects

U.S. Federal regulations : **United States inventory (TSCA 8b):** This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: hex-1-ene
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: hex-1-ene: Fire hazard, Immediate (acute) health hazard

Clean Water Act (CWA) 307: No products were found.

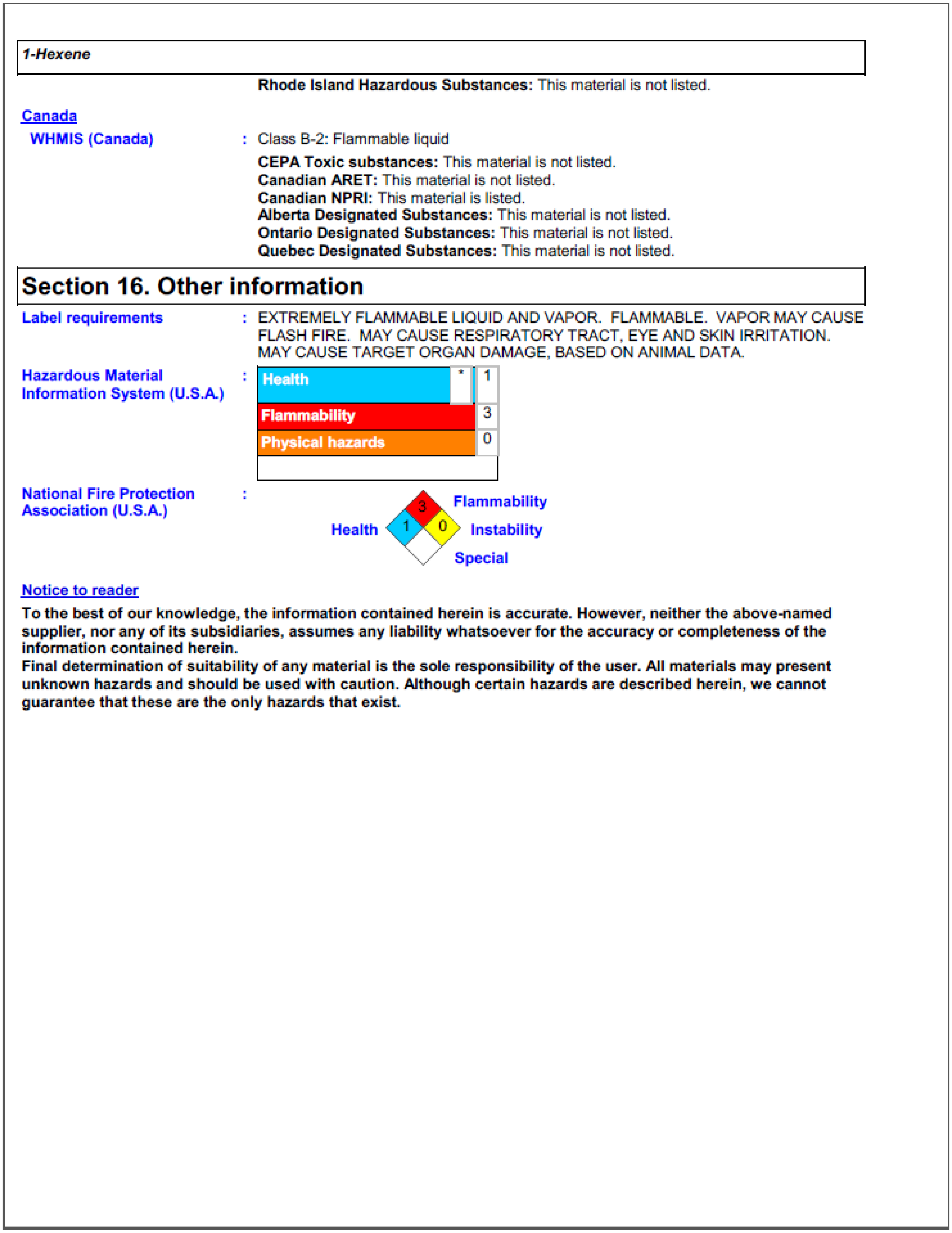
Clean Water Act (CWA) 311: No products were found.

Clean Air Act (CAA) 112 accidental release prevention: No products were found.

Clean Air Act (CAA) 112 regulated flammable substances: No products were found.

Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

State regulations : **Connecticut Carcinogen Reporting:** This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.



1-Hexene

Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class B-2: Flammable liquid

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

Label requirements : EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. MAY CAUSE RESPIRATORY TRACT, EYE AND SKIN IRRITATION. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

Hazardous Material Information System (U.S.A.) :

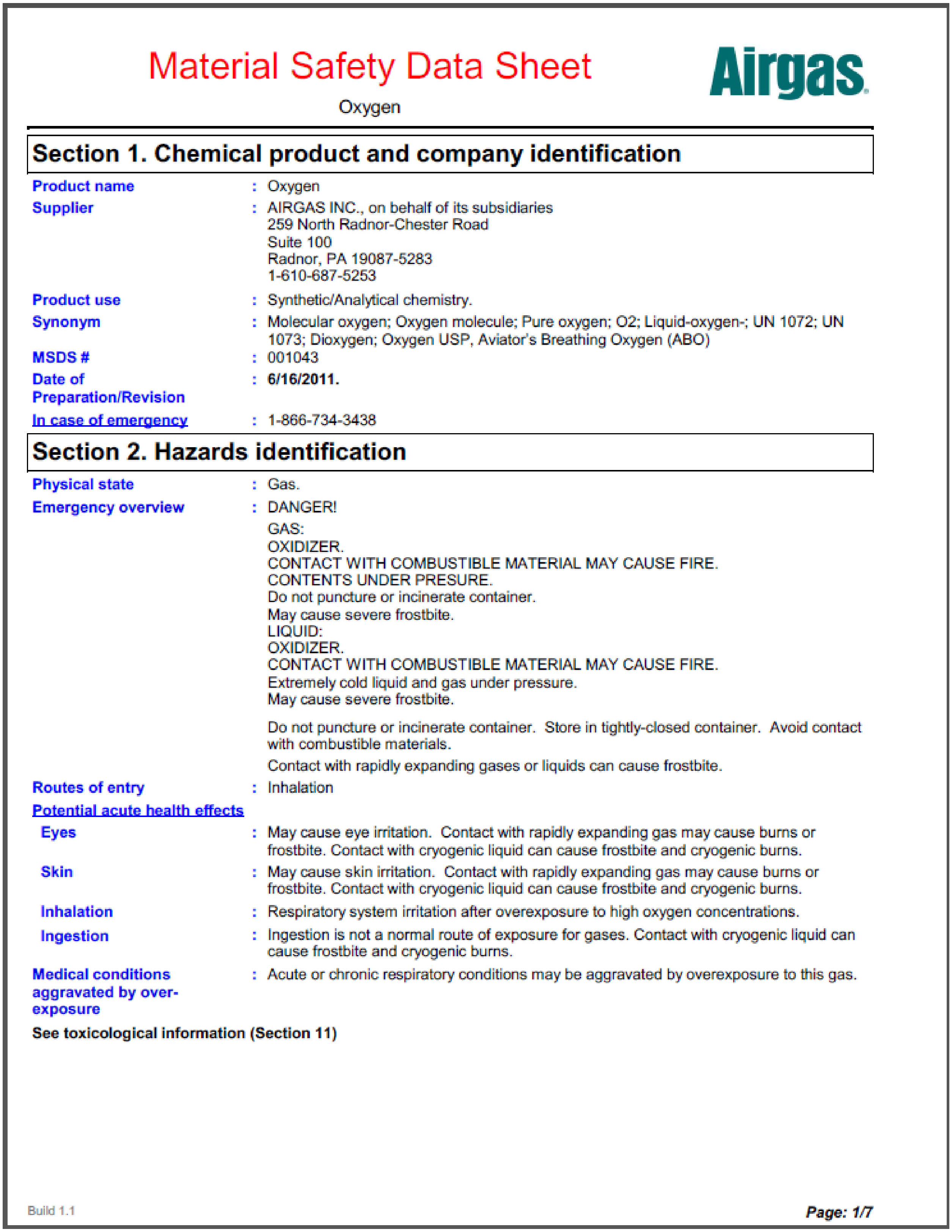
Health	*	1
Flammability		3
Physical hazards		0

National Fire Protection Association (U.S.A.) :

Flammability 3
Health 1
Instability 0
Special

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.



Material Safety Data Sheet

Oxygen

Airgas

Section 1. Chemical product and company identification

Product name : Oxygen

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : Molecular oxygen; Oxygen molecule; Pure oxygen; O2; Liquid-oxygen-; UN 1072; UN 1073; Dioxygen; Oxygen USP, Aviator's Breathing Oxygen (ABO)

MSDS # : 001043

Date of Preparation/Revision : **6/16/2011.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas.

Emergency overview : DANGER!

GAS:
OXIDIZER.
CONTACT WITH COMBUSTIBLE MATERIAL MAY CAUSE FIRE.
CONTENTS UNDER PRESURE.
Do not puncture or incinerate container.
May cause severe frostbite.
LIQUID:
OXIDIZER.
CONTACT WITH COMBUSTIBLE MATERIAL MAY CAUSE FIRE.
Extremely cold liquid and gas under pressure.
May cause severe frostbite.

Do not puncture or incinerate container. Store in tightly-closed container. Avoid contact with combustible materials.

Contact with rapidly expanding gases or liquids can cause frostbite.

Routes of entry : Inhalation

Potential acute health effects

Eyes : May cause eye irritation. Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Skin : May cause skin irritation. Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Inhalation : Respiratory system irritation after overexposure to high oxygen concentrations.

Ingestion : Ingestion is not a normal route of exposure for gases. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Medical conditions aggravated by over-exposure : Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.

See toxicological information (Section 11)

Build 1.1

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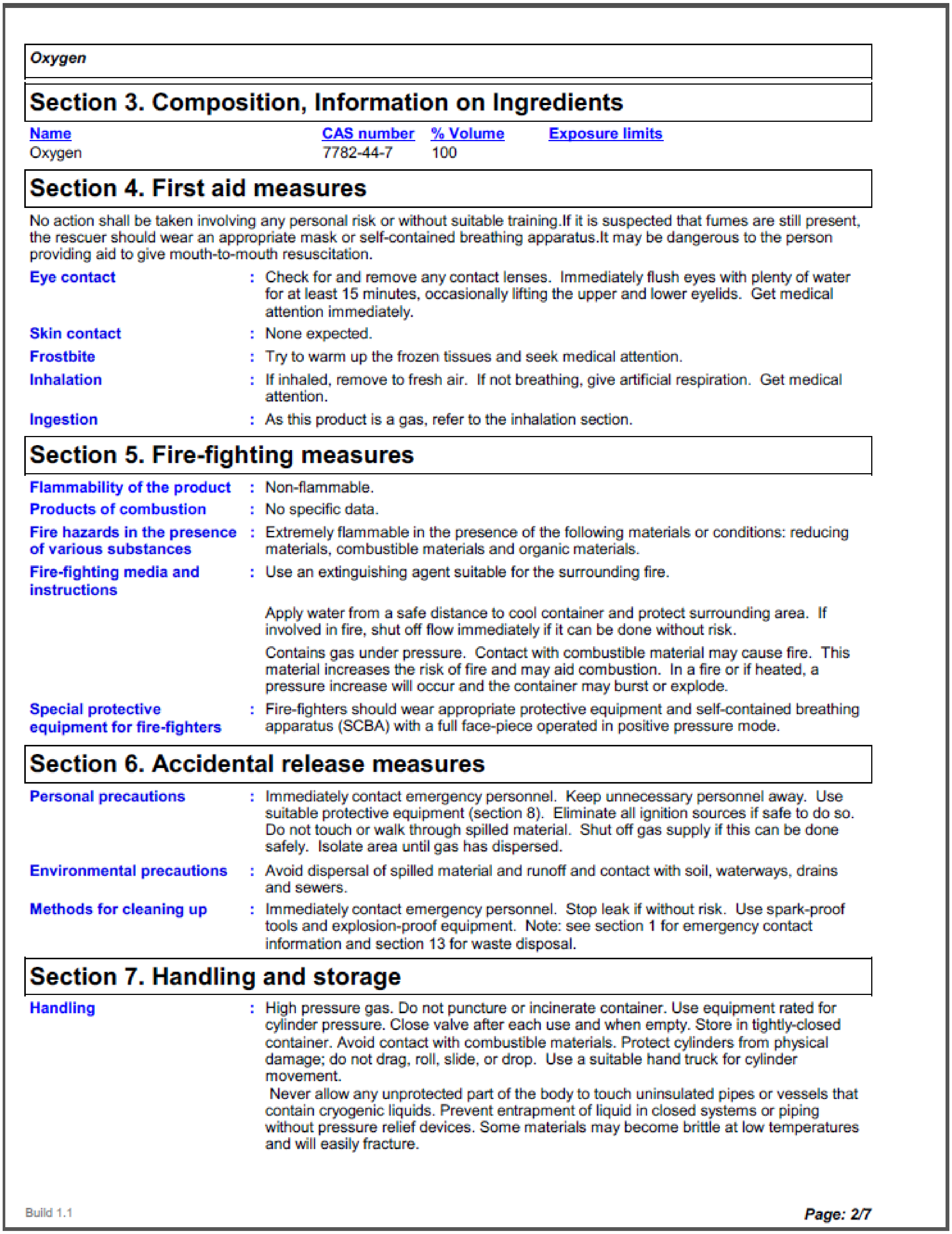


Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Oxygen	7782-44-7	100	

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact	Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.
Skin contact	None expected.
Frostbite	Try to warm up the frozen tissues and seek medical attention.
Inhalation	If inhaled, remove to fresh air. If not breathing, give artificial respiration. Get medical attention.
Ingestion	As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

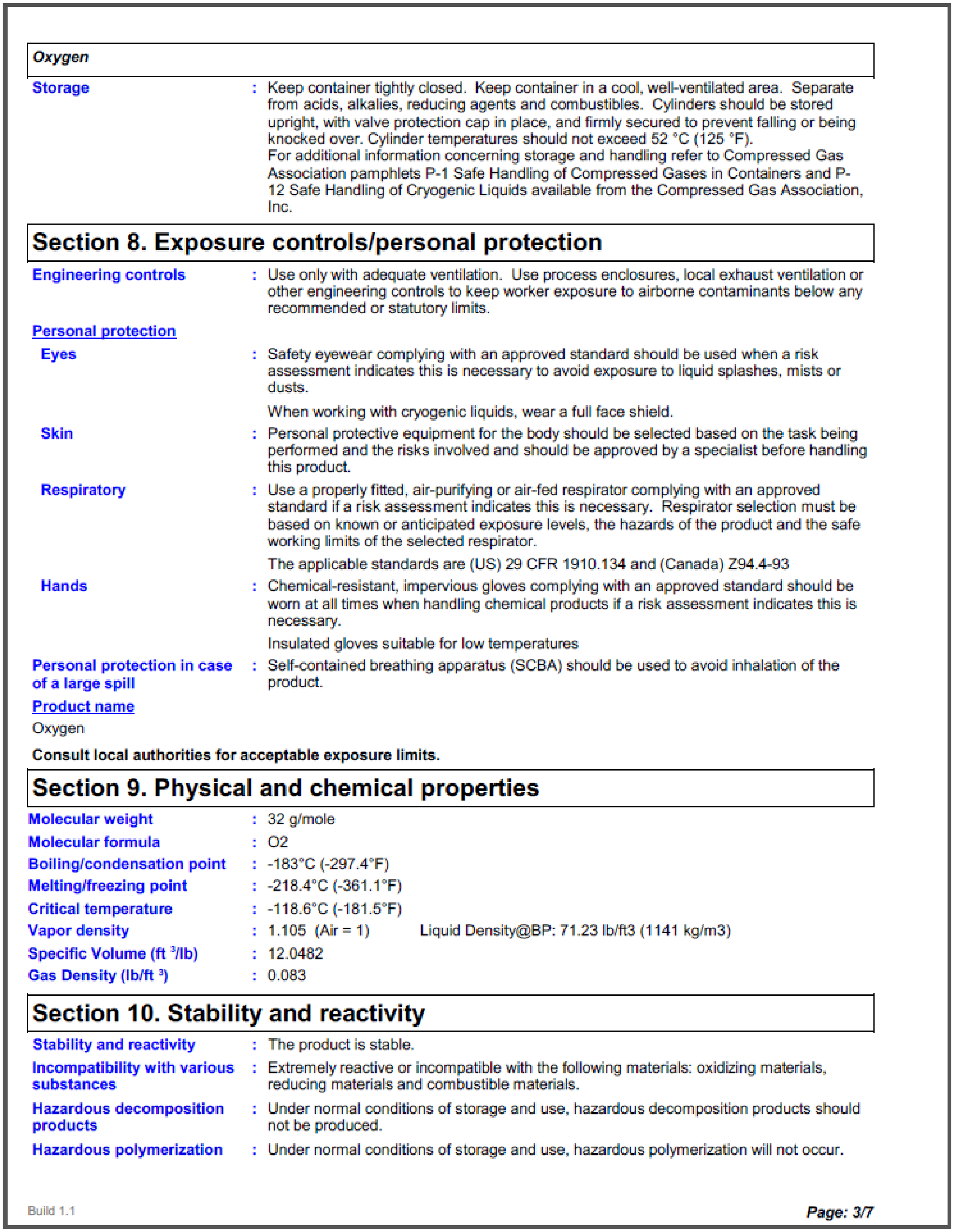
Flammability of the product	Non-flammable.
Products of combustion	No specific data.
Fire hazards in the presence of various substances	Extremely flammable in the presence of the following materials or conditions: reducing materials, combustible materials and organic materials.
Fire-fighting media and instructions	Use an extinguishing agent suitable for the surrounding fire. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk. Contains gas under pressure. Contact with combustible material may cause fire. This material increases the risk of fire and may aid combustion. In a fire or if heated, a pressure increase will occur and the container may burst or explode.
Special protective equipment for fire-fighters	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions	Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Eliminate all ignition sources if safe to do so. Do not touch or walk through spilled material. Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.
Environmental precautions	Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.
Methods for cleaning up	Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling	High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Store in tightly-closed container. Avoid contact with combustible materials. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement. Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.



Oxygen

Storage	:	Keep container tightly closed. Keep container in a cool, well-ventilated area. Separate from acids, alkalies, reducing agents and combustibles. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F). For additional information concerning storage and handling refer to Compressed Gas Association pamphlets P-1 Safe Handling of Compressed Gases in Containers and P-12 Safe Handling of Cryogenic Liquids available from the Compressed Gas Association, Inc.

Section 8. Exposure controls/personal protection

Engineering controls	:	Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits.
Personal protection		
Eyes	:	Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts. When working with cryogenic liquids, wear a full face shield.
Skin	:	Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.
Respiratory	:	Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator. The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93
Hands	:	Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Insulated gloves suitable for low temperatures
Personal protection in case of a large spill	:	Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name

Oxygen

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight	:	32 g/mole
Molecular formula	:	$O2$
Boiling/condensation point	:	-183°C (-297.4°F)
Melting/freezing point	:	-218.4°C (-361.1°F)
Critical temperature	:	-118.6°C (-181.5°F)
Vapor density	:	1.105 (Air = 1) Liquid Density@BP: 71.23 lb/ft3 (1141 kg/m3)
Specific Volume (ft ^{3}/lb)	:	12.0482
Gas Density (lb/ft ^{3})	:	0.083

Section 10. Stability and reactivity

Stability and reactivity	:	The product is stable.
Incompatibility with various substances	:	Extremely reactive or incompatible with the following materials: oxidizing materials, reducing materials and combustible materials.
Hazardous decomposition products	:	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization	:	Under normal conditions of storage and use, hazardous polymerization will not occur.

Build 1.1

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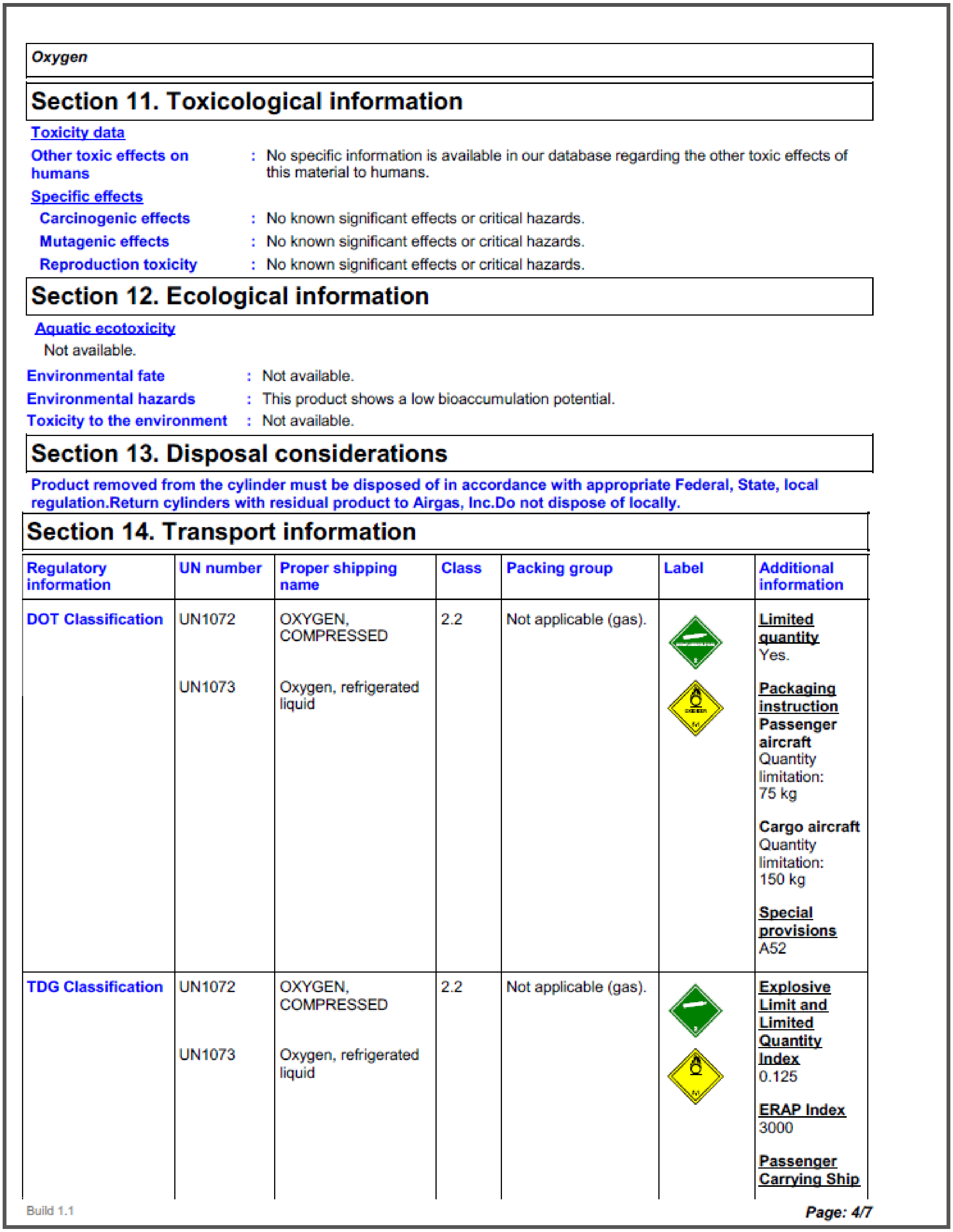


Oxygen

Section 11. Toxicological information

Toxicity data

Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.

Mutagenic effects : No known significant effects or critical hazards.

Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Environmental fate : Not available.

Environmental hazards : This product shows a low bioaccumulation potential.

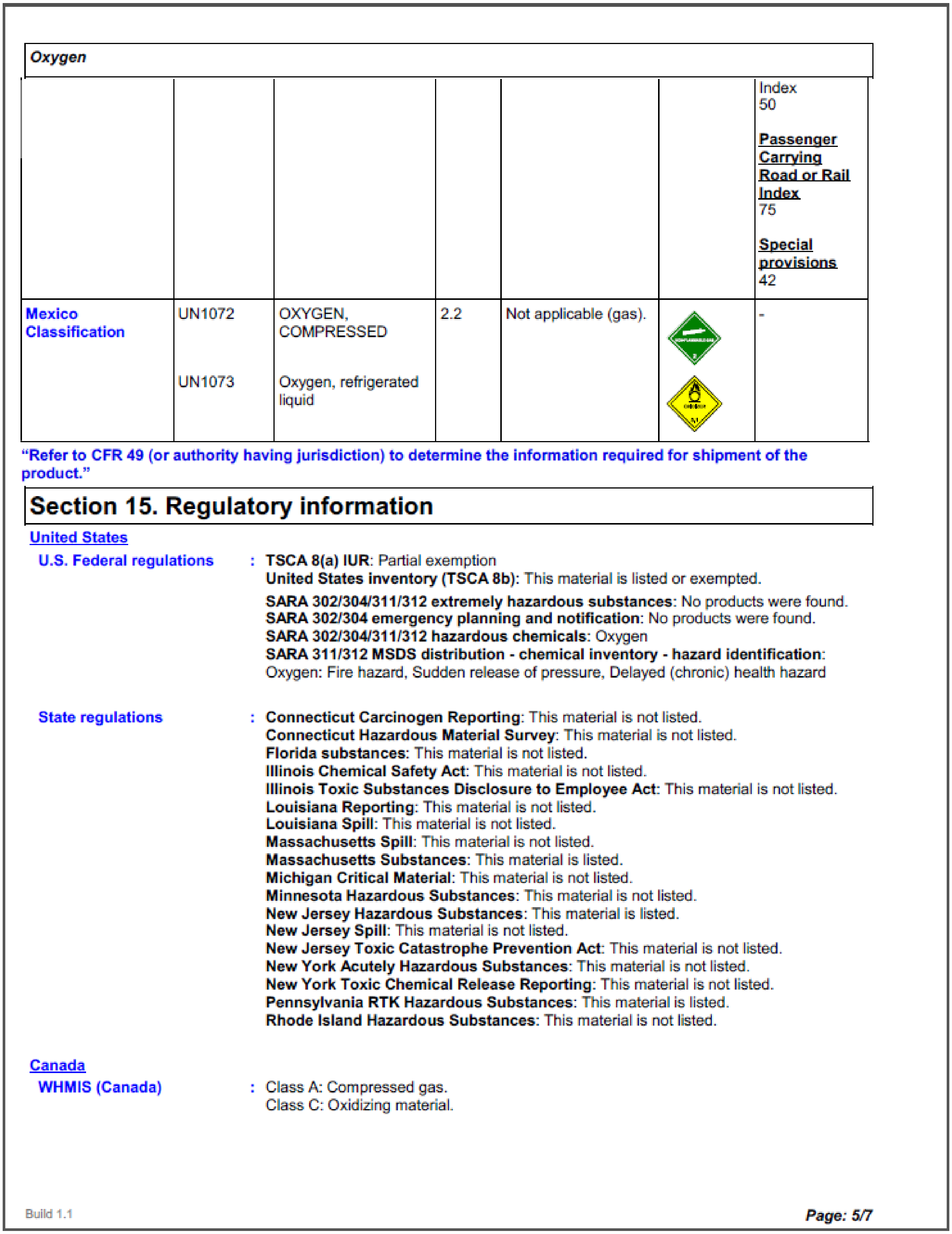
Toxicity to the environment : Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1072 UN1073	OXYGEN, COMPRESSED Oxygen, refrigerated liquid	2.2	Not applicable (gas).		**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: 75 kg **Cargo aircraft** Quantity limitation: 150 kg **Special provisions** A52
TDG Classification	UN1072 UN1073	OXYGEN, COMPRESSED Oxygen, refrigerated liquid	2.2	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0.125 **ERAP Index** 3000 **Passenger Carrying Ship**



Oxygen

						Index 50 **Passenger Carrying Road or Rail Index** 75 **Special provisions** 42
Mexico Classification	UN1072 UN1073	OXYGEN, COMPRESSED Oxygen, refrigerated liquid	2.2	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

U.S. Federal regulations : **TSCA 8(a) IUR**: Partial exemption
United States inventory (TSCA 8b): This material is listed or exempted.
SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: Oxygen
SARA 311/312 MSDS distribution - chemical inventory - hazard identification:
Oxygen: Fire hazard, Sudden release of pressure, Delayed (chronic) health hazard

State regulations : **Connecticut Carcinogen Reporting**: This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class C: Oxidizing material.

Build 1.1

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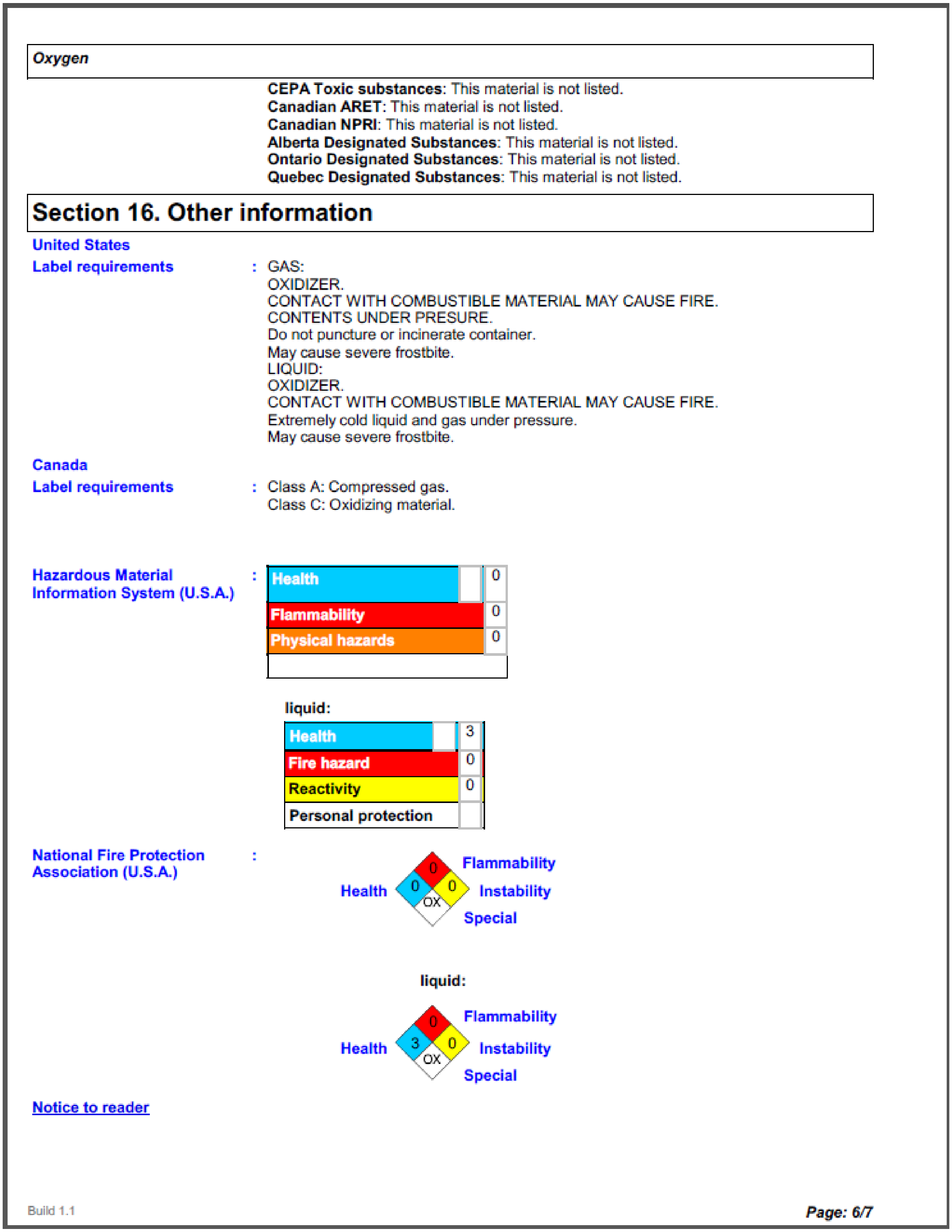


Oxygen

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is not listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

United States

Label requirements : GAS:
OXIDIZER.
CONTACT WITH COMBUSTIBLE MATERIAL MAY CAUSE FIRE.
CONTENTS UNDER PRESURE.
Do not puncture or incinerate container.
May cause severe frostbite.
LIQUID:
OXIDIZER.
CONTACT WITH COMBUSTIBLE MATERIAL MAY CAUSE FIRE.
Extremely cold liquid and gas under pressure.
May cause severe frostbite.

Canada

Label requirements : Class A: Compressed gas.
Class C: Oxidizing material.

Hazardous Material Information System (U.S.A.) :

Health	0
Flammability	0
Physical hazards	0

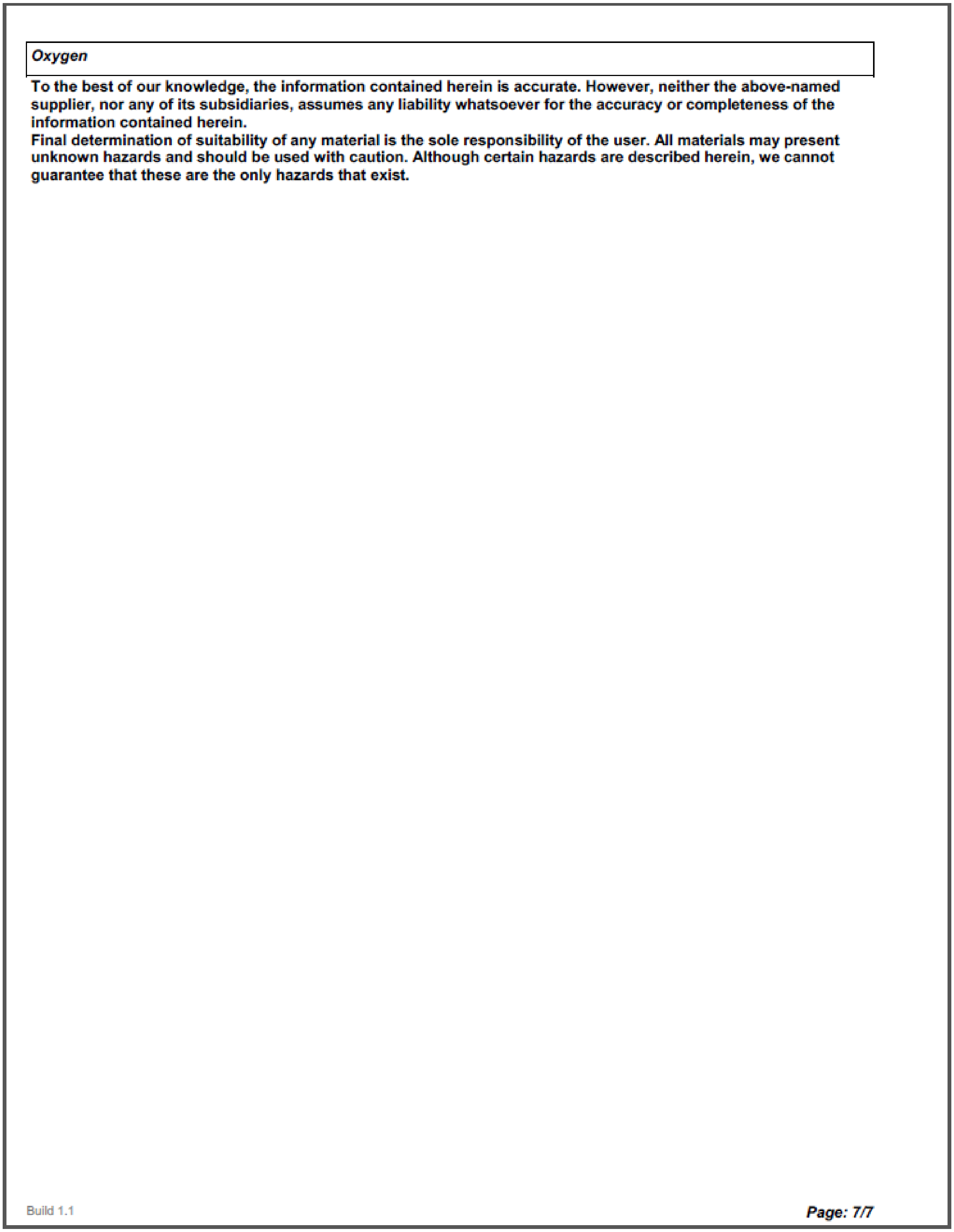
liquid:

Health	3
Fire hazard	0
Reactivity	0
Personal protection	

National Fire Protection Association (U.S.A.) :

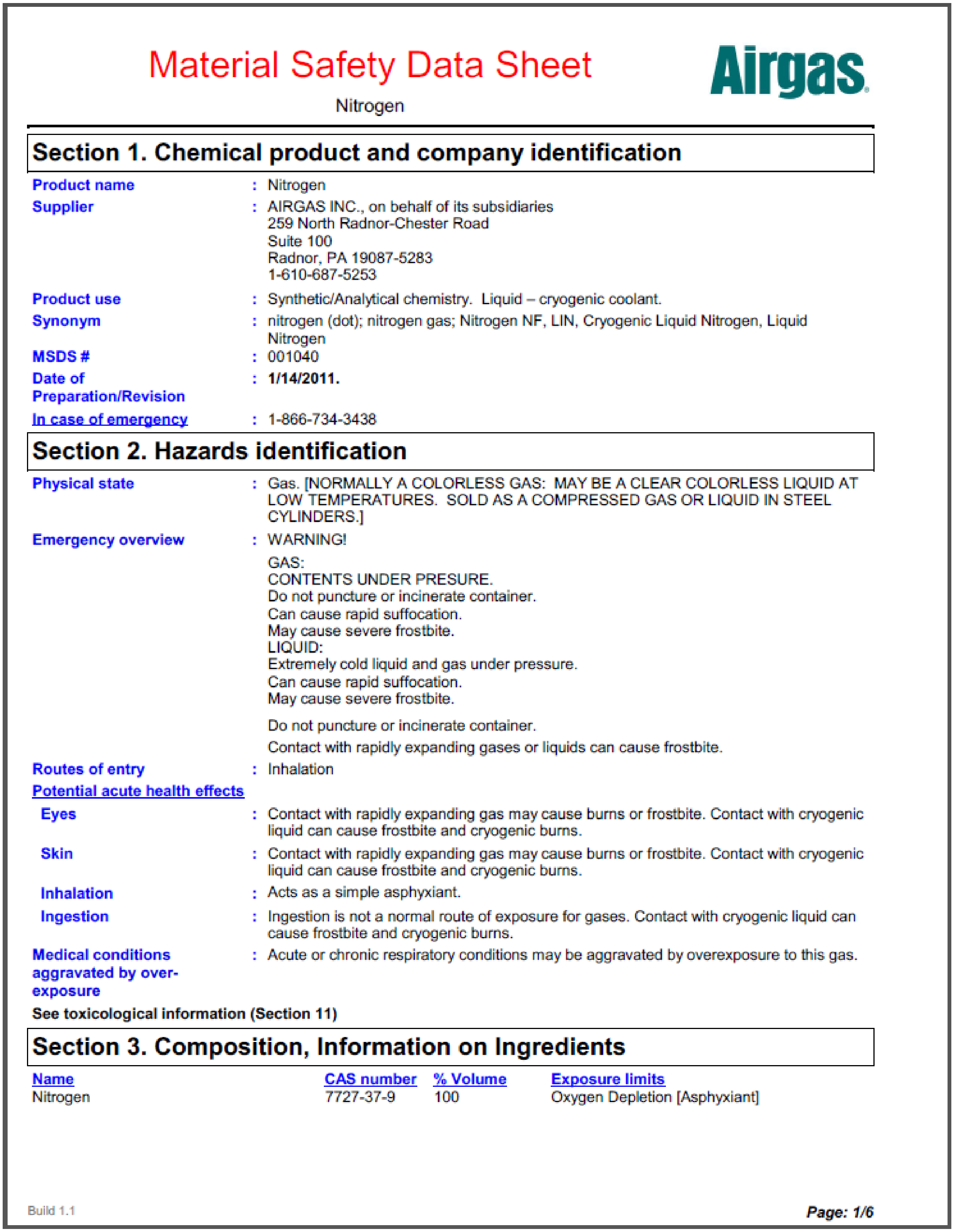
liquid:

Notice to reader



Oxygen

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.



Material Safety Data Sheet

Airgas

Nitrogen

Section 1. Chemical product and company identification

Product name : Nitrogen

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry. Liquid – cryogenic coolant.

Synonym : nitrogen (dot); nitrogen gas; Nitrogen NF, LIN, Cryogenic Liquid Nitrogen, Liquid Nitrogen

MSDS # : 001040

Date of Preparation/Revision : **1/14/2011.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas. [NORMALLY A COLORLESS GAS: MAY BE A CLEAR COLORLESS LIQUID AT LOW TEMPERATURES. SOLD AS A COMPRESSED GAS OR LIQUID IN STEEL CYLINDERS.]

Emergency overview : WARNING!

GAS:
CONTENTS UNDER PRESURE.
Do not puncture or incinerate container.
Can cause rapid suffocation.
May cause severe frostbite.
LIQUID:
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.

Do not puncture or incinerate container.

Contact with rapidly expanding gases or liquids can cause frostbite.

Routes of entry : Inhalation

Potential acute health effects

Eyes : Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Skin : Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Inhalation : Acts as a simple asphyxiant.

Ingestion : Ingestion is not a normal route of exposure for gases. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Medical conditions aggravated by over-exposure : Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.

See toxicological information (Section 11)

Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Nitrogen	7727-37-9	100	Oxygen Depletion [Asphyxiant]

Build 1.1

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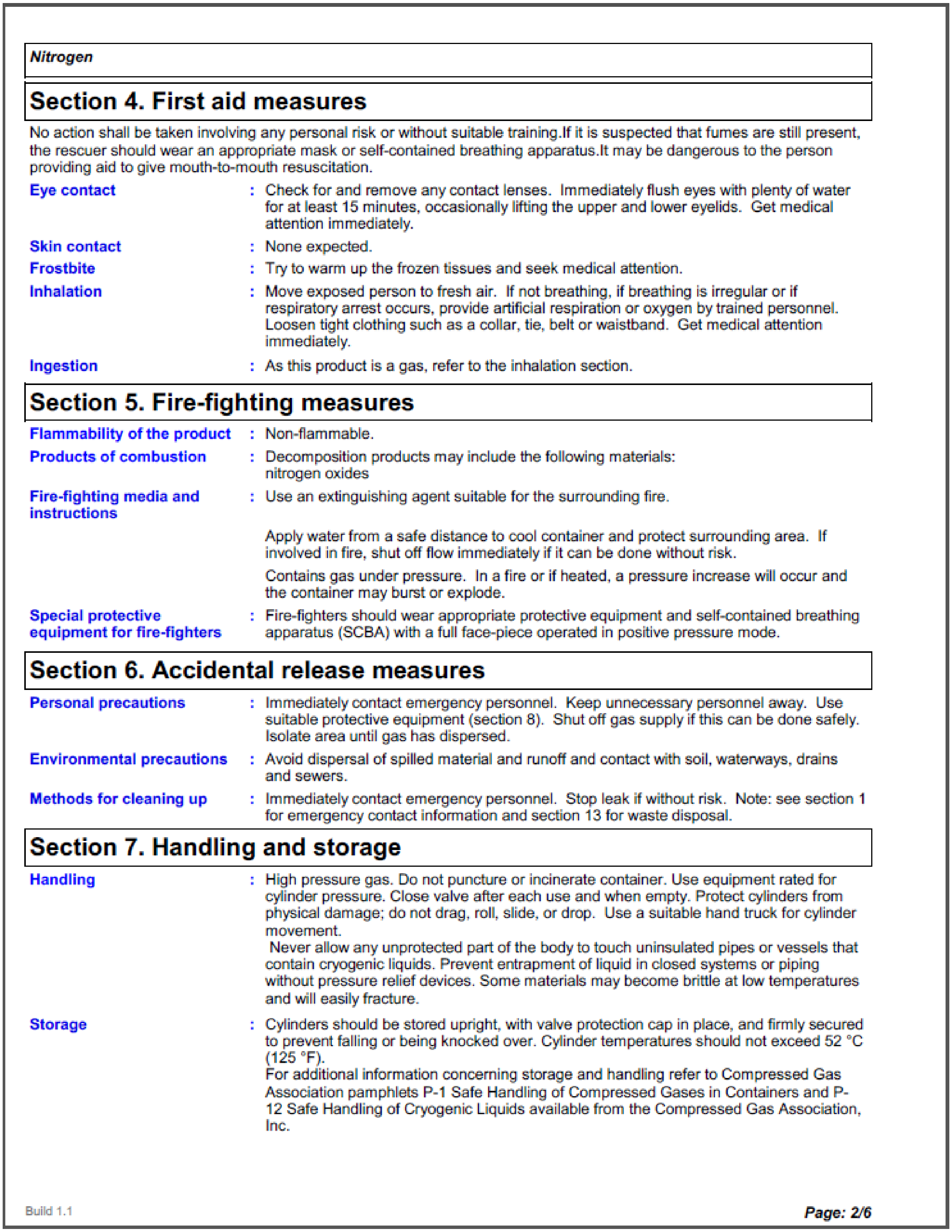

Nitrogen

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : None expected.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Non-flammable.

Products of combustion : Decomposition products may include the following materials:
nitrogen oxides

Fire-fighting media and instructions : Use an extinguishing agent suitable for the surrounding fire.

Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. In a fire or if heated, a pressure increase will occur and the container may burst or explode.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.
Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.

Storage : Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).
For additional information concerning storage and handling refer to Compressed Gas Association pamphlets P-1 Safe Handling of Compressed Gases in Containers and P-12 Safe Handling of Cryogenic Liquids available from the Compressed Gas Association, Inc.

Build 1.1

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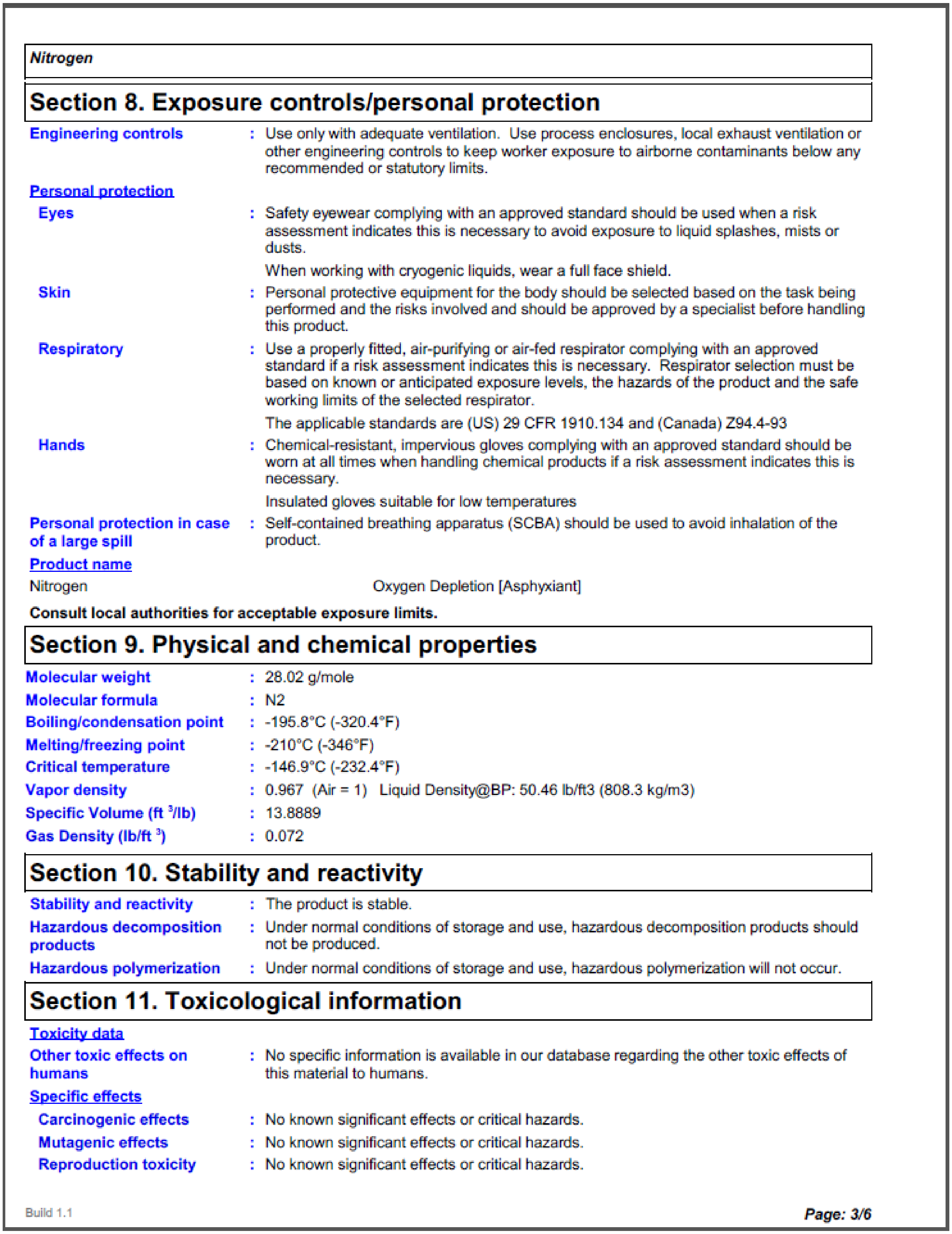

Nitrogen

Section 8. Exposure controls/personal protection

Engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

When working with cryogenic liquids, wear a full face shield.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Insulated gloves suitable for low temperatures

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name	
Nitrogen	Oxygen Depletion [Asphyxiant]

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight : 28.02 g/mole

Molecular formula : N2

Boiling/condensation point : -195.8°C (-320.4°F)

Melting/freezing point : -210°C (-346°F)

Critical temperature : -146.9°C (-232.4°F)

Vapor density : 0.967 (Air = 1) Liquid Density@BP: 50.46 lb/ft3 (808.3 kg/m3)

Specific Volume (ft ^{3}/lb) : 13.8889

Gas Density (lb/ft ^{3}) : 0.072

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.

Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.

Mutagenic effects : No known significant effects or critical hazards.

Reproduction toxicity : No known significant effects or critical hazards.

Build 1.1

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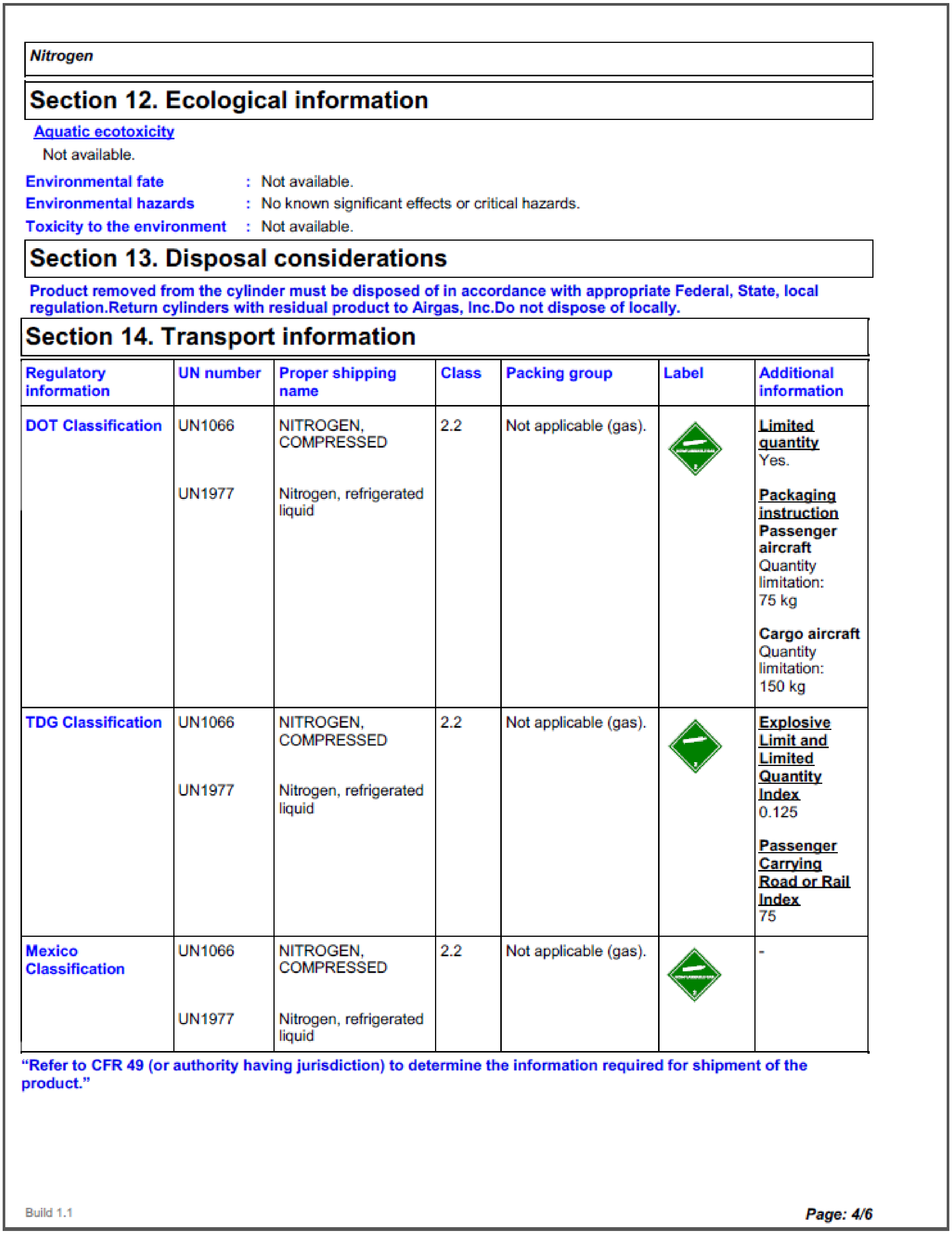


Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Environmental fate : Not available.
Environmental hazards : No known significant effects or critical hazards.
Toxicity to the environment : Not available.

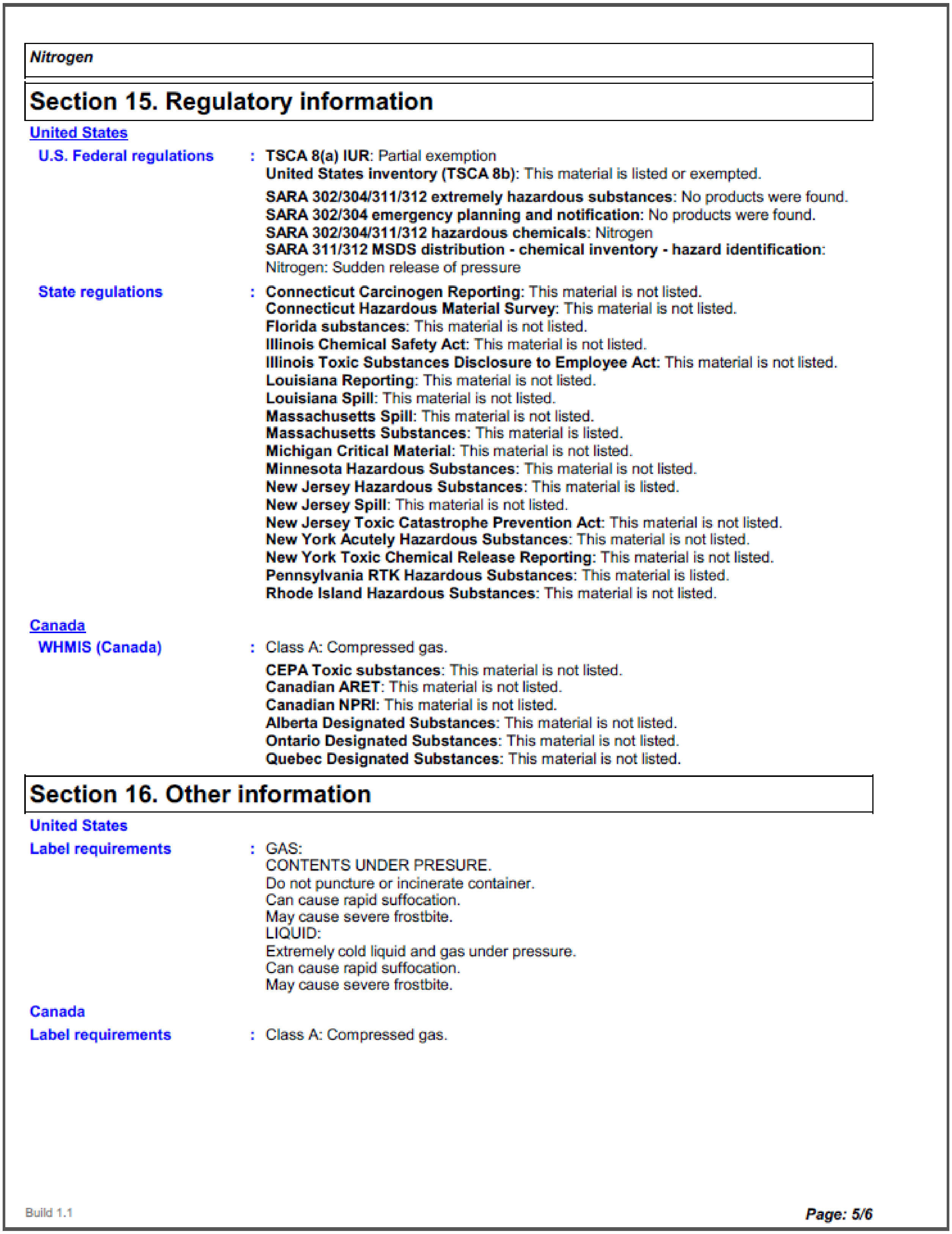
Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1066	NITROGEN, COMPRESSED	2.2	Not applicable (gas).		**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: 75 kg **Cargo aircraft** Quantity limitation: 150 kg
	UN1977	Nitrogen, refrigerated liquid				
TDG Classification	UN1066	NITROGEN, COMPRESSED	2.2	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0.125 **Passenger Carrying Road or Rail Index** 75
	UN1977	Nitrogen, refrigerated liquid				
Mexico Classification	UN1066	NITROGEN, COMPRESSED	2.2	Not applicable (gas).		-
	UN1977	Nitrogen, refrigerated liquid				

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."



Section 15. Regulatory information

United States

U.S. Federal regulations :
TSCA 8(a) IUR: Partial exemption
United States inventory (TSCA 8b): This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: Nitrogen
SARA 311/312 MSDS distribution - chemical inventory - hazard identification:
Nitrogen: Sudden release of pressure

State regulations :
Connecticut Carcinogen Reporting: This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class A: Compressed gas.

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is not listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

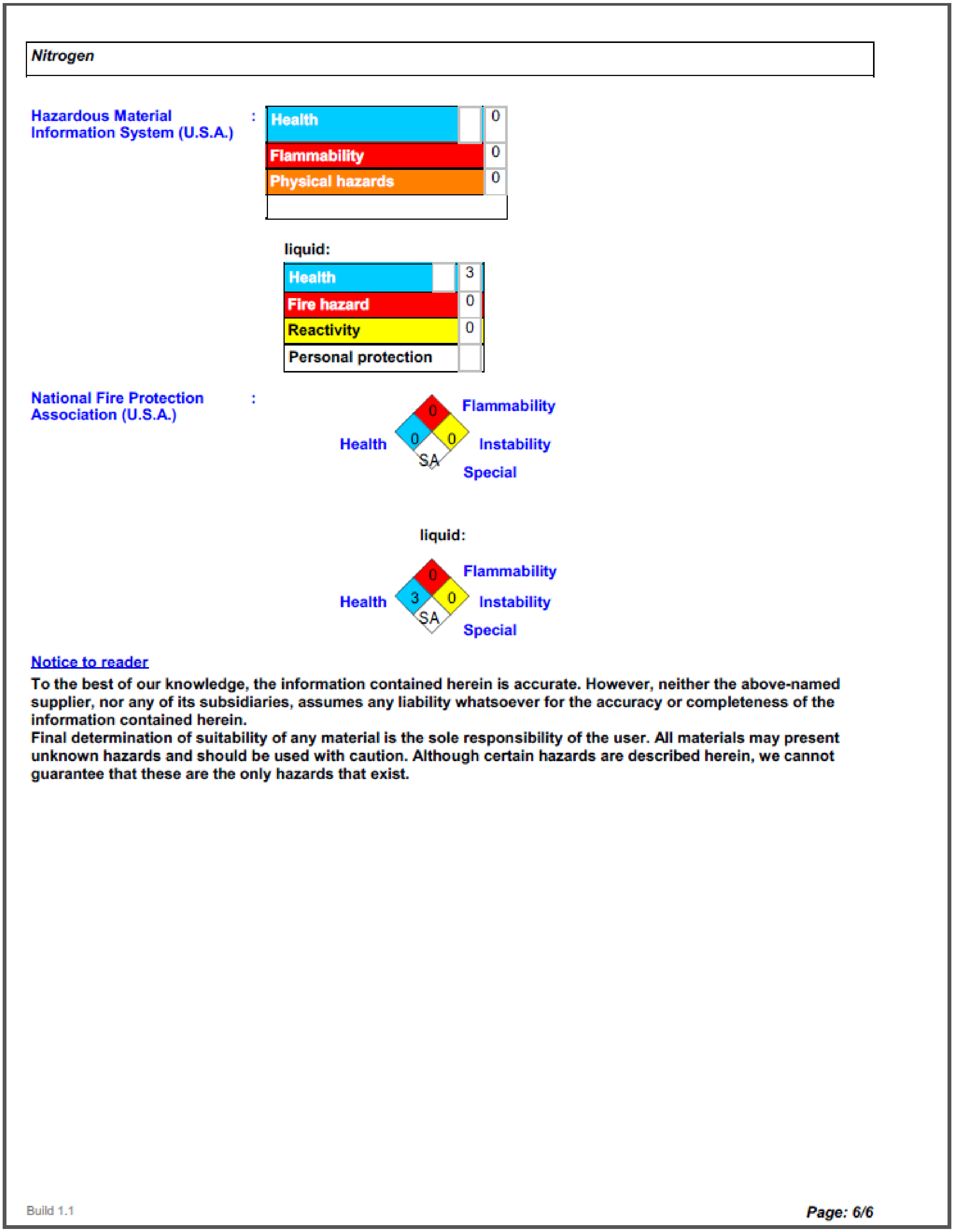
Section 16. Other information

United States

Label requirements :
GAS:
CONTENTS UNDER PRESURE.
Do not puncture or incinerate container.
Can cause rapid suffocation.
May cause severe frostbite.
LIQUID:
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.

Canada

Label requirements : Class A: Compressed gas.



Nitrogen

Hazardous Material Information System (U.S.A.) :

Health	0
Flammability	0
Physical hazards	0

liquid:

Health	3
Fire hazard	0
Reactivity	0
Personal protection	

National Fire Protection Association (U.S.A.) :

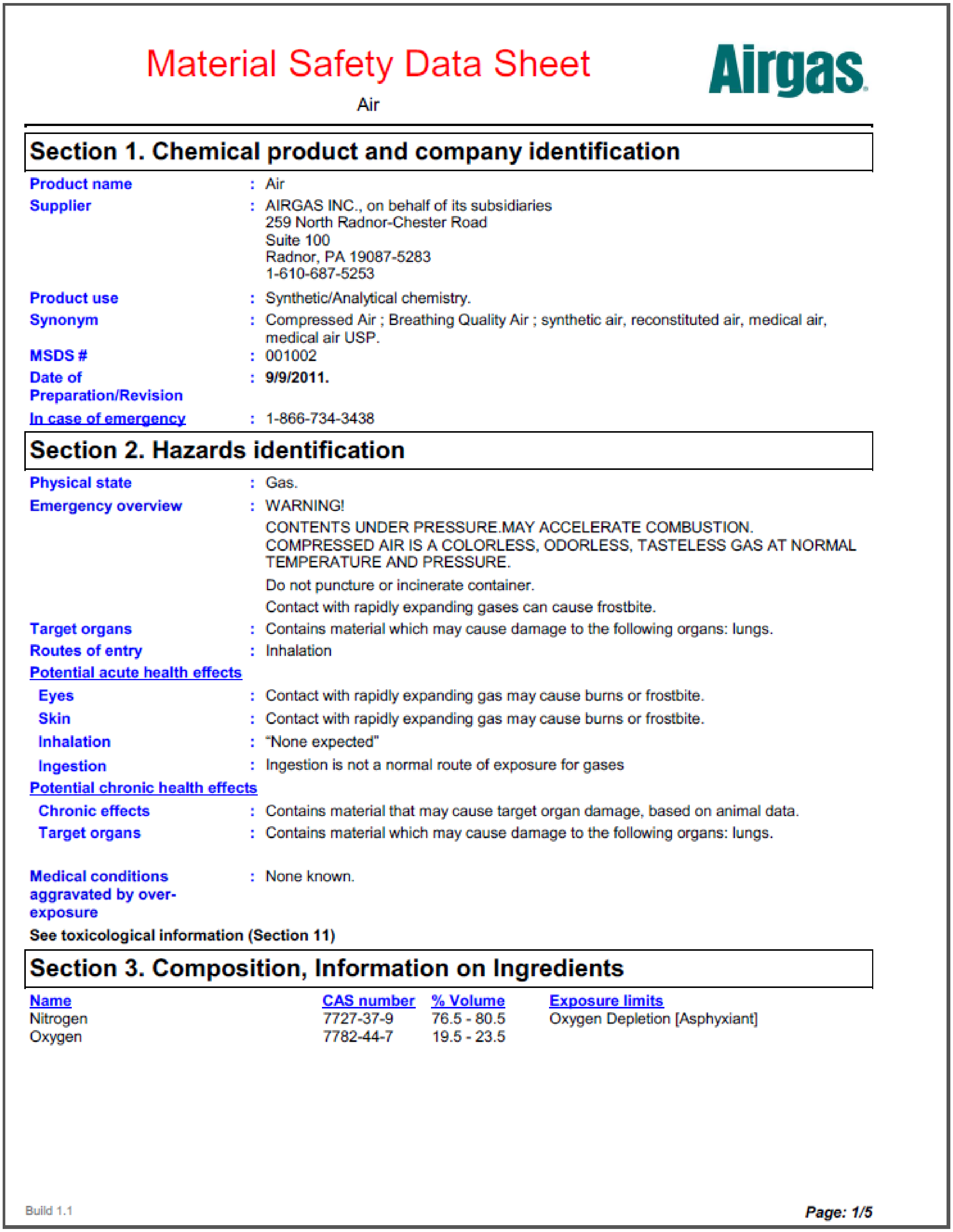
Flammability	0
Health	0
Instability	0
Special	SA

liquid:

Flammability	0
Health	3
Instability	0
Special	SA

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.



Material Safety Data Sheet

Air

Section 1. Chemical product and company identification

Product name : Air

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : Compressed Air ; Breathing Quality Air ; synthetic air, reconstituted air, medical air, medical air USP.

MSDS # : 001002

Date of Preparation/Revision : **9/9/2011.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas.

Emergency overview : WARNING!

CONTENTS UNDER PRESSURE.MAY ACCELERATE COMBUSTION.
COMPRESSED AIR IS A COLORLESS, ODORLESS, TASTELESS GAS AT NORMAL TEMPERATURE AND PRESSURE.

Do not puncture or incinerate container.

Contact with rapidly expanding gases can cause frostbite.

Target organs : Contains material which may cause damage to the following organs: lungs.

Routes of entry : Inhalation

Potential acute health effects

Eyes : Contact with rapidly expanding gas may cause burns or frostbite.

Skin : Contact with rapidly expanding gas may cause burns or frostbite.

Inhalation : "None expected"

Ingestion : Ingestion is not a normal route of exposure for gases

Potential chronic health effects

Chronic effects : Contains material that may cause target organ damage, based on animal data.

Target organs : Contains material which may cause damage to the following organs: lungs.

Medical conditions aggravated by over-exposure : None known.

See toxicological information (Section 11)

Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Nitrogen	7727-37-9	76.5 - 80.5	Oxygen Depletion [Asphyxiant]
Oxygen	7782-44-7	19.5 - 23.5	

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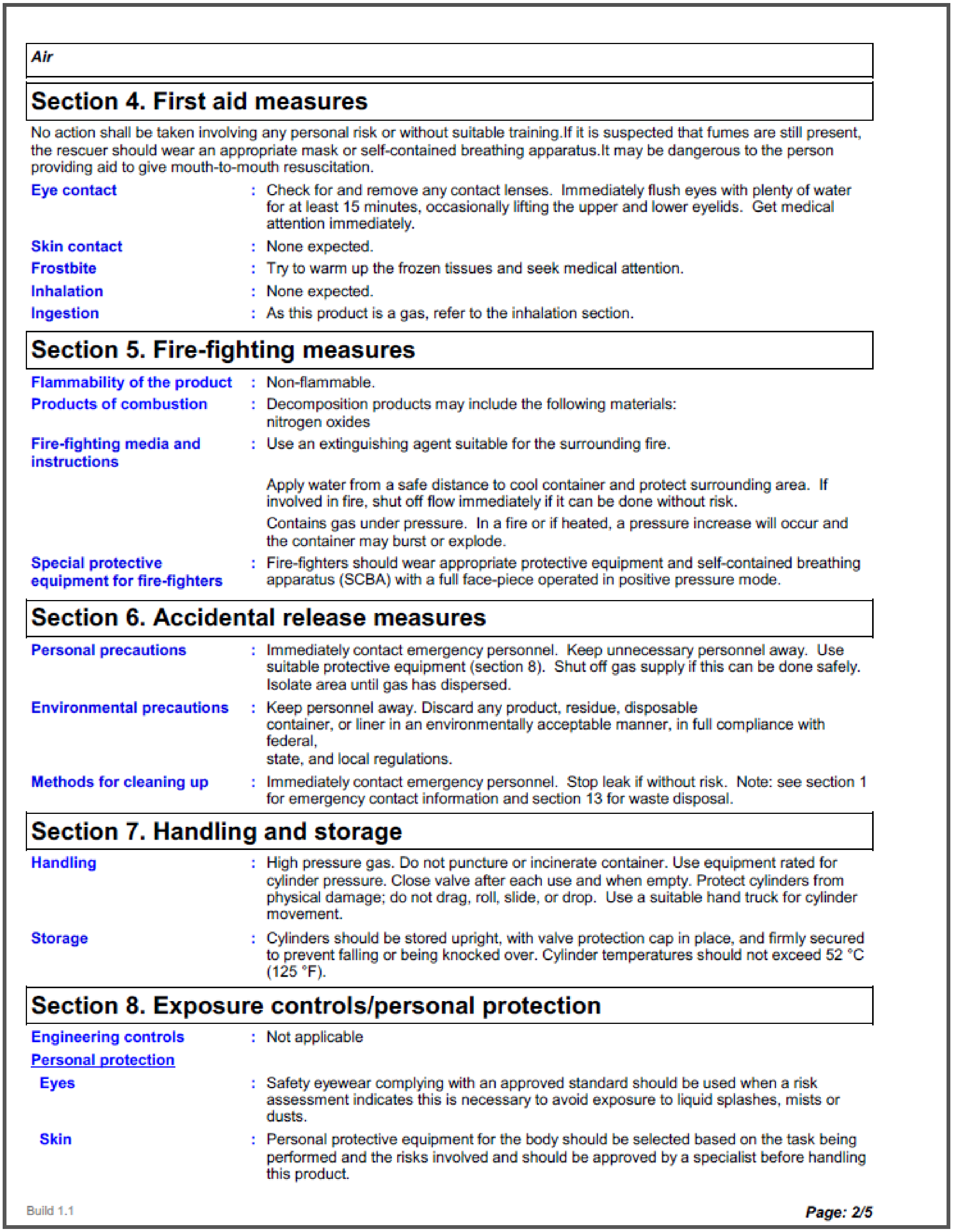

Air

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : None expected.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : None expected.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Non-flammable.

Products of combustion : Decomposition products may include the following materials:
nitrogen oxides

Fire-fighting media and instructions : Use an extinguishing agent suitable for the surrounding fire.

Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. In a fire or if heated, a pressure increase will occur and the container may burst or explode.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions : Keep personnel away. Discard any product, residue, disposable
container, or liner in an environmentally acceptable manner, in full compliance with
federal,
state, and local regulations.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Storage : Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

Section 8. Exposure controls/personal protection

Engineering controls : Not applicable

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

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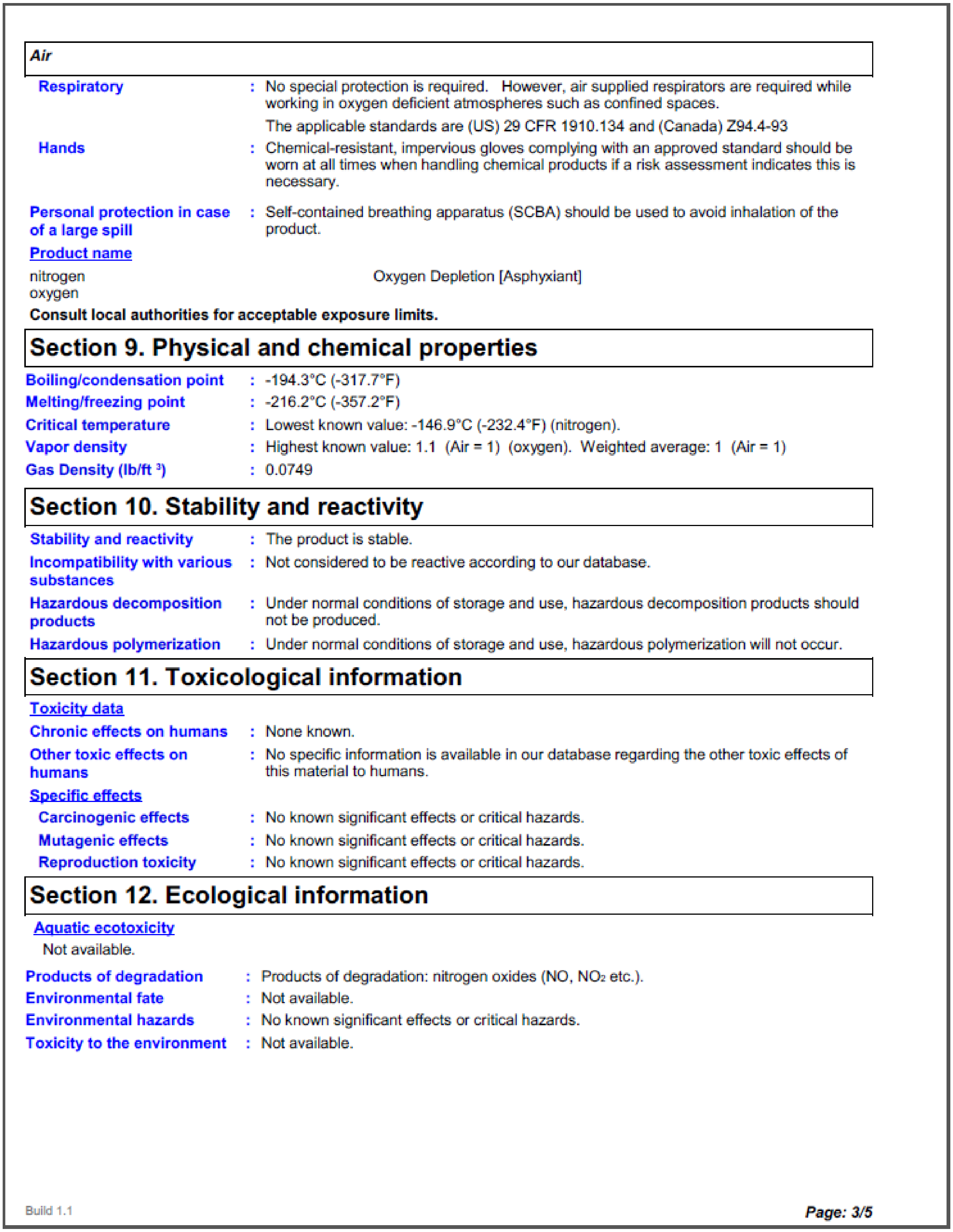


Air

Respiratory : No special protection is required. However, air supplied respirators are required while working in oxygen deficient atmospheres such as confined spaces.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Product name	
nitrogen	Oxygen Depletion [Asphyxiant]
oxygen	

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Boiling/condensation point : -194.3°C (-317.7°F)

Melting/freezing point : -216.2°C (-357.2°F)

Critical temperature : Lowest known value: -146.9°C (-232.4°F) (nitrogen).

Vapor density : Highest known value: 1.1 (Air = 1) (oxygen). Weighted average: 1 (Air = 1)

Gas Density (lb/ft^3) : 0.0749

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.

Incompatibility with various substances : Not considered to be reactive according to our database.

Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Chronic effects on humans : None known.

Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.

Mutagenic effects : No known significant effects or critical hazards.

Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

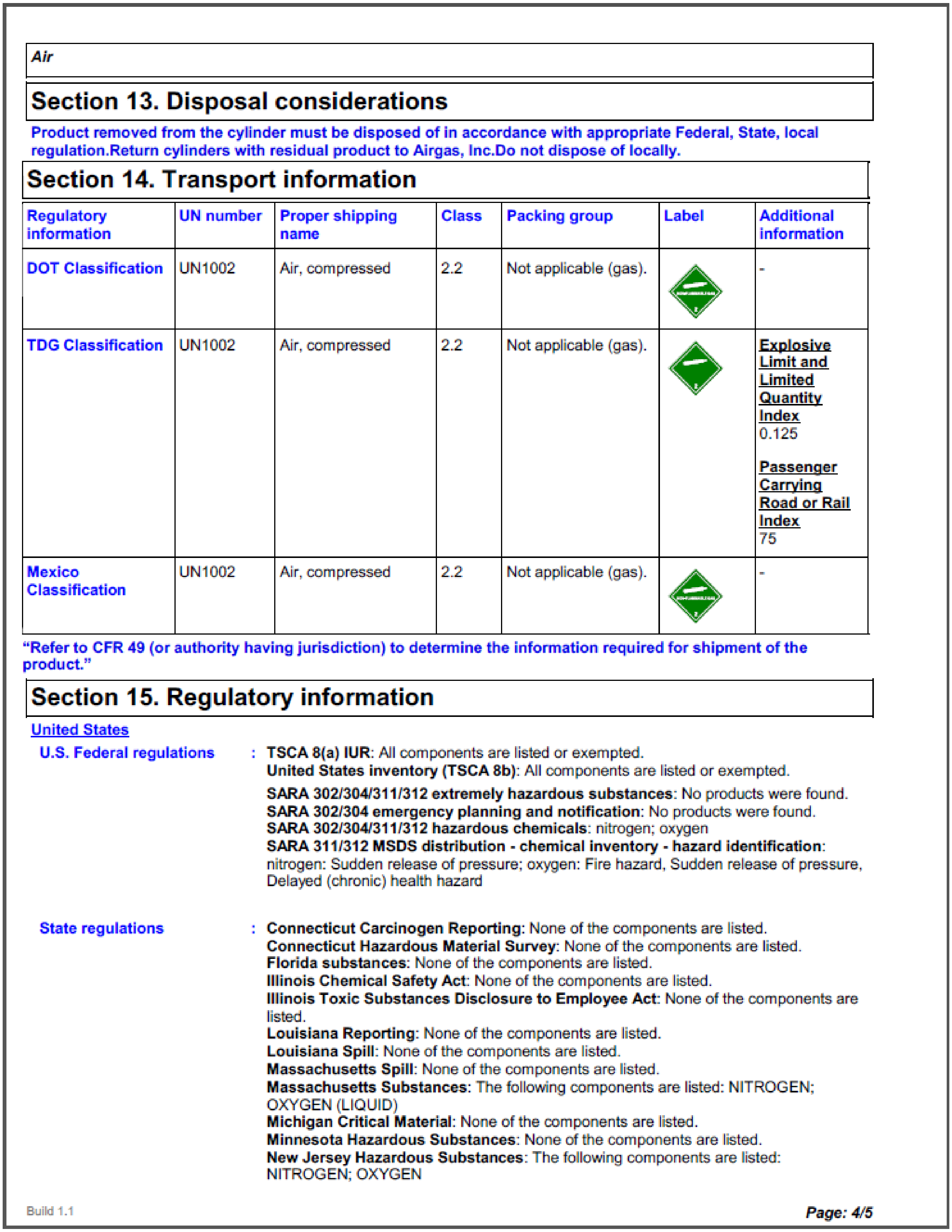
Not available.

Products of degradation : Products of degradation: nitrogen oxides (NO, NO_2 etc.).

Environmental fate : Not available.

Environmental hazards : No known significant effects or critical hazards.

Toxicity to the environment : Not available.



Air

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1002	Air, compressed	2.2	Not applicable (gas).		-
TDG Classification	UN1002	Air, compressed	2.2	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0.125 **Passenger Carrying Road or Rail Index** 75
Mexico Classification	UN1002	Air, compressed	2.2	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

U.S. Federal regulations : **TSCA 8(a) IUR**: All components are listed or exempted.
United States inventory (TSCA 8b): All components are listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: nitrogen; oxygen
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: nitrogen: Sudden release of pressure; oxygen: Fire hazard, Sudden release of pressure, Delayed (chronic) health hazard

State regulations : **Connecticut Carcinogen Reporting**: None of the components are listed.
Connecticut Hazardous Material Survey: None of the components are listed.
Florida substances: None of the components are listed.
Illinois Chemical Safety Act: None of the components are listed.
Illinois Toxic Substances Disclosure to Employee Act: None of the components are listed.
Louisiana Reporting: None of the components are listed.
Louisiana Spill: None of the components are listed.
Massachusetts Spill: None of the components are listed.
Massachusetts Substances: The following components are listed: NITROGEN; OXYGEN (LIQUID)
Michigan Critical Material: None of the components are listed.
Minnesota Hazardous Substances: None of the components are listed.
New Jersey Hazardous Substances: The following components are listed: NITROGEN; OXYGEN

Build 1.1

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Air

New Jersey Spill: None of the components are listed.
New Jersey Toxic Catastrophe Prevention Act: None of the components are listed.
New York Acutely Hazardous Substances: None of the components are listed.
New York Toxic Chemical Release Reporting: None of the components are listed.
Pennsylvania RTK Hazardous Substances: The following components are listed: NITROGEN; OXYGEN
Rhode Island Hazardous Substances: None of the components are listed.

Canada

WHMIS (Canada) : Class A: Compressed gas.

CEPA Toxic substances: None of the components are listed.
Canadian ARET: None of the components are listed.
Canadian NPRI: None of the components are listed.
Alberta Designated Substances: None of the components are listed.
Ontario Designated Substances: None of the components are listed.
Quebec Designated Substances: None of the components are listed.

Section 16. Other information

United States

Label requirements : CONTENTS UNDER PRESSURE.MAY ACCELERATE COMBUSTION. COMPRESSED AIR IS A COLORLESS, ODORLESS, TASTELESS GAS AT NORMAL TEMPERATURE AND PRESSURE.

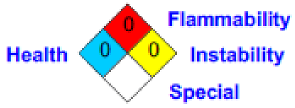
Canada

Label requirements : Class A: Compressed gas.

Hazardous Material Information System (U.S.A.) :

Health	0
Flammability	0
Physical hazards	0

National Fire Protection Association (U.S.A.) :



Notice to reader

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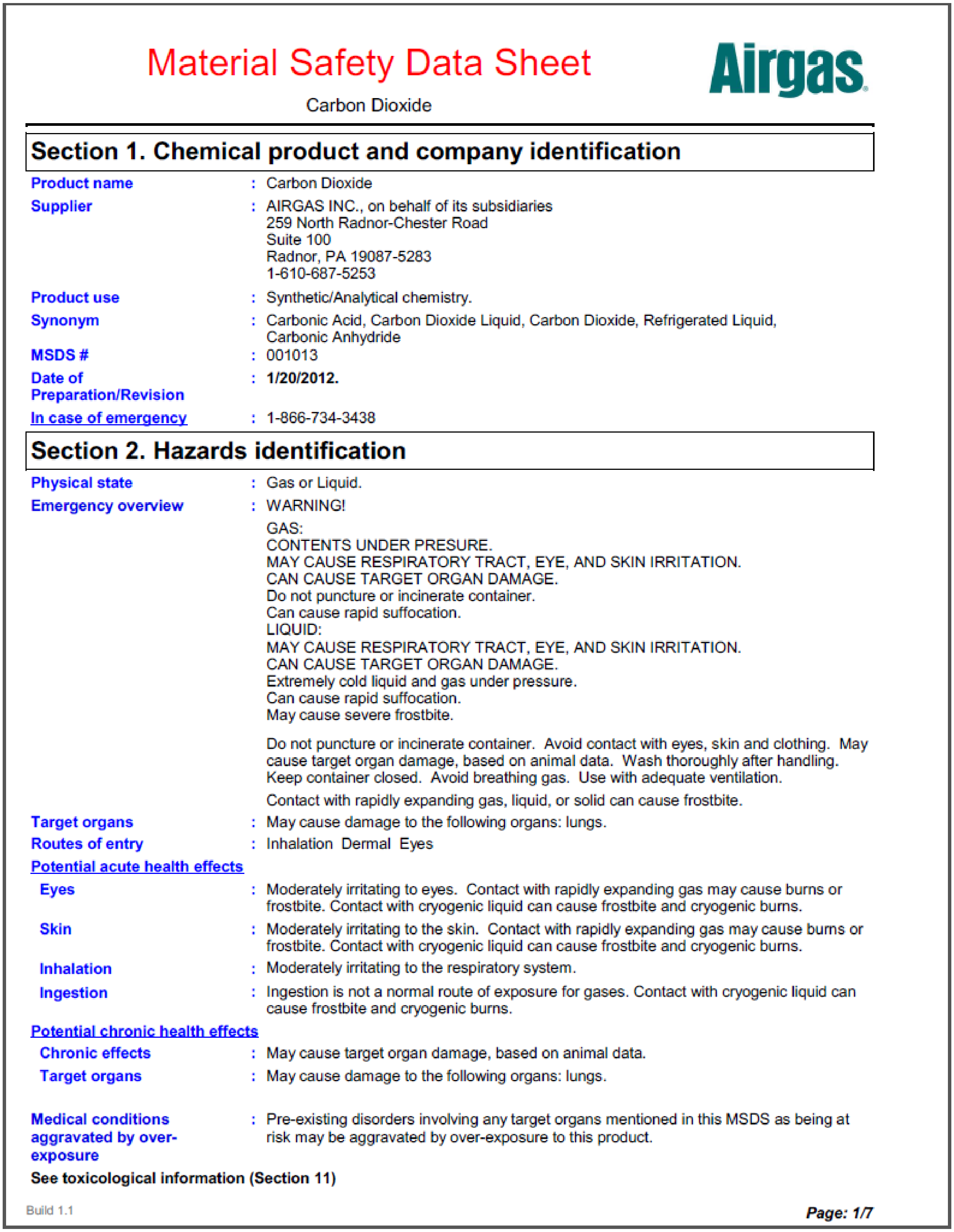

Material Safety Data Sheet

Airgas.

Carbon Dioxide

Section 1. Chemical product and company identification

Product name : Carbon Dioxide

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : Carbonic Acid, Carbon Dioxide Liquid, Carbon Dioxide, Refrigerated Liquid, Carbonic Anhydride

MSDS # : 001013

Date of Preparation/Revision : **1/20/2012.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas or Liquid.

Emergency overview : WARNING!

GAS:
CONTENTS UNDER PRESURE.
MAY CAUSE RESPIRATORY TRACT, EYE, AND SKIN IRRITATION.
CAN CAUSE TARGET ORGAN DAMAGE.
Do not puncture or incinerate container.
Can cause rapid suffocation.
LIQUID:
MAY CAUSE RESPIRATORY TRACT, EYE, AND SKIN IRRITATION.
CAN CAUSE TARGET ORGAN DAMAGE.
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.

Do not puncture or incinerate container. Avoid contact with eyes, skin and clothing. May cause target organ damage, based on animal data. Wash thoroughly after handling. Keep container closed. Avoid breathing gas. Use with adequate ventilation.

Contact with rapidly expanding gas, liquid, or solid can cause frostbite.

Target organs : May cause damage to the following organs: lungs.

Routes of entry : Inhalation Dermal Eyes

Potential acute health effects

Eyes : Moderately irritating to eyes. Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Skin : Moderately irritating to the skin. Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Inhalation : Moderately irritating to the respiratory system.

Ingestion : Ingestion is not a normal route of exposure for gases. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Potential chronic health effects

Chronic effects : May cause target organ damage, based on animal data.

Target organs : May cause damage to the following organs: lungs.

Medical conditions aggravated by over-exposure : Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (Section 11)

Build 1.1

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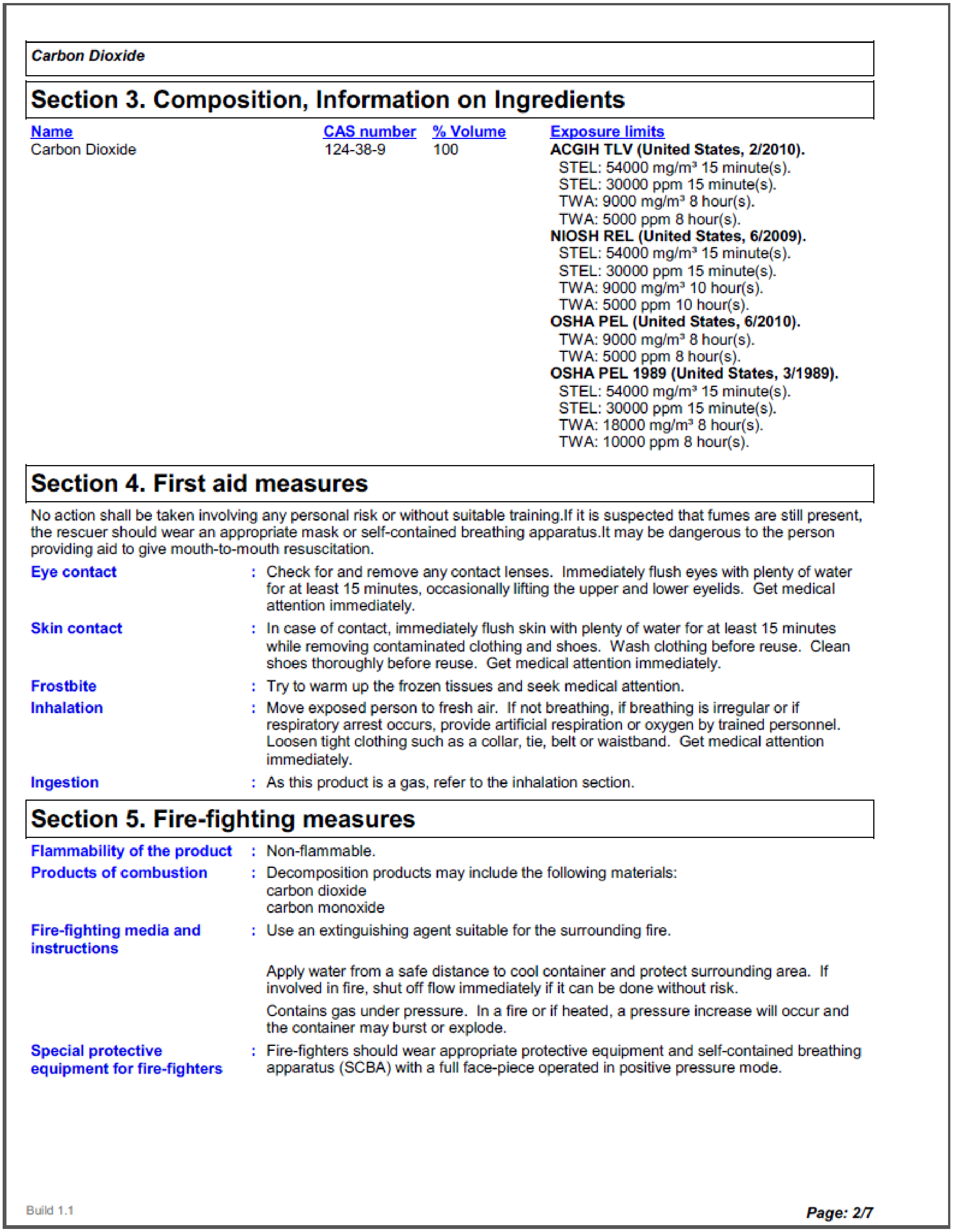


Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Carbon Dioxide	124-38-9	100	**ACGIH TLV (United States, 2/2010).** STEL: 54000 mg/m³ 15 minute(s). STEL: 30000 ppm 15 minute(s). TWA: 9000 mg/m³ 8 hour(s). TWA: 5000 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** STEL: 54000 mg/m³ 15 minute(s). STEL: 30000 ppm 15 minute(s). TWA: 9000 mg/m³ 10 hour(s). TWA: 5000 ppm 10 hour(s). **OSHA PEL (United States, 6/2010).** TWA: 9000 mg/m³ 8 hour(s). TWA: 5000 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** STEL: 54000 mg/m³ 15 minute(s). STEL: 30000 ppm 15 minute(s). TWA: 18000 mg/m³ 8 hour(s). TWA: 10000 ppm 8 hour(s).

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Non-flammable.

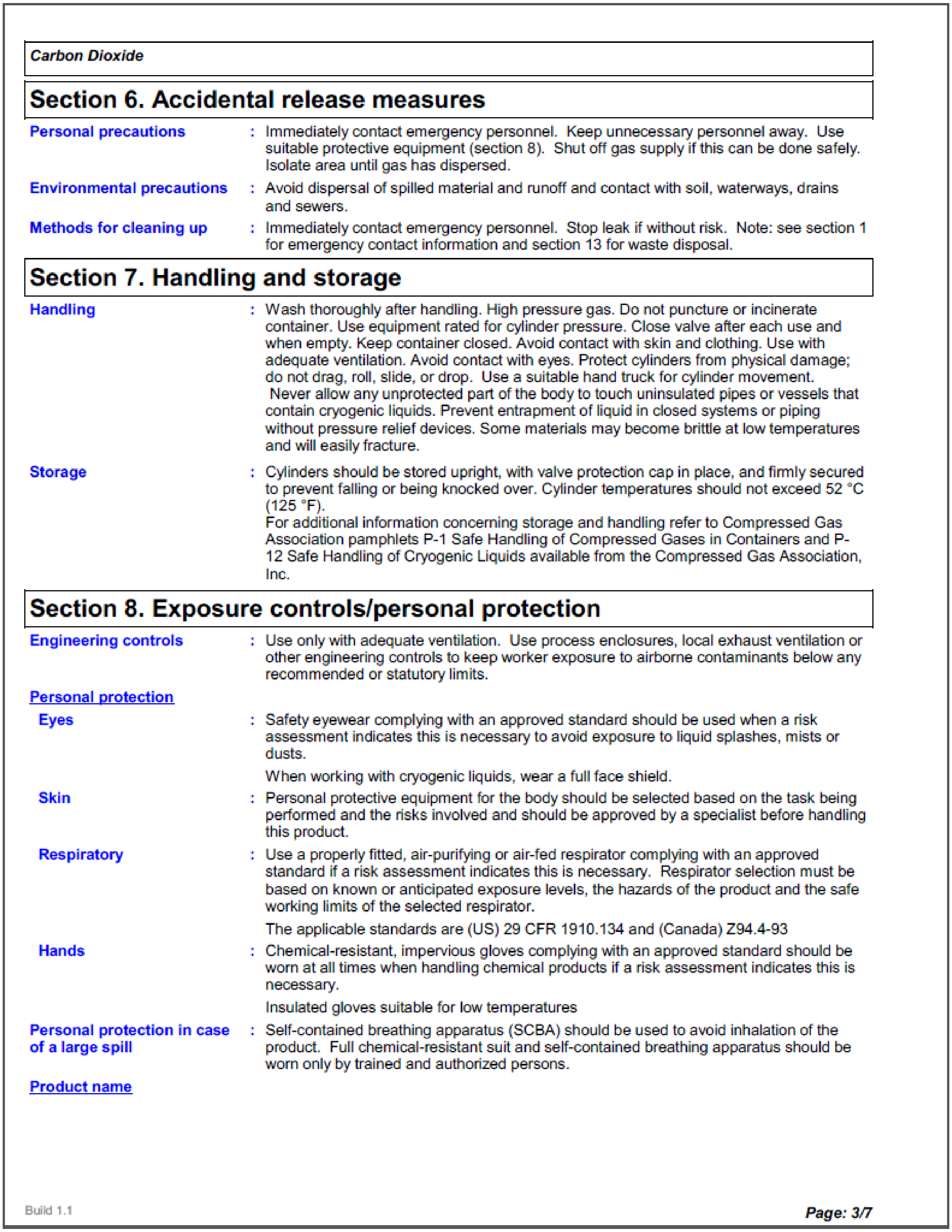
Products of combustion : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Fire-fighting media and instructions : Use an extinguishing agent suitable for the surrounding fire.

Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. In a fire or if heated, a pressure increase will occur and the container may burst or explode.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.



Carbon Dioxide

Section 6. Accidental release measures

Personal precautions	Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.
Environmental precautions	Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.
Methods for cleaning up	Immediately contact emergency personnel. Stop leak if without risk. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling	Wash thoroughly after handling. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Avoid contact with skin and clothing. Use with adequate ventilation. Avoid contact with eyes. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement. Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.
Storage	Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F). For additional information concerning storage and handling refer to Compressed Gas Association pamphlets P-1 Safe Handling of Compressed Gases in Containers and P-12 Safe Handling of Cryogenic Liquids available from the Compressed Gas Association, Inc.

Section 8. Exposure controls/personal protection

Engineering controls	Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits.
Personal protection	
Eyes	Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts. When working with cryogenic liquids, wear a full face shield.
Skin	Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.
Respiratory	Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator. The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93
Hands	Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Insulated gloves suitable for low temperatures
Personal protection in case of a large spill	Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product. Full chemical-resistant suit and self-contained breathing apparatus should be worn only by trained and authorized persons.
Product name	

Build 1.1

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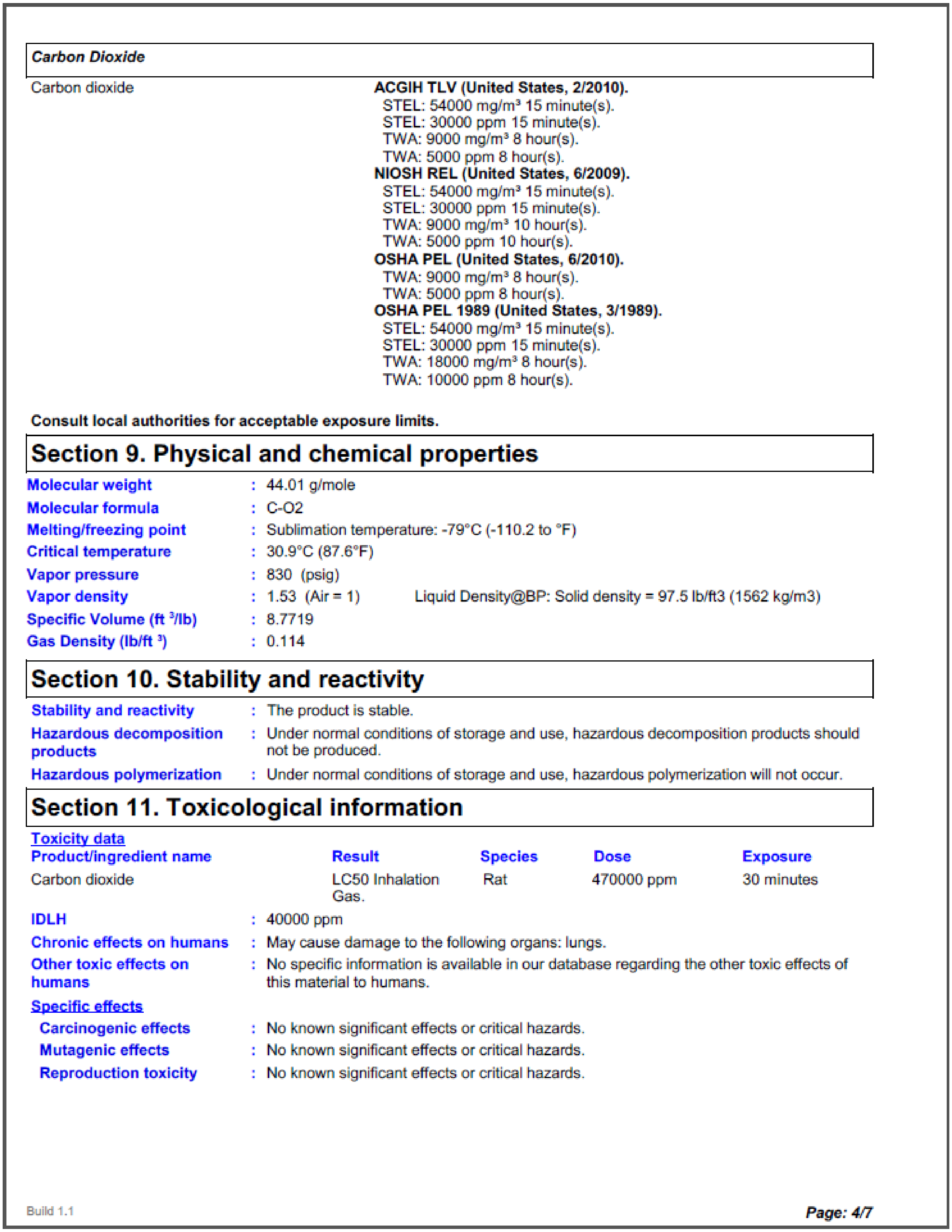

Carbon Dioxide

Carbon dioxide	**ACGIH TLV (United States, 2/2010).** STEL: 54000 mg/m³ 15 minute(s). STEL: 30000 ppm 15 minute(s). TWA: 9000 mg/m³ 8 hour(s). TWA: 5000 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** STEL: 54000 mg/m³ 15 minute(s). STEL: 30000 ppm 15 minute(s). TWA: 9000 mg/m³ 10 hour(s). TWA: 5000 ppm 10 hour(s). **OSHA PEL (United States, 6/2010).** TWA: 9000 mg/m³ 8 hour(s). TWA: 5000 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** STEL: 54000 mg/m³ 15 minute(s). STEL: 30000 ppm 15 minute(s). TWA: 18000 mg/m³ 8 hour(s). TWA: 10000 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight : 44.01 g/mole
Molecular formula : C-O2
Melting/freezing point : Sublimation temperature: -79°C (-110.2 to °F)
Critical temperature : 30.9°C (87.6°F)
Vapor pressure : 830 (psig)
Vapor density : 1.53 (Air = 1) Liquid Density@BP: Solid density = 97.5 lb/ft3 (1562 kg/m3)
Specific Volume (ft ^{3}/lb) : 8.7719
Gas Density (lb/ft ^{3}) : 0.114

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.
Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Product/ingredient name	**Result**	**Species**	**Dose**	**Exposure**
Carbon dioxide	LC50 Inhalation Gas.	Rat	470000 ppm	30 minutes

IDLH : 40000 ppm
Chronic effects on humans : May cause damage to the following organs: lungs.
Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.
Mutagenic effects : No known significant effects or critical hazards.
Reproduction toxicity : No known significant effects or critical hazards.

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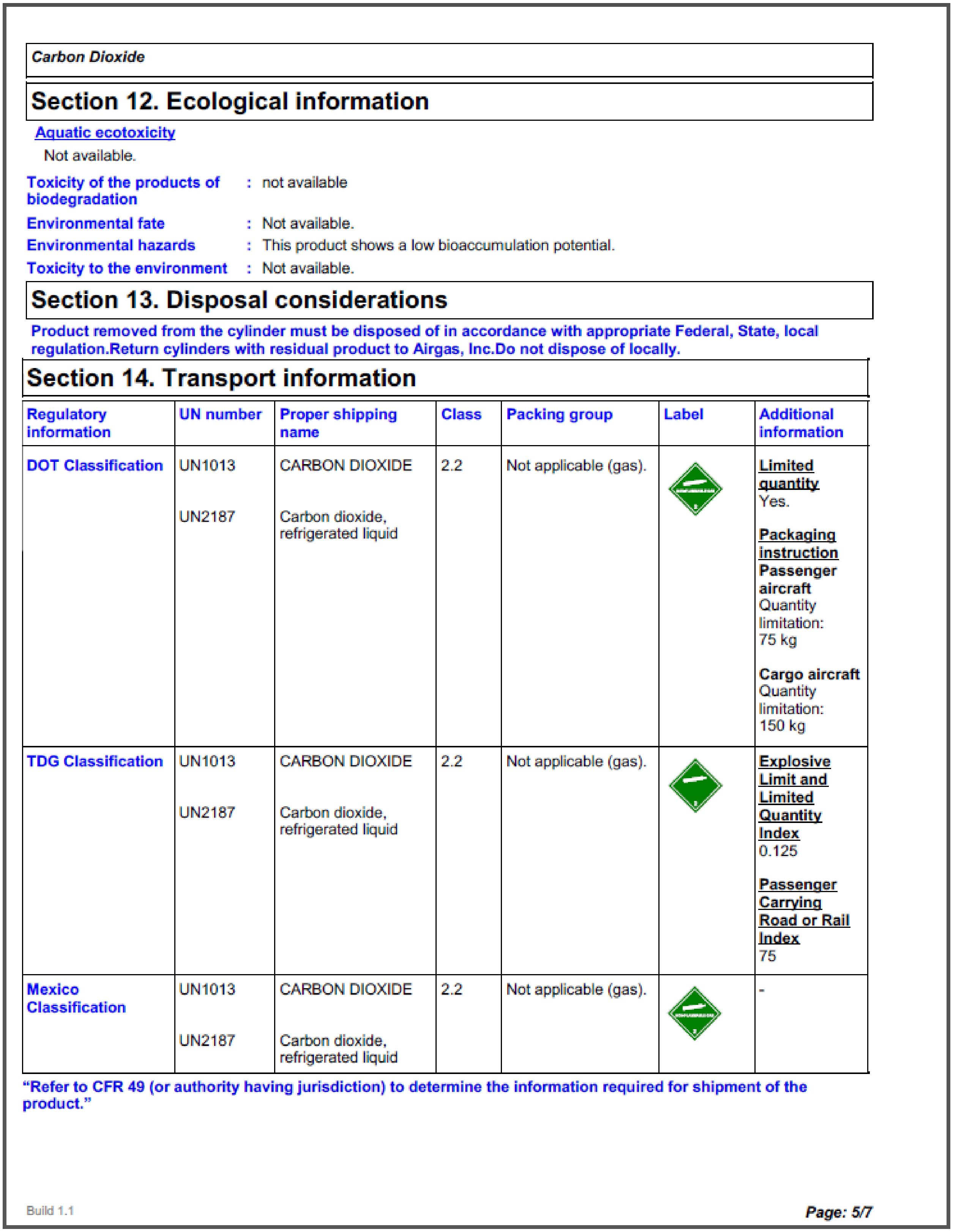

Carbon Dioxide

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Toxicity of the products of biodegradation : not available

Environmental fate : Not available.

Environmental hazards : This product shows a low bioaccumulation potential.

Toxicity to the environment : Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1013 UN2187	CARBON DIOXIDE Carbon dioxide, refrigerated liquid	2.2	Not applicable (gas).		**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: 75 kg **Cargo aircraft** Quantity limitation: 150 kg
TDG Classification	UN1013 UN2187	CARBON DIOXIDE Carbon dioxide, refrigerated liquid	2.2	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0.125 **Passenger Carrying Road or Rail Index** 75
Mexico Classification	UN1013 UN2187	CARBON DIOXIDE Carbon dioxide, refrigerated liquid	2.2	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

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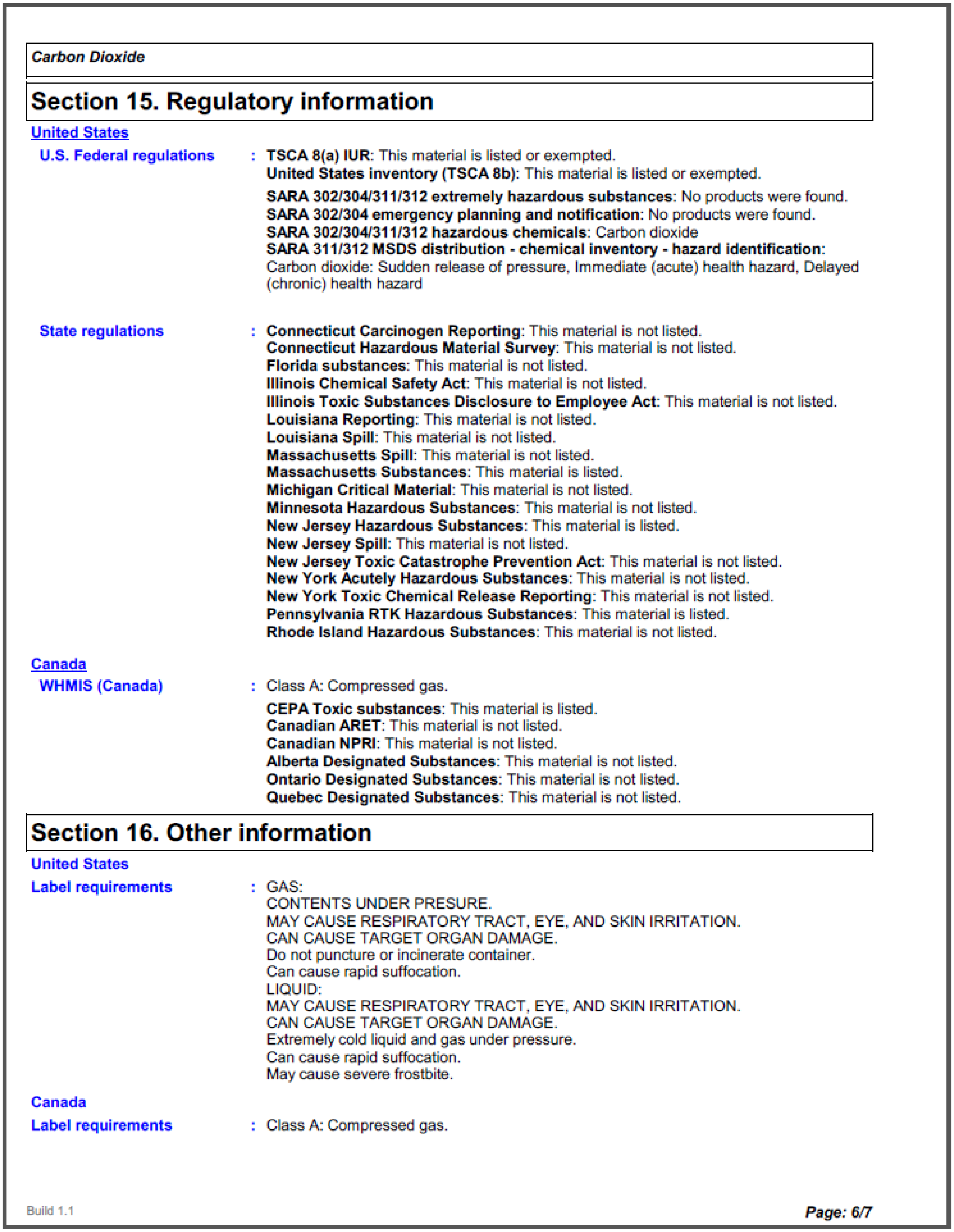

Carbon Dioxide

Section 15. Regulatory information

United States

U.S. Federal regulations : **TSCA 8(a) IUR**: This material is listed or exempted.
United States inventory (TSCA 8b): This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: Carbon dioxide
SARA 311/312 MSDS distribution - chemical inventory - hazard identification:
Carbon dioxide: Sudden release of pressure, Immediate (acute) health hazard, Delayed (chronic) health hazard

State regulations : **Connecticut Carcinogen Reporting**: This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada) : Class A: Compressed gas.

CEPA Toxic substances: This material is listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is not listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

United States

Label requirements : GAS:
CONTENTS UNDER PRESURE.
MAY CAUSE RESPIRATORY TRACT, EYE, AND SKIN IRRITATION.
CAN CAUSE TARGET ORGAN DAMAGE.
Do not puncture or incinerate container.
Can cause rapid suffocation.
LIQUID:
MAY CAUSE RESPIRATORY TRACT, EYE, AND SKIN IRRITATION.
CAN CAUSE TARGET ORGAN DAMAGE.
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.

Canada

Label requirements : Class A: Compressed gas.

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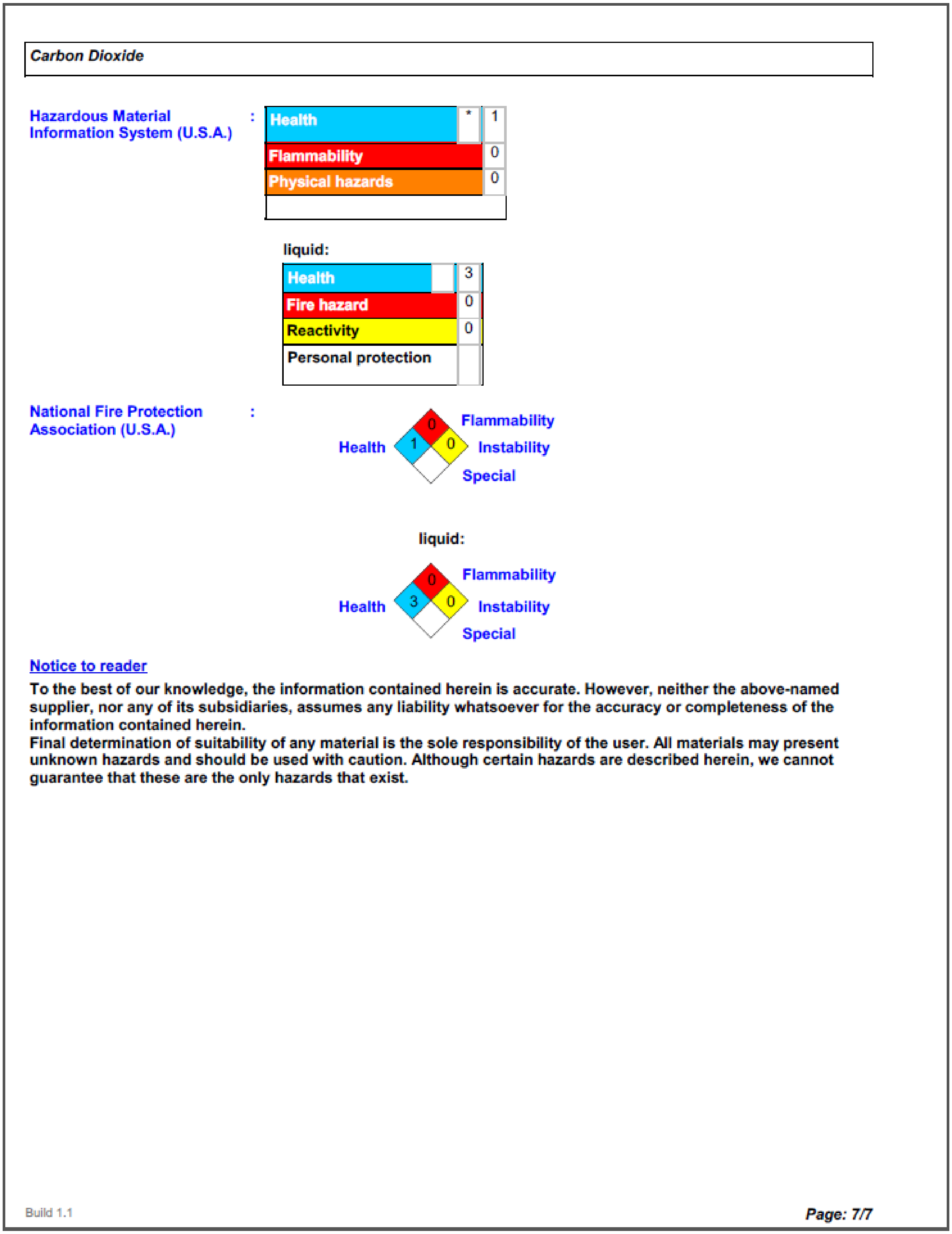

Carbon Dioxide

Hazardous Material Information System (U.S.A.) :

Health	*	1
Flammability		0
Physical hazards		0

liquid:

Health		3
Fire hazard		0
Reactivity		0
Personal protection		

National Fire Protection Association (U.S.A.) :

liquid:

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

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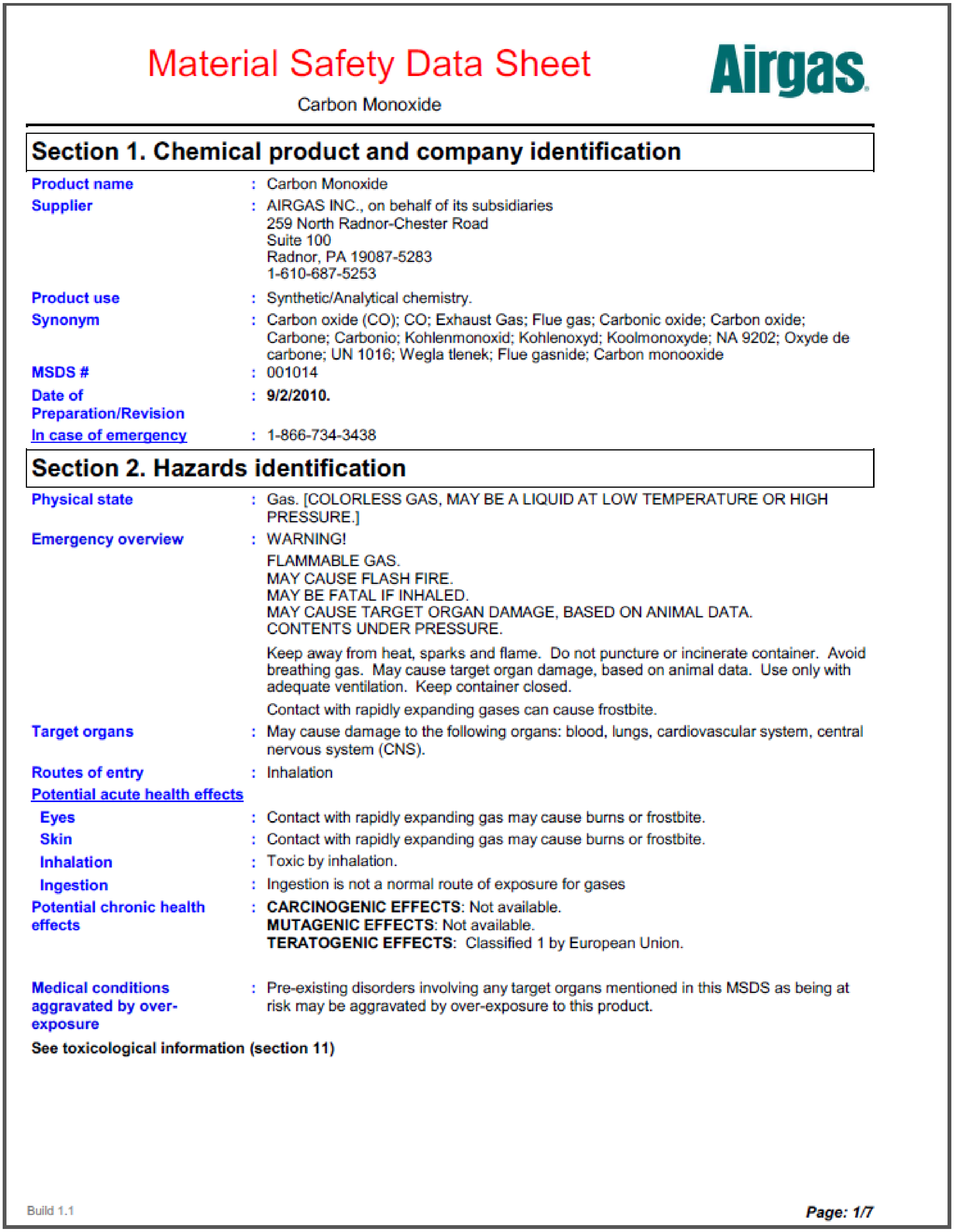

Material Safety Data Sheet

Carbon Monoxide

Section 1. Chemical product and company identification

Product name : Carbon Monoxide

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : Carbon oxide (CO); CO; Exhaust Gas; Flue gas; Carbonic oxide; Carbon oxide; Carbone; Carbonio; Kohlenmonoxid; Kohlenoxyd; Koolmonoxyde; NA 9202; Oxyde de carbone; UN 1016; Wegla tlenek; Flue gasnide; Carbon monooxide

MSDS # : 001014

Date of Preparation/Revision : **9/2/2010.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas. [COLORLESS GAS, MAY BE A LIQUID AT LOW TEMPERATURE OR HIGH PRESSURE.]

Emergency overview : WARNING!

FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
MAY BE FATAL IF INHALED.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.

Keep away from heat, sparks and flame. Do not puncture or incinerate container. Avoid breathing gas. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container closed.

Contact with rapidly expanding gases can cause frostbite.

Target organs : May cause damage to the following organs: blood, lungs, cardiovascular system, central nervous system (CNS).

Routes of entry : Inhalation

Potential acute health effects

- **Eyes** : Contact with rapidly expanding gas may cause burns or frostbite.
- **Skin** : Contact with rapidly expanding gas may cause burns or frostbite.
- **Inhalation** : Toxic by inhalation.
- **Ingestion** : Ingestion is not a normal route of exposure for gases

Potential chronic health effects : **CARCINOGENIC EFFECTS**: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Classified 1 by European Union.

Medical conditions aggravated by over-exposure : Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (section 11)

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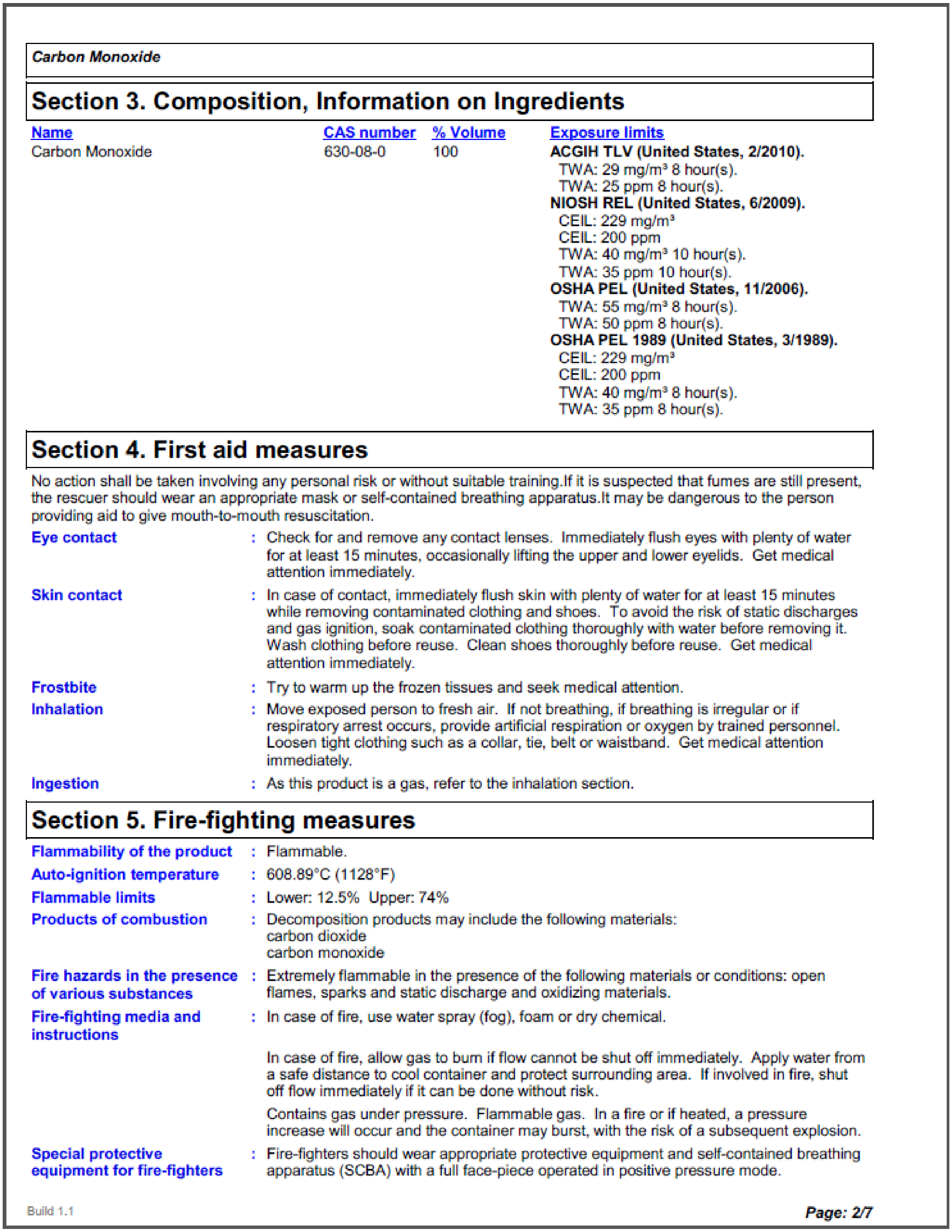

Carbon Monoxide

Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Carbon Monoxide	630-08-0	100	**ACGIH TLV (United States, 2/2010).** TWA: 29 mg/m^3 8 hour(s). TWA: 25 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** CEIL: 229 mg/m^3 CEIL: 200 ppm TWA: 40 mg/m^3 10 hour(s). TWA: 35 ppm 10 hour(s). **OSHA PEL (United States, 11/2006).** TWA: 55 mg/m^3 8 hour(s). TWA: 50 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** CEIL: 229 mg/m^3 CEIL: 200 ppm TWA: 40 mg/m^3 8 hour(s). TWA: 35 ppm 8 hour(s).

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 608.89°C (1128°F)

Flammable limits : Lower: 12.5% Upper: 74%

Products of combustion : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Fire hazards in the presence of various substances : Extremely flammable in the presence of the following materials or conditions: open flames, sparks and static discharge and oxidizing materials.

Fire-fighting media and instructions : In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

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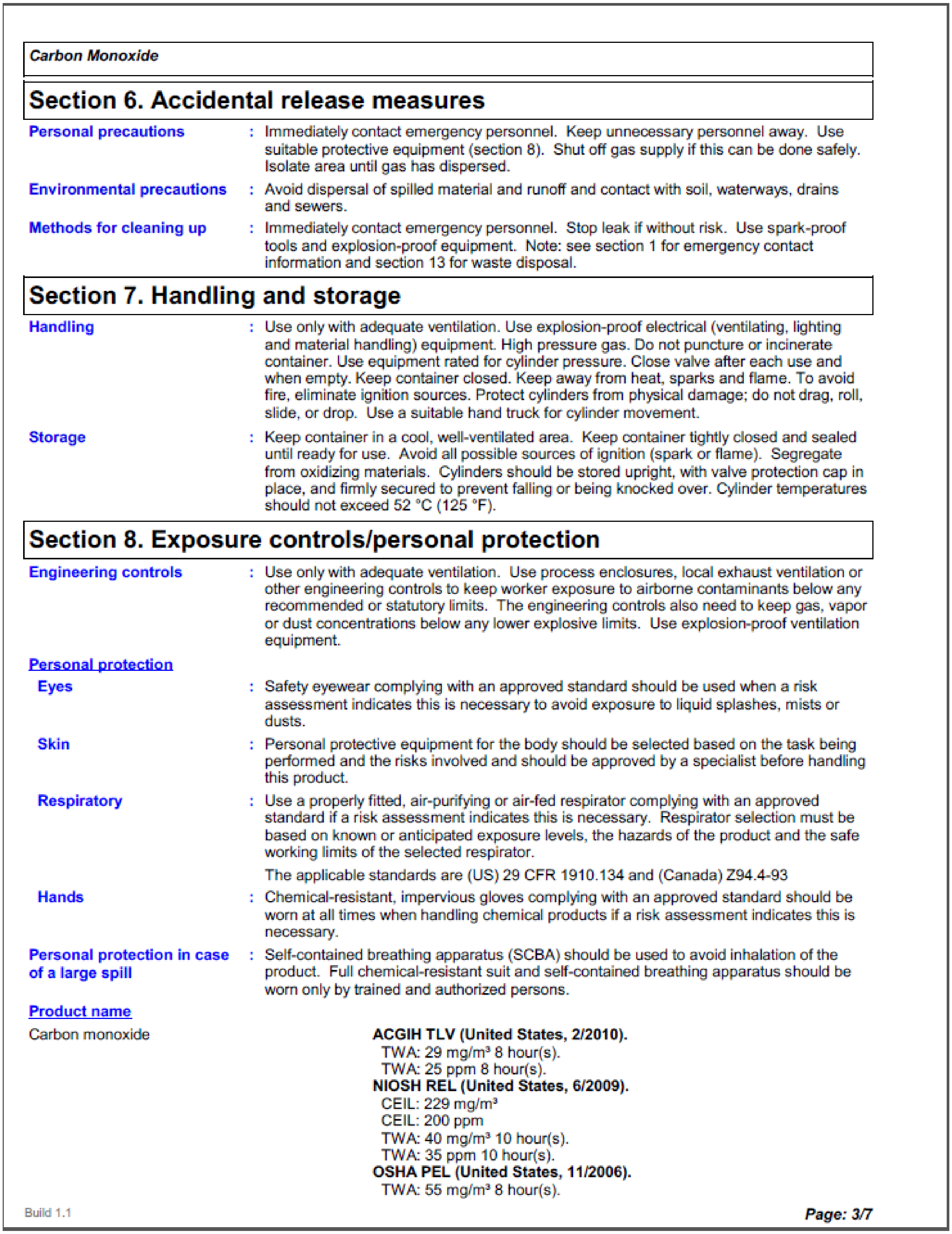


Carbon Monoxide

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Storage : Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

Section 8. Exposure controls/personal protection

Engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

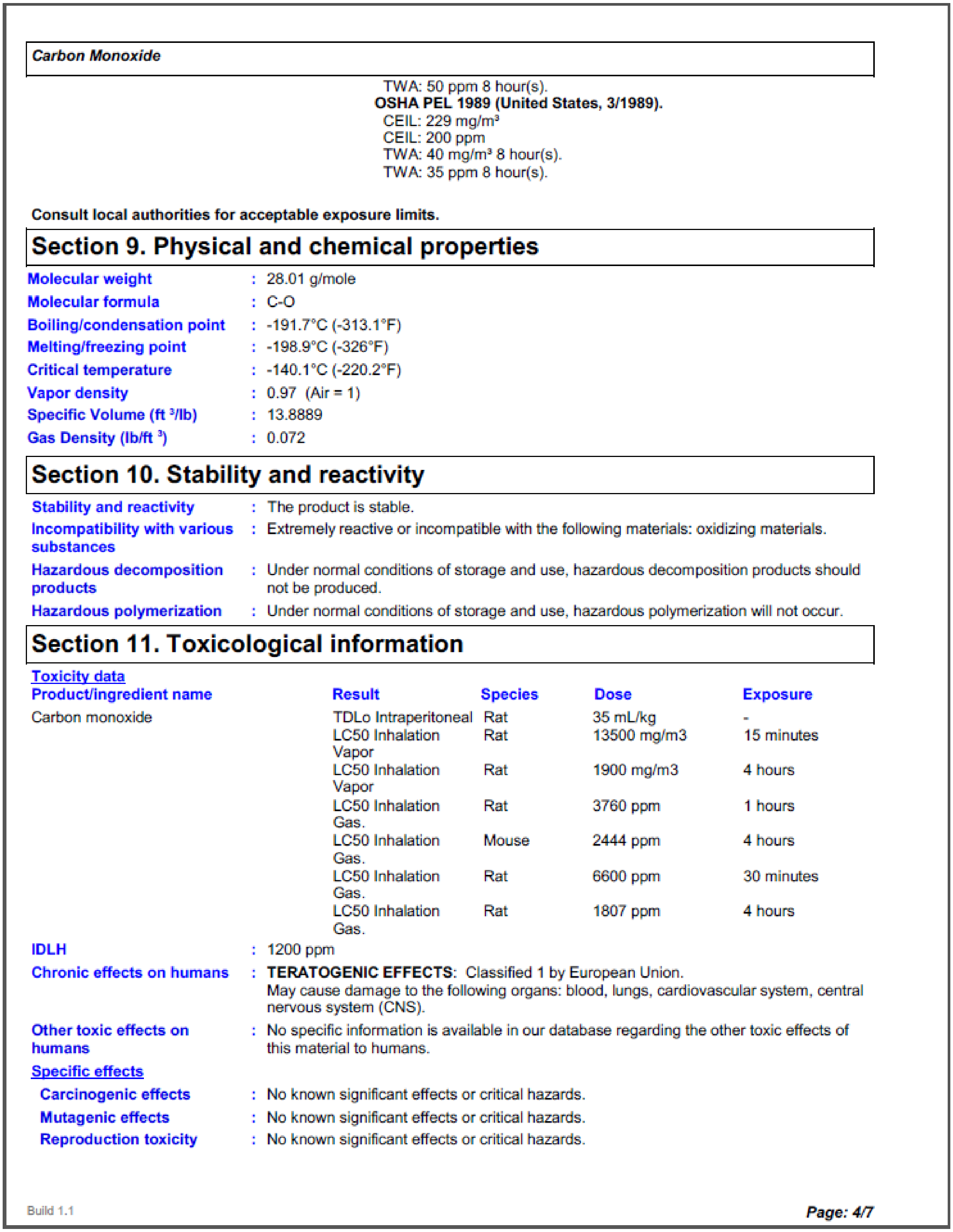
Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product. Full chemical-resistant suit and self-contained breathing apparatus should be worn only by trained and authorized persons.

Product name	
Carbon monoxide	**ACGIH TLV (United States, 2/2010).** TWA: 29 mg/m³ 8 hour(s). TWA: 25 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** CEIL: 229 mg/m³ CEIL: 200 ppm TWA: 40 mg/m³ 10 hour(s). TWA: 35 ppm 10 hour(s). **OSHA PEL (United States, 11/2006).** TWA: 55 mg/m³ 8 hour(s).



Carbon Monoxide

TWA: 50 ppm 8 hour(s).
OSHA PEL 1989 (United States, 3/1989).
CEIL: 229 mg/m^3
CEIL: 200 ppm
TWA: 40 mg/m^3 8 hour(s).
TWA: 35 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight	: 28.01 g/mole
Molecular formula	: C-O
Boiling/condensation point	: -191.7°C (-313.1°F)
Melting/freezing point	: -198.9°C (-326°F)
Critical temperature	: -140.1°C (-220.2°F)
Vapor density	: 0.97 (Air = 1)
Specific Volume (ft ^{3}/lb)	: 13.8889
Gas Density (lb/ft ^{3})	: 0.072

Section 10. Stability and reactivity

Stability and reactivity	: The product is stable.
Incompatibility with various substances	: Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products	: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization	: Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Product/ingredient name	**Result**	**Species**	**Dose**	**Exposure**
Carbon monoxide	TDLo Intraperitoneal	Rat	35 mL/kg	-
	LC50 Inhalation Vapor	Rat	13500 mg/m3	15 minutes
	LC50 Inhalation Vapor	Rat	1900 mg/m3	4 hours
	LC50 Inhalation Gas.	Rat	3760 ppm	1 hours
	LC50 Inhalation Gas.	Mouse	2444 ppm	4 hours
	LC50 Inhalation Gas.	Rat	6600 ppm	30 minutes
	LC50 Inhalation Gas.	Rat	1807 ppm	4 hours

IDLH	: 1200 ppm
Chronic effects on humans	: **TERATOGENIC EFFECTS**: Classified 1 by European Union. May cause damage to the following organs: blood, lungs, cardiovascular system, central nervous system (CNS).
Other toxic effects on humans	: No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects	: No known significant effects or critical hazards.
Mutagenic effects	: No known significant effects or critical hazards.
Reproduction toxicity	: No known significant effects or critical hazards.

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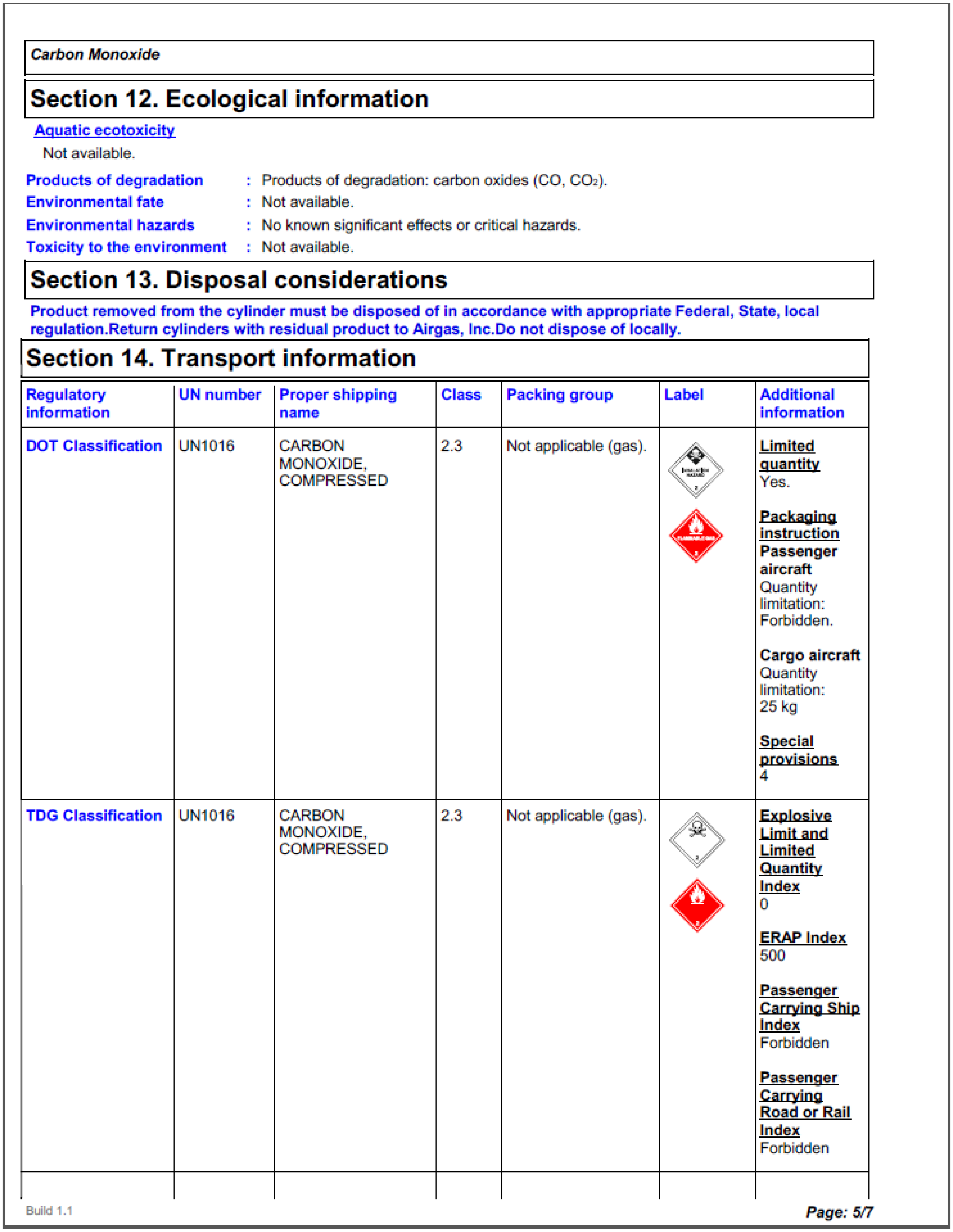


Section 12. Ecological information

Aquatic ecotoxicity

Not available.

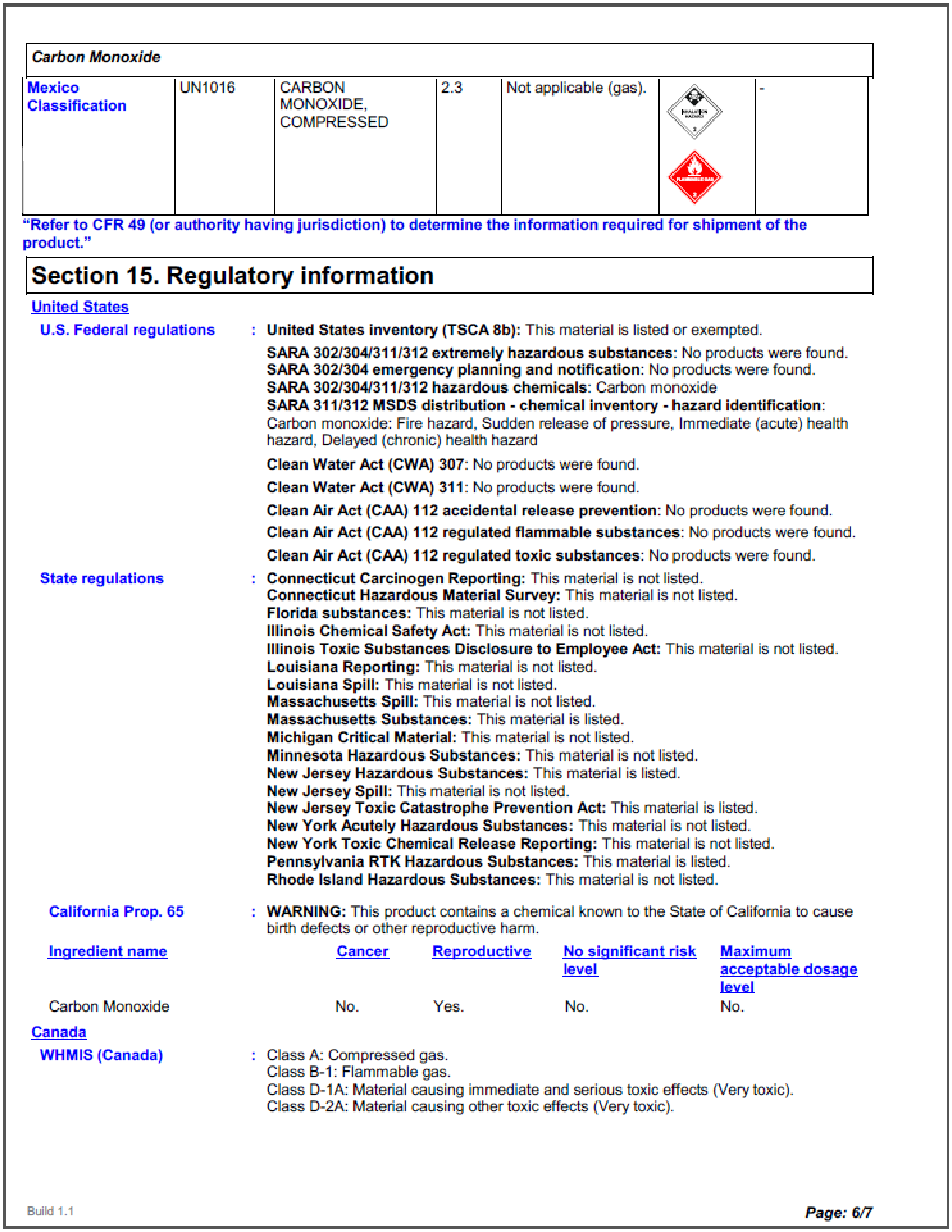
Products of degradation : Products of degradation: carbon oxides (CO, CO_2).
Environmental fate : Not available.
Environmental hazards : No known significant effects or critical hazards.
Toxicity to the environment : Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1016	CARBON MONOXIDE, COMPRESSED	2.3	Not applicable (gas).		**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: Forbidden. **Cargo aircraft** Quantity limitation: 25 kg **Special provisions** 4
TDG Classification	UN1016	CARBON MONOXIDE, COMPRESSED	2.3	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0 **ERAP Index** 500 **Passenger Carrying Ship Index** Forbidden **Passenger Carrying Road or Rail Index** Forbidden



Carbon Monoxide						
Mexico Classification	UN1016	CARBON MONOXIDE, COMPRESSED	2.3	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

U.S. Federal regulations : **United States inventory (TSCA 8b):** This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: Carbon monoxide
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Carbon monoxide: Fire hazard, Sudden release of pressure, Immediate (acute) health hazard, Delayed (chronic) health hazard

Clean Water Act (CWA) 307: No products were found.

Clean Water Act (CWA) 311: No products were found.

Clean Air Act (CAA) 112 accidental release prevention: No products were found.

Clean Air Act (CAA) 112 regulated flammable substances: No products were found.

Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

State regulations : **Connecticut Carcinogen Reporting:** This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

California Prop. 65 : **WARNING:** This product contains a chemical known to the State of California to cause birth defects or other reproductive harm.

Ingredient name	**Cancer**	**Reproductive**	**No significant risk level**	**Maximum acceptable dosage level**
Carbon Monoxide	No.	Yes.	No.	No.

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class B-1: Flammable gas.
Class D-1A: Material causing immediate and serious toxic effects (Very toxic).
Class D-2A: Material causing other toxic effects (Very toxic).

Build 1.1

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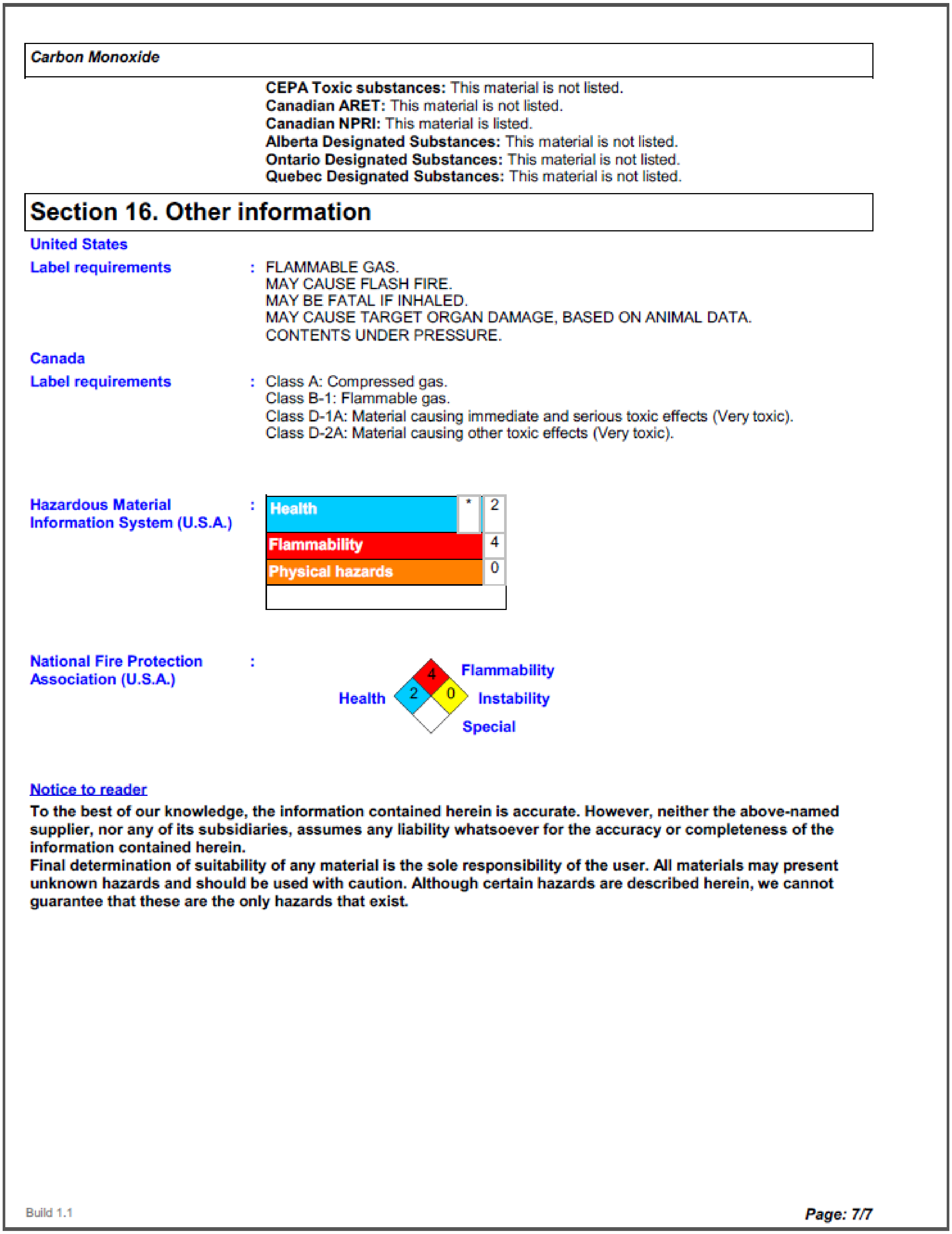


Carbon Monoxide

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

United States

Label requirements : FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
MAY BE FATAL IF INHALED.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.

Canada

Label requirements : Class A: Compressed gas.
Class B-1: Flammable gas.
Class D-1A: Material causing immediate and serious toxic effects (Very toxic).
Class D-2A: Material causing other toxic effects (Very toxic).

Hazardous Material Information System (U.S.A.) :

Health	*	2
Flammability		4
Physical hazards		0

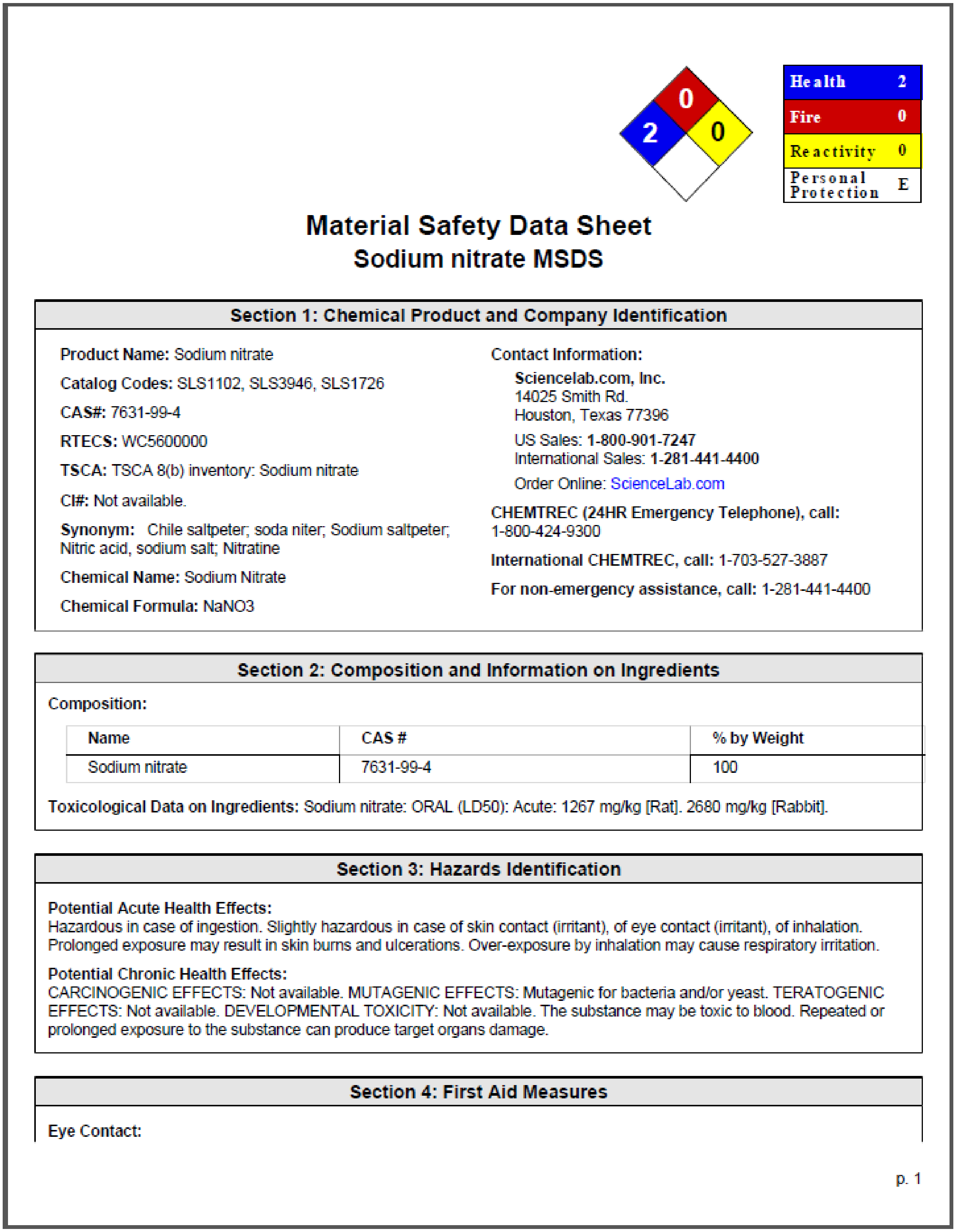
National Fire Protection Association (U.S.A.) :

Flammability 4
Health 2
Instability 0
Special

Notice to reader

Build 1.1

Page: 7/7



Health	2
Fire	0
Reactivity	0
Personal Protection	E

Material Safety Data Sheet
Sodium nitrate MSDS

Section 1: Chemical Product and Company Identification

Product Name: Sodium nitrate

Catalog Codes: SLS1102, SLS3946, SLS1726

CAS#: 7631-99-4

RTECS: WC5600000

TSCA: TSCA 8(b) inventory: Sodium nitrate

CI#: Not available.

Synonym: Chile saltpeter; soda niter; Sodium saltpeter; Nitric acid, sodium salt; Nitratine

Chemical Name: Sodium Nitrate

Chemical Formula: NaNO3

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Sodium nitrate	7631-99-4	100

Toxicological Data on Ingredients: Sodium nitrate: ORAL (LD50): Acute: 1267 mg/kg [Rat]. 2680 mg/kg [Rabbit].

Section 3: Hazards Identification

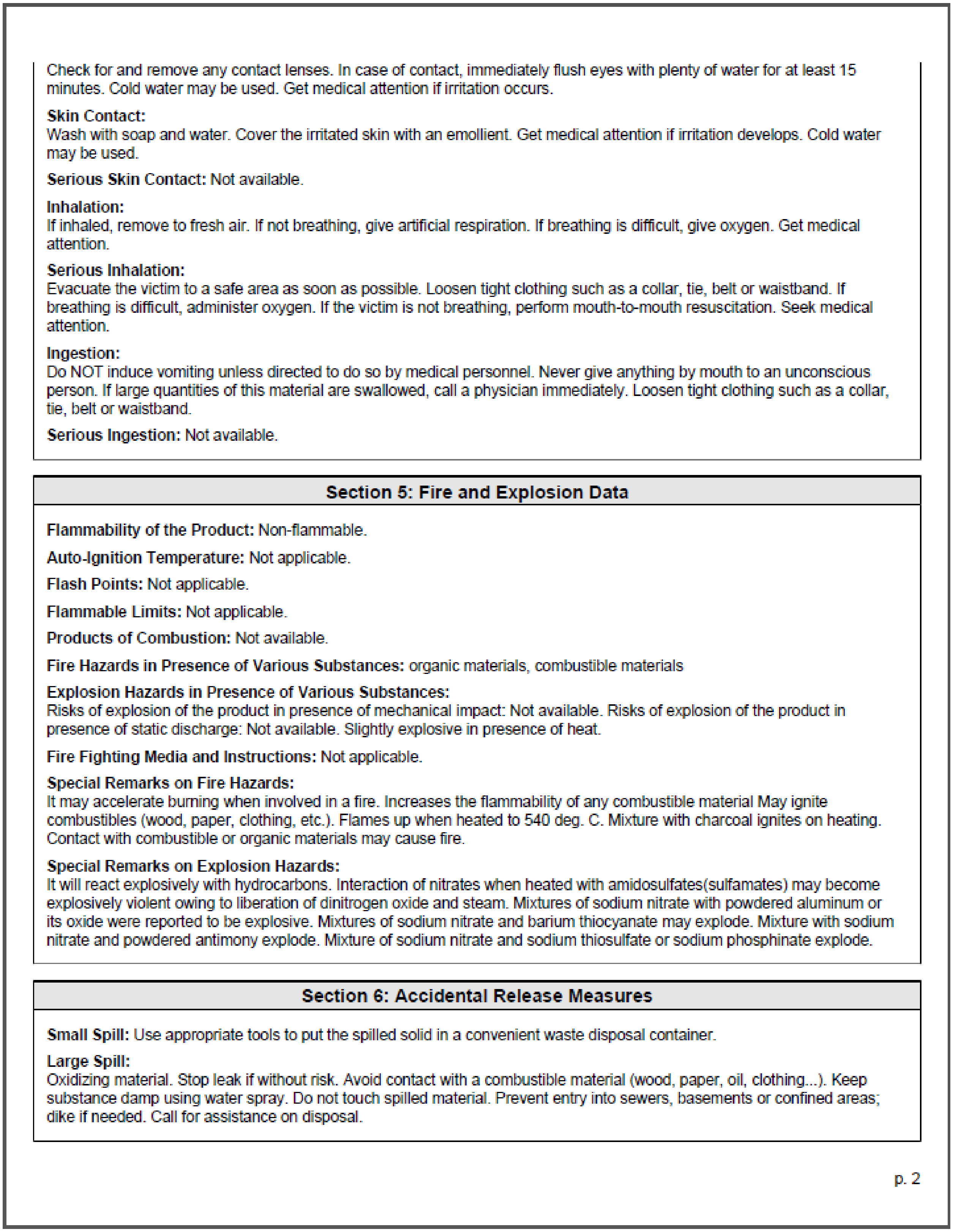
Potential Acute Health Effects:
Hazardous in case of ingestion. Slightly hazardous in case of skin contact (irritant), of eye contact (irritant), of inhalation. Prolonged exposure may result in skin burns and ulcerations. Over-exposure by inhalation may cause respiratory irritation.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to blood. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:

p. 1



Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention if irritation occurs.

Skin Contact:
Wash with soap and water. Cover the irritated skin with an emollient. Get medical attention if irritation develops. Cold water may be used.

Serious Skin Contact: Not available.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

Fire Hazards in Presence of Various Substances: organic materials, combustible materials

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available. Slightly explosive in presence of heat.

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards:
It may accelerate burning when involved in a fire. Increases the flammability of any combustible material May ignite combustibles (wood, paper, clothing, etc.). Flames up when heated to 540 deg. C. Mixture with charcoal ignites on heating. Contact with combustible or organic materials may cause fire.

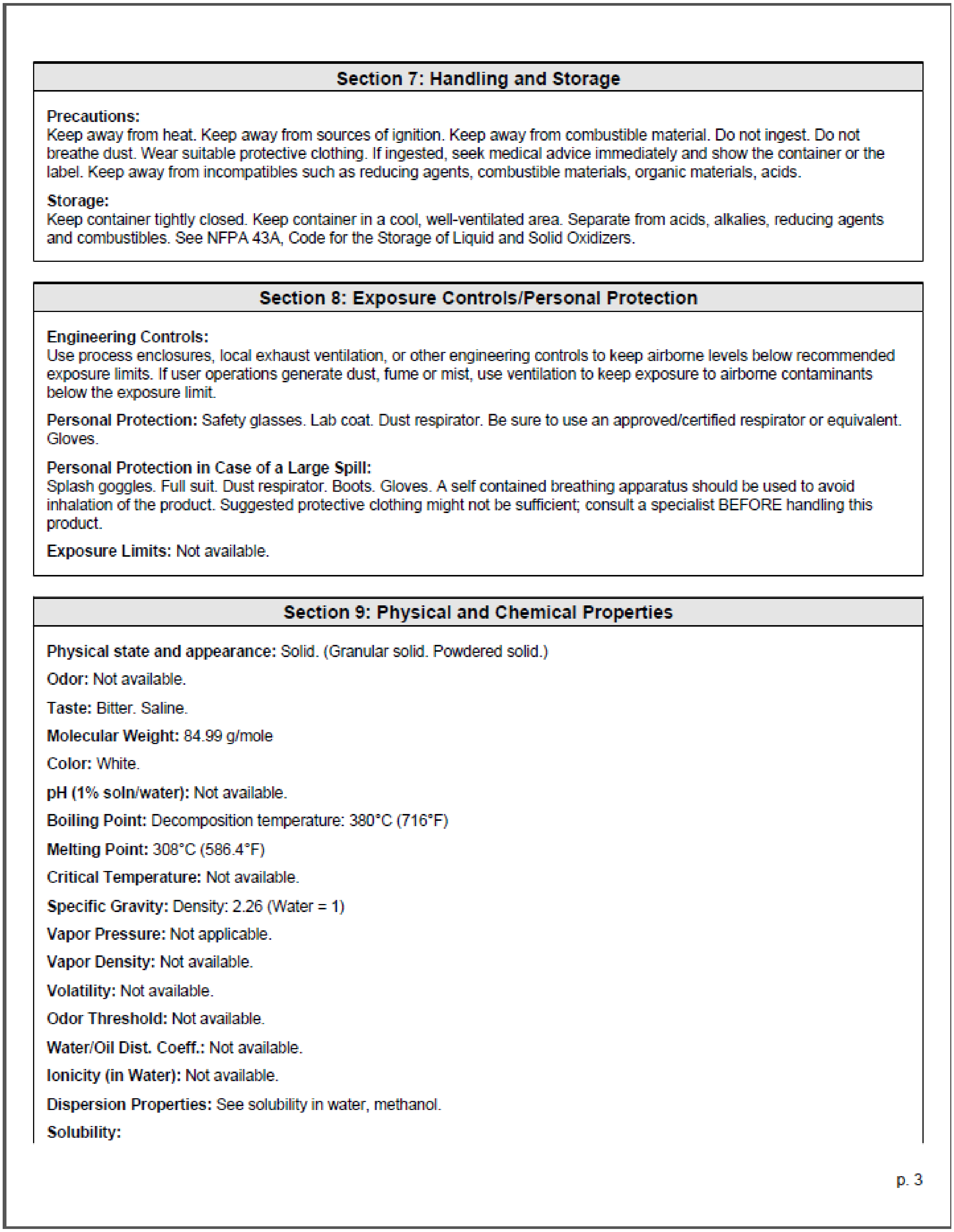
Special Remarks on Explosion Hazards:
It will react explosively with hydrocarbons. Interaction of nitrates when heated with amidosulfates(sulfamates) may become explosively violent owing to liberation of dinitrogen oxide and steam. Mixtures of sodium nitrate with powdered aluminum or its oxide were reported to be explosive. Mixtures of sodium nitrate and barium thiocyanate may explode. Mixture with sodium nitrate and powdered antimony explode. Mixture of sodium nitrate and sodium thiosulfate or sodium phosphinate explode.

Section 6: Accidental Release Measures

Small Spill: Use appropriate tools to put the spilled solid in a convenient waste disposal container.

Large Spill:
Oxidizing material. Stop leak if without risk. Avoid contact with a combustible material (wood, paper, oil, clothing...). Keep substance damp using water spray. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal.

p. 2



Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Keep away from combustible material. Do not ingest. Do not breathe dust. Wear suitable protective clothing. If ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibles such as reducing agents, combustible materials, organic materials, acids.

Storage:
Keep container tightly closed. Keep container in a cool, well-ventilated area. Separate from acids, alkalies, reducing agents and combustibles. See NFPA 43A, Code for the Storage of Liquid and Solid Oxidizers.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection: Safety glasses. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid. (Granular solid. Powdered solid.)

Odor: Not available.

Taste: Bitter. Saline.

Molecular Weight: 84.99 g/mole

Color: White.

pH (1% soln/water): Not available.

Boiling Point: Decomposition temperature: 380°C (716°F)

Melting Point: 308°C (586.4°F)

Critical Temperature: Not available.

Specific Gravity: Density: 2.26 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

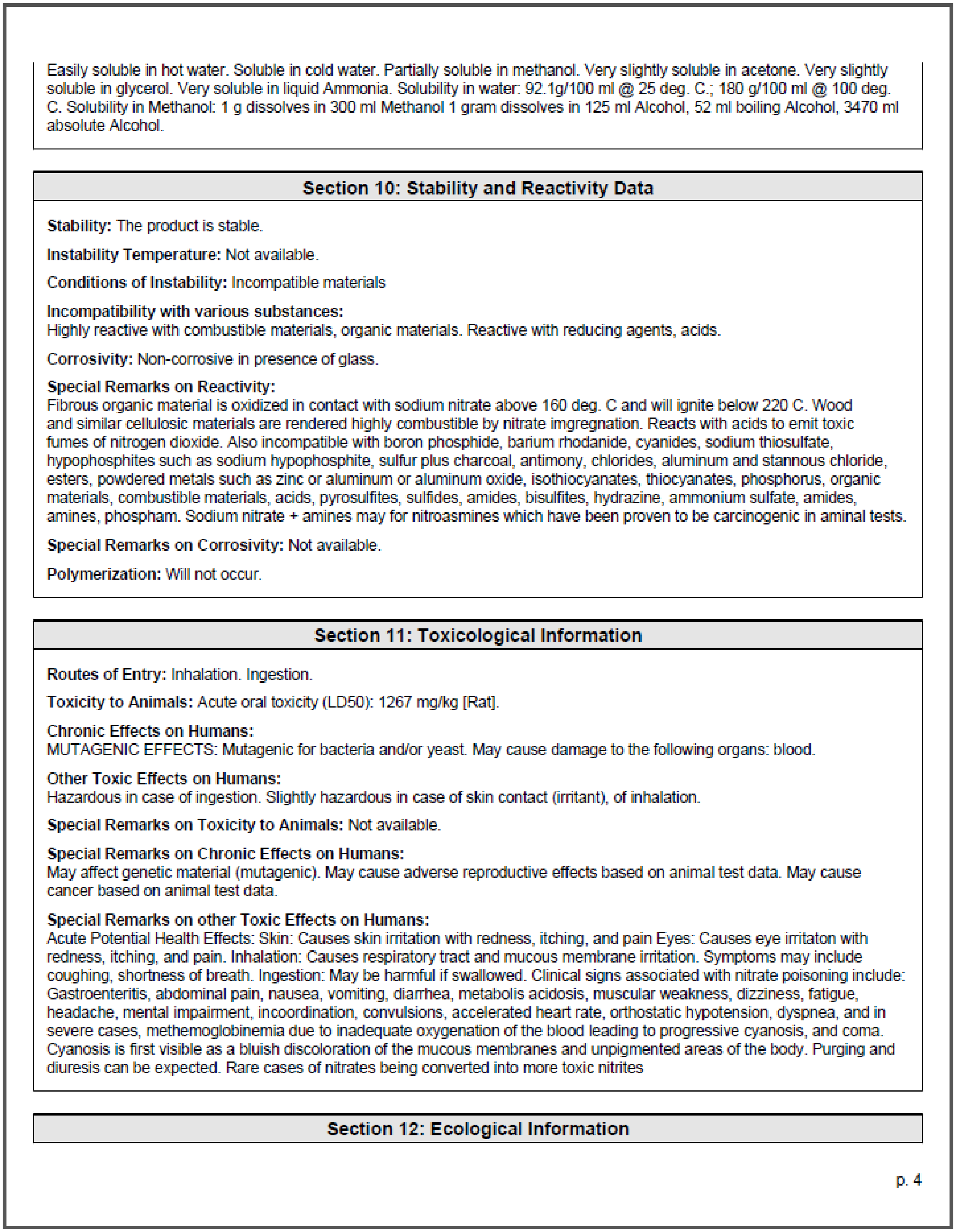
Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, methanol.

Solubility:

p. 3



Easily soluble in hot water. Soluble in cold water. Partially soluble in methanol. Very slightly soluble in acetone. Very slightly soluble in glycerol. Very soluble in liquid Ammonia. Solubility in water: 92.1g/100 ml @ 25 deg. C.; 180 g/100 ml @ 100 deg. C. Solubility in Methanol: 1 g dissolves in 300 ml Methanol 1 gram dissolves in 125 ml Alcohol, 52 ml boiling Alcohol, 3470 ml absolute Alcohol.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Incompatible materials

Incompatibility with various substances:
Highly reactive with combustible materials, organic materials. Reactive with reducing agents, acids.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Fibrous organic material is oxidized in contact with sodium nitrate above 160 deg. C and will ignite below 220 C. Wood and similar cellulosic materials are rendered highly combustible by nitrate imgregnation. Reacts with acids to emit toxic fumes of nitrogen dioxide. Also incompatible with boron phosphide, barium rhodanide, cyanides, sodium thiosulfate, hypophosphites such as sodium hypophosphite, sulfur plus charcoal, antimony, chlorides, aluminum and stannous chloride, esters, powdered metals such as zinc or aluminum or aluminum oxide, isothiocyanates, thiocyanates, phosphorus, organic materials, combustible materials, acids, pyrosulfites, sulfides, amides, bisulfites, hydrazine, ammonium sulfate, amides, amines, phospham. Sodium nitrate + amines may for nitroasmines which have been proven to be carcinogenic in aminal tests.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Inhalation. Ingestion.

Toxicity to Animals: Acute oral toxicity (LD50): 1267 mg/kg [Rat].

Chronic Effects on Humans:
MUTAGENIC EFFECTS: Mutagenic for bacteria and/or yeast. May cause damage to the following organs: blood.

Other Toxic Effects on Humans:
Hazardous in case of ingestion. Slightly hazardous in case of skin contact (irritant), of inhalation.

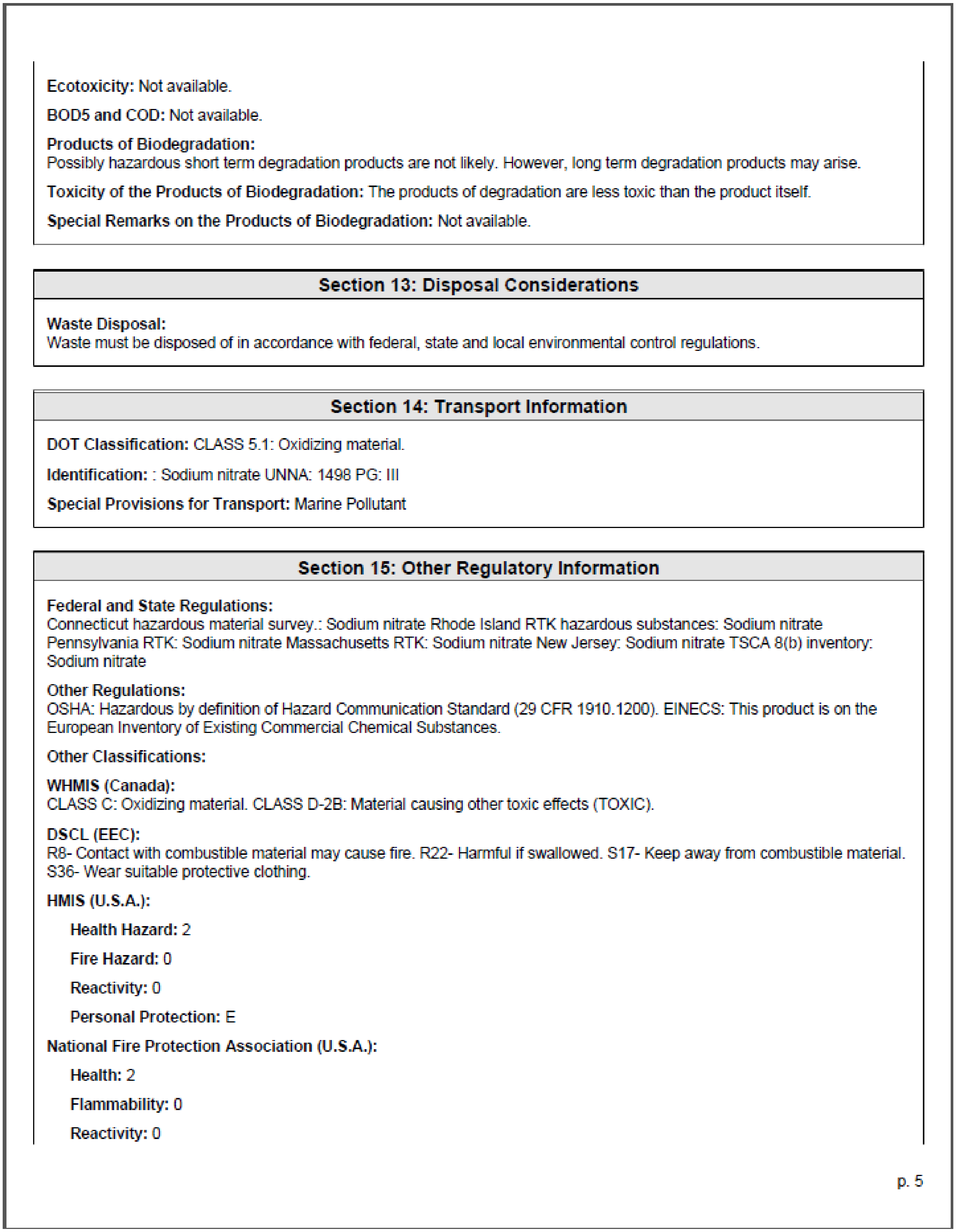
Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May affect genetic material (mutagenic). May cause adverse reproductive effects based on animal test data. May cause cancer based on animal test data.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes skin irritation with redness, itching, and pain Eyes: Causes eye irritaton with redness, itching, and pain. Inhalation: Causes respiratory tract and mucous membrane irritation. Symptoms may include coughing, shortness of breath. Ingestion: May be harmful if swallowed. Clinical signs associated with nitrate poisoning include: Gastroenteritis, abdominal pain, nausea, vomiting, diarrhea, metabolis acidosis, muscular weakness, dizziness, fatigue, headache, mental impairment, incoordination, convulsions, accelerated heart rate, orthostatic hypotension, dyspnea, and in severe cases, methemoglobinemia due to inadequate oxygenation of the blood leading to progressive cyanosis, and coma. Cyanosis is first visible as a bluish discoloration of the mucous membranes and unpigmented areas of the body. Purging and diuresis can be expected. Rare cases of nitrates being converted into more toxic nitrites

Section 12: Ecological Information

p. 4



Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 5.1: Oxidizing material.

Identification: : Sodium nitrate UNNA: 1498 PG: III

Special Provisions for Transport: Marine Pollutant

Section 15: Other Regulatory Information

Federal and State Regulations:
Connecticut hazardous material survey.: Sodium nitrate Rhode Island RTK hazardous substances: Sodium nitrate Pennsylvania RTK: Sodium nitrate Massachusetts RTK: Sodium nitrate New Jersey: Sodium nitrate TSCA 8(b) inventory: Sodium nitrate

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS C: Oxidizing material. CLASS D-2B: Material causing other toxic effects (TOXIC).

DSCL (EEC):
R8- Contact with combustible material may cause fire. R22- Harmful if swallowed. S17- Keep away from combustible material. S36- Wear suitable protective clothing.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 0

Reactivity: 0

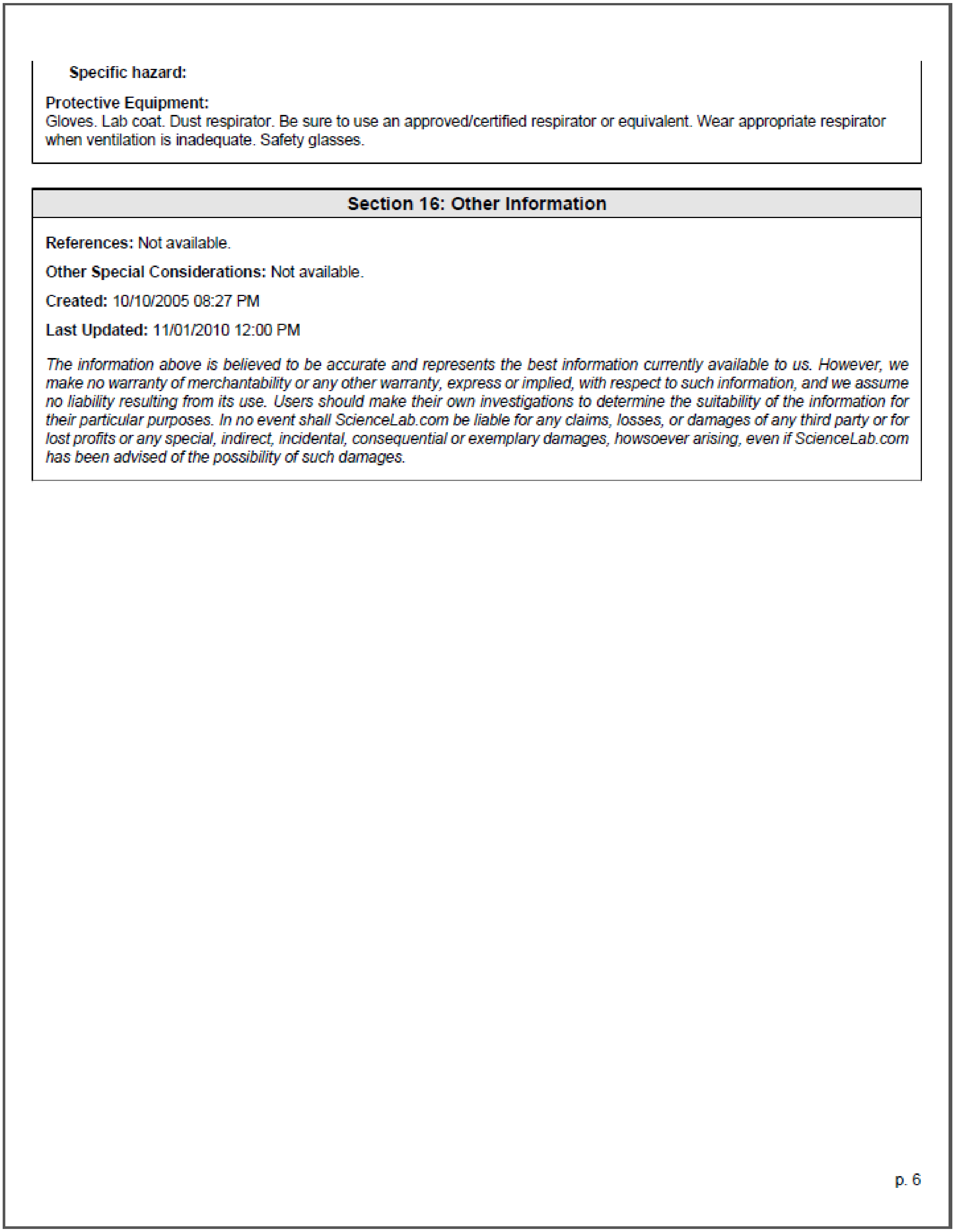
Personal Protection: E

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 0

Reactivity: 0



Specific hazard:

Protective Equipment:
Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Safety glasses.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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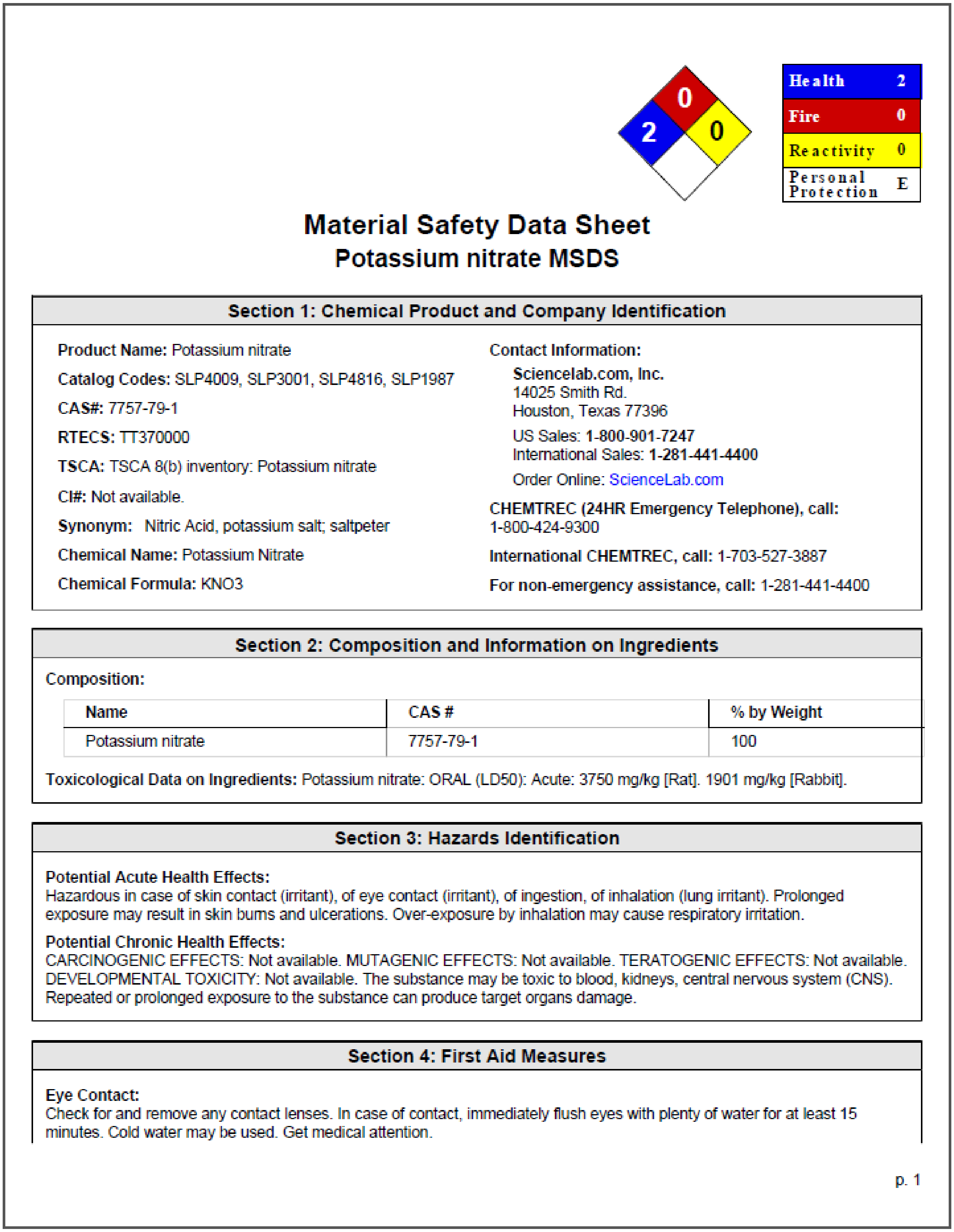

Health	2
Fire	0
Reactivity	0
Personal Protection	E

Material Safety Data Sheet
Potassium nitrate MSDS

Section 1: Chemical Product and Company Identification

Product Name: Potassium nitrate

Catalog Codes: SLP4009, SLP3001, SLP4816, SLP1987

CAS#: 7757-79-1

RTECS: TT370000

TSCA: TSCA 8(b) inventory: Potassium nitrate

CI#: Not available.

Synonym: Nitric Acid, potassium salt; saltpeter

Chemical Name: Potassium Nitrate

Chemical Formula: KNO3

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Potassium nitrate	7757-79-1	100

Toxicological Data on Ingredients: Potassium nitrate: ORAL (LD50): Acute: 3750 mg/kg [Rat]. 1901 mg/kg [Rabbit].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, of inhalation (lung irritant). Prolonged exposure may result in skin burns and ulcerations. Over-exposure by inhalation may cause respiratory irritation.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to blood, kidneys, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention.

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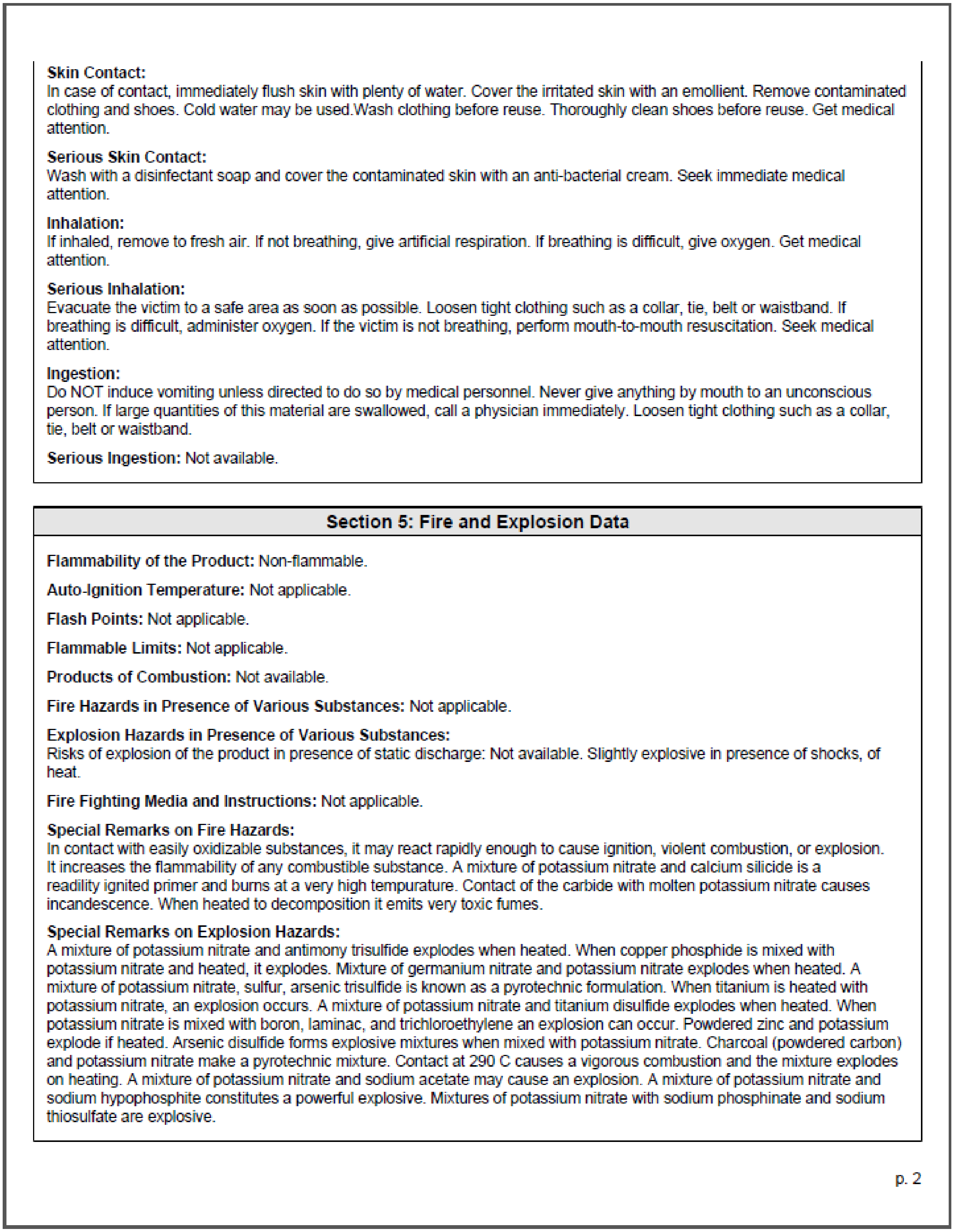


Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Cold water may be used.Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

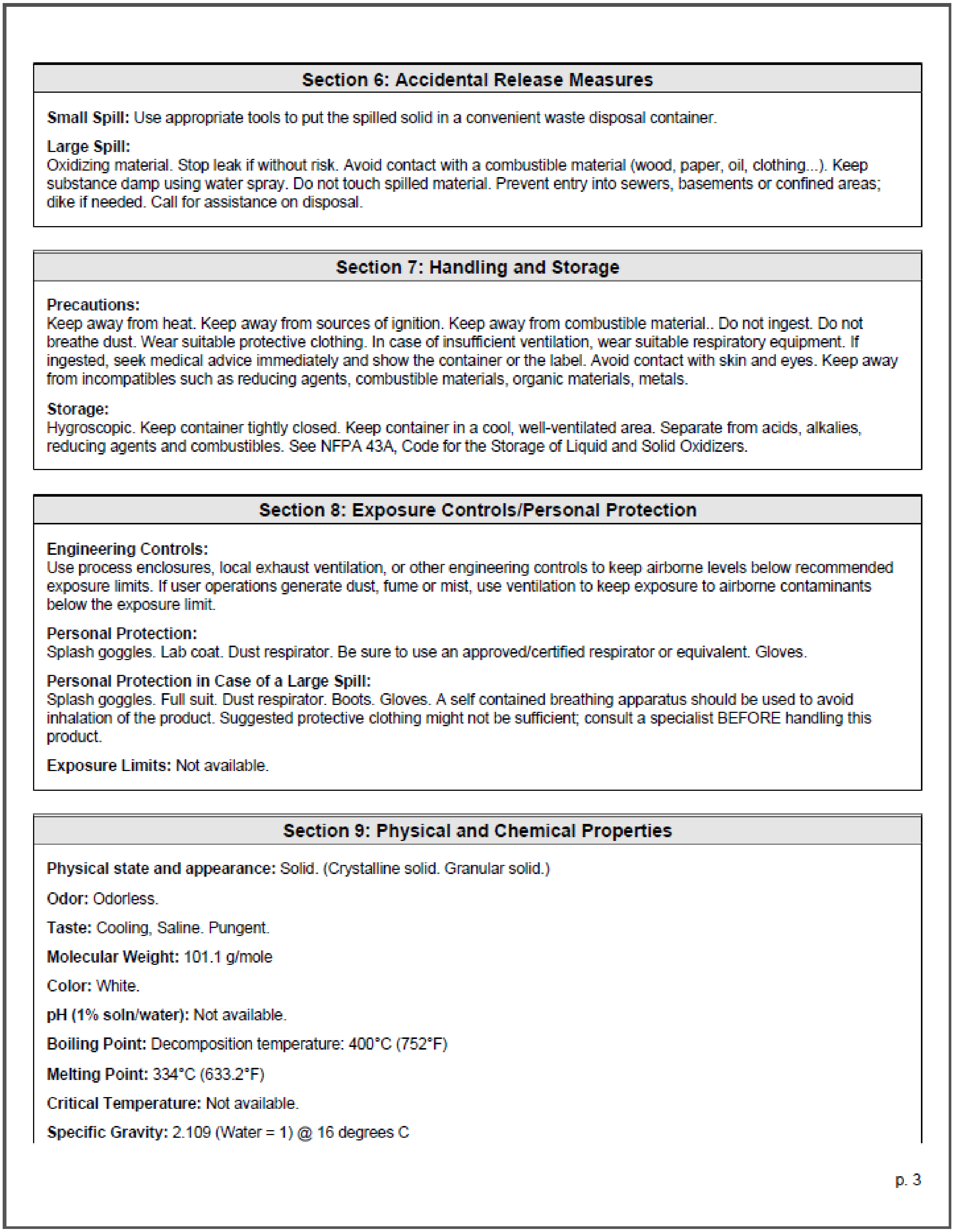
Fire Hazards in Presence of Various Substances: Not applicable.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of static discharge: Not available. Slightly explosive in presence of shocks, of heat.

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards:
In contact with easily oxidizable substances, it may react rapidly enough to cause ignition, violent combustion, or explosion. It increases the flammability of any combustible substance. A mixture of potassium nitrate and calcium silicide is a readility ignited primer and burns at a very high tempurature. Contact of the carbide with molten potassium nitrate causes incandescence. When heated to decomposition it emits very toxic fumes.

Special Remarks on Explosion Hazards:
A mixture of potassium nitrate and antimony trisulfide explodes when heated. When copper phosphide is mixed with potassium nitrate and heated, it explodes. Mixture of germanium nitrate and potassium nitrate explodes when heated. A mixture of potassium nitrate, sulfur, arsenic trisulfide is known as a pyrotechnic formulation. When titanium is heated with potassium nitrate, an explosion occurs. A mixture of potassium nitrate and titanium disulfide explodes when heated. When potassium nitrate is mixed with boron, laminac, and trichloroethylene an explosion can occur. Powdered zinc and potassium explode if heated. Arsenic disulfide forms explosive mixtures when mixed with potassium nitrate. Charcoal (powdered carbon) and potassium nitrate make a pyrotechnic mixture. Contact at 290 C causes a vigorous combustion and the mixture explodes on heating. A mixture of potassium nitrate and sodium acetate may cause an explosion. A mixture of potassium nitrate and sodium hypophosphite constitutes a powerful explosive. Mixtures of potassium nitrate with sodium phosphinate and sodium thiosulfate are explosive.



Section 6: Accidental Release Measures

Small Spill: Use appropriate tools to put the spilled solid in a convenient waste disposal container.

Large Spill:
Oxidizing material. Stop leak if without risk. Avoid contact with a combustible material (wood, paper, oil, clothing...). Keep substance damp using water spray. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal.

Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Keep away from combustible material.. Do not ingest. Do not breathe dust. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as reducing agents, combustible materials, organic materials, metals.

Storage:
Hygroscopic. Keep container tightly closed. Keep container in a cool, well-ventilated area. Separate from acids, alkalies, reducing agents and combustibles. See NFPA 43A, Code for the Storage of Liquid and Solid Oxidizers.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid. (Crystalline solid. Granular solid.)

Odor: Odorless.

Taste: Cooling, Saline. Pungent.

Molecular Weight: 101.1 g/mole

Color: White.

pH (1% soln/water): Not available.

Boiling Point: Decomposition temperature: 400°C (752°F)

Melting Point: 334°C (633.2°F)

Critical Temperature: Not available.

Specific Gravity: 2.109 (Water = 1) @ 16 degrees C

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water.

Solubility:
Easily soluble in hot water. Soluble in cold water. Insoluble in diethyl ether. Soluble in liquid ammonia, glycerin, and absolute alcohol. Solubility in water: 1g/2.8 ml water @ 25 C.; 13.3 g/100 ml water @ 0 C; 1g/0.5 ml boiling water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Incompatible materials, dust generation

Incompatibility with various substances: Reactive with reducing agents, combustible materials, organic materials, metals.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Hygroscopic; keep container tightly closed. Potassium nitrate reacts vigorously when heated with sulfides of the alkaline earth group including barium sulfide and calcium sulfide. Also incompatible with boron, and finely powdered metals, chromium nitride, aluminum, titanium, anitimony, germanium, zinc, zirconium, calcium disilicide, metal sulfides, carbon, sulfur, phosphorus, phosphides, sodium phosphinate, sodium thiosulfate, citric acid, tin chloride, sodium acetate, throium carbide.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Inhalation. Ingestion.

Toxicity to Animals: Acute oral toxicity (LD50): 1901 mg/kg [Rabbit].

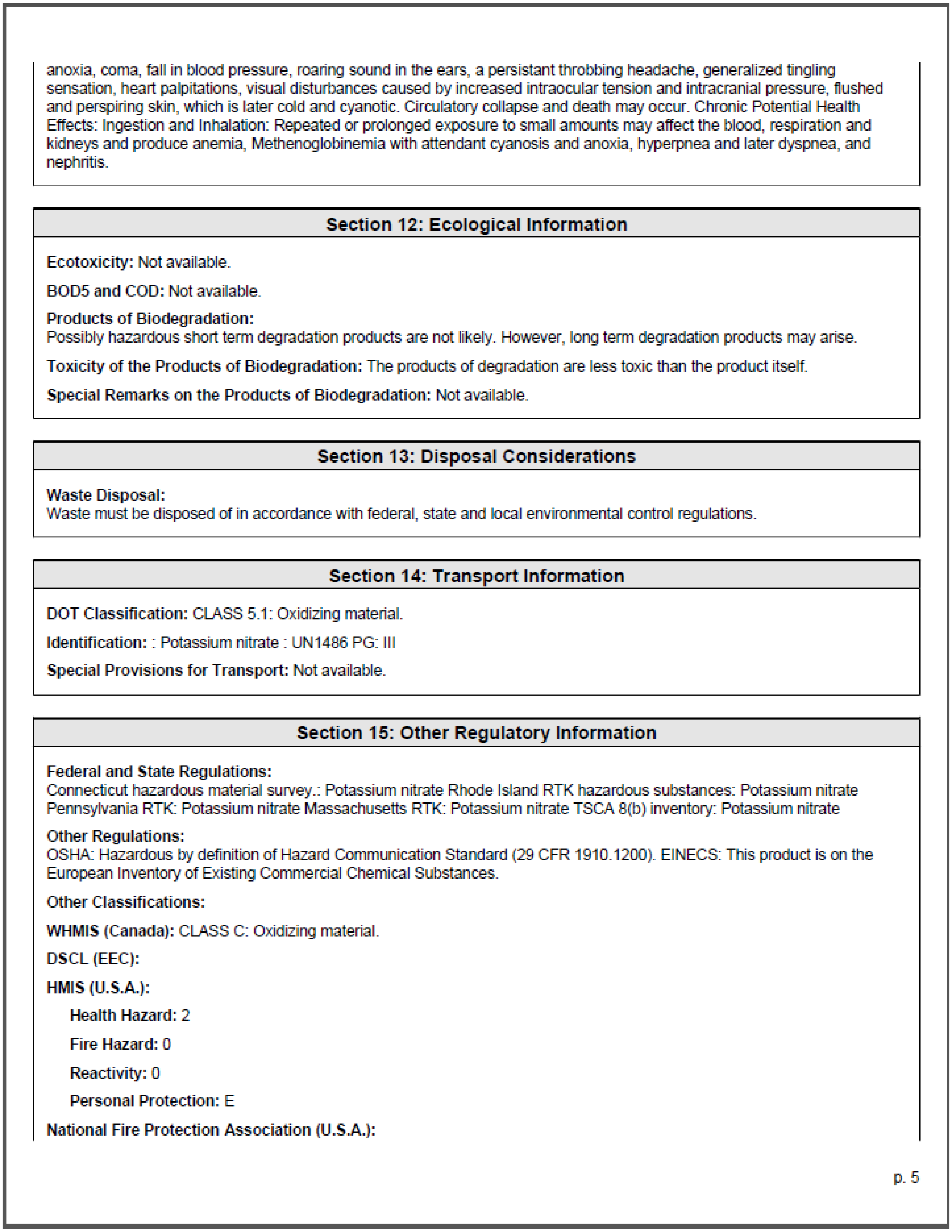
Chronic Effects on Humans: May cause damage to the following organs: blood, kidneys, central nervous system (CNS).

Other Toxic Effects on Humans: Hazardous in case of skin contact (irritant), of ingestion, of inhalation (lung irritant).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects based on animal test data. May affect genetic material (mutagenic)

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes skin irritation. Eyes: Causes eye irritation Inhalation: Breathing Potassium Nitrate can irritate the nose and throat causing sneezing and coughing. High levels can interfere with the ability of the blood to carry oxygen causing headache, dizziness and a blue color to the skin and lips (methemoglobinemia), and other symtoms of methemoglobinemia (see other symptoms under ingestion). Higher levels can cause trouble breathing, circulatory collapse and even death. Ingestion: Ingestion of large quantities may cause violent gastroenteritis with nausea, vomiting, severe abdominal pain. It may also cause colic and diarrhea. Acute toxicity of nitrate occurs as a result of reduction to nitrite. The nitrite acts in the blood to oxidize hemoglobin to methemoglobin which does not perform as an oxygen carrier to tissues causing Methenoglobinemia. Symptoms may include vertigo, muscular weakness, syncope, irregular pulse, convulsions,



anoxia, coma, fall in blood pressure, roaring sound in the ears, a persistant throbbing headache, generalized tingling sensation, heart palpitations, visual disturbances caused by increased intraocular tension and intracranial pressure, flushed and perspiring skin, which is later cold and cyanotic. Circulatory collapse and death may occur. Chronic Potential Health Effects: Ingestion and Inhalation: Repeated or prolonged exposure to small amounts may affect the blood, respiration and kidneys and produce anemia, Methenoglobinemia with attendant cyanosis and anoxia, hyperpnea and later dyspnea, and nephritis.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 5.1: Oxidizing material.

Identification: : Potassium nitrate : UN1486 PG: III

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Connecticut hazardous material survey.: Potassium nitrate Rhode Island RTK hazardous substances: Potassium nitrate Pennsylvania RTK: Potassium nitrate Massachusetts RTK: Potassium nitrate TSCA 8(b) inventory: Potassium nitrate

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

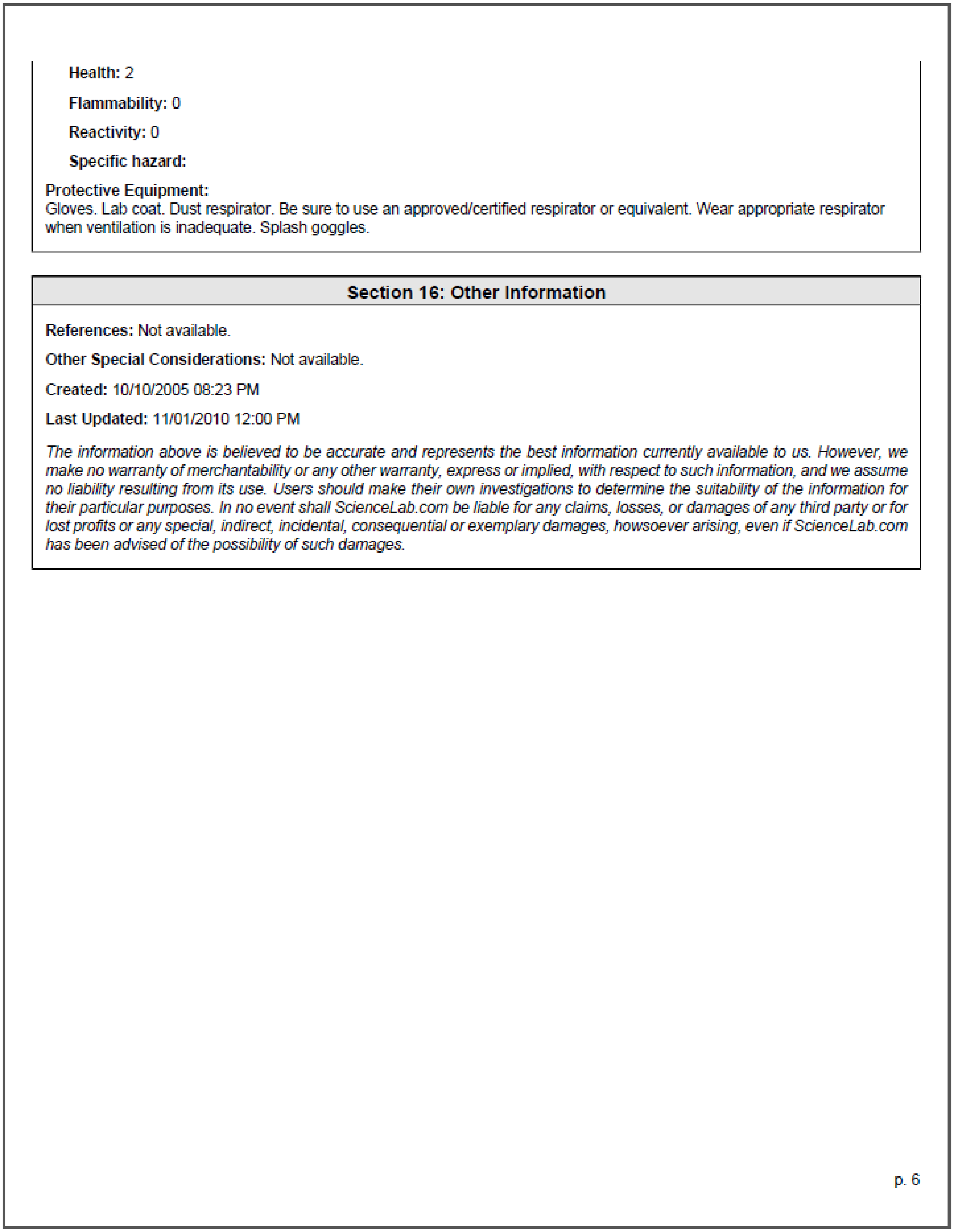
WHMIS (Canada): CLASS C: Oxidizing material.

DSCL (EEC):

HMIS (U.S.A.):

- **Health Hazard:** 2
- **Fire Hazard:** 0
- **Reactivity:** 0
- **Personal Protection:** E

National Fire Protection Association (U.S.A.):



Health: 2

Flammability: 0

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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Last Updated: 11/01/2010 12:00 PM

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Appendix E: Sample ASPEN Block Reports

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 BLOCK:  CMP-300  MODEL: MCOMPR
 ------------------------------
   INLET STREAMS:    S-325       TO STAGE   1
   OUTLET STREAMS:   S-314      FROM STAGE   4
   PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                 ***  MASS AND ENERGY BALANCE  ***
                             IN            OUT       RELATIVE DIFF.
    TOTAL BALANCE
      MOLE(LBMOL/HR)           3681.00        3681.00        0.00000
      MASS(LB/HR   )           7420.46        7420.46        0.00000
      ENTHALPY(BTU/HR  )       0.160078E+07    0.278814E+08   -0.942586

                 ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E            0.00000      LB/HR
    PRODUCT STREAMS CO2E         0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION    0.00000      LB/HR
    TOTAL CO2E PRODUCTION        0.00000      LB/HR

                   ***  INPUT DATA  ***

   ISENTROPIC CENTRIFUGAL COMPRESSOR
   NUMBER OF STAGES                                4
   FINAL PRESSURE, PSIA                         1,166.30

                COMPRESSOR SPECIFICATIONS PER STAGE

   STAGE               MECHANICAL     ISENTROPIC
   NUMBER                EFFICIENCY     EFFICIENCY



     1                 1.000         0.7200
     2                 1.000         0.7200
     3                 1.000         0.7200
     4                 1.000         0.7200

                COOLER SPECIFICATIONS PER STAGE

   STAGE     PRESSURE DROP     TEMPERATURE
   NUMBER    PSI              F
```

```
  1      2.000           493.0
  2      2.000           767.0
  3      2.000           1041.
  4      2.000           1150.

                    ***  RESULTS  ***

FINAL PRESSURE, PSIA                             1,164.30
TOTAL WORK REQUIRED, HP                              22,340.3
TOTAL COOLING DUTY , BTU/HR                              -0.305628+08

                    ***  PROFILE  ***

                    COMPRESSOR PROFILE

STAGE      OUTLET       PRESSURE     OUTLET
NUMBER     PRESSURE     RATIO        TEMPERATURE
         PSIA                   F

  1       43.86       2.985       444.3
  2       130.9       3.127       996.9
  3       390.8       3.031       1387.
  4       1166.       3.000       1775.

STAGE      INDICATED      BRAKE
NUMBER     HORSEPOWER     HORSEPOWER
         HP             HP
  1       3073.         3073.
  2       5124.         5124.
  3       6392.         6392.
  4       7751.         7751.

STAGE      HEAD          VOLUMETRIC
NUMBER     DEVELOPED      FLOW
         FT-LBF/LB     CUFT/HR
  1      0.5905E+06    0.1613E+07
  2      0.9844E+06    0.8998E+06
  3      0.1228E+07    0.3767E+06
  4      0.1489E+07    0.1533E+06

                    COOLER PROFILE
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  STAGE    OUTLET        OUTLET     COOLING    VAPOR
  NUMBER   TEMPERATURE   PRESSURE   LOAD       FRACTION
           F             PSIA       BTU/HR

    1       493.0         41.86      0.1254E+07   1.000
    2       767.0         128.9      -.5957E+07   1.000
    3       1041.         388.8      -.9116E+07   1.000
    4       1150.         1164.      -.1674E+08   1.000

 BLOCK:  DC-500   MODEL: RADFRAC
 -------------------------------
   INLETS   - S-504    STAGE  12
   OUTLETS  - S-512    STAGE   1
              S-505    STAGE  30
              HS-706   STAGE  30
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                                IN            OUT       RELATIVE DIFF.
   TOTAL BALANCE
     MOLE(LBMOL/HR)          3769.17        3769.17        0.00000
     MASS(LB/HR   )          358212.        358212.       0.399806E-07
     ENTHALPY(BTU/HR  )    -0.502864E+08  -0.809244E+08    0.378600

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000      LB/HR
   PRODUCT STREAMS CO2E         0.00000      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION         0.00000      LB/HR




                    **********************
                    ****  INPUT DATA  ****
                    **********************

  ****   INPUT PARAMETERS   ****

   NUMBER OF STAGES                               30
   ALGORITHM OPTION                              STANDARD
   ABSORBER OPTION                               NO
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 INITIALIZATION OPTION                        STANDARD
 HYDRAULIC PARAMETER CALCULATIONS                    NO
 INSIDE LOOP CONVERGENCE METHOD                    BROYDEN
 DESIGN SPECIFICATION METHOD                   NESTED
 MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS              200
 MAXIMUM NO. OF INSIDE LOOP ITERATIONS              10
 MAXIMUM NUMBER OF FLASH ITERATIONS                  30
 FLASH TOLERANCE                              0.000100000
 OUTSIDE LOOP CONVERGENCE TOLERANCE                 0.000100000

****   COL-SPECS   ****

 MOLAR VAPOR DIST / TOTAL DIST                      1.00000
 MASS REFLUX RATIO                             0.86000
 MASS DISTILLATE TO FEED RATIO                      0.60000

****    PROFILES   ****

 P-SPEC         STAGE   1  PRES, PSIA                14.6959

**** TRAY MURPHREE EFFICIENCY ****

                STAGE   2  EFFICIENCY               0.56000
                   3                      0.56000
                   4                      0.56000
                   5                      0.56000
                   6                      0.56000
                   7                      0.56000
                   8                      0.57000
                   9                      0.57000
                  10                      0.57000
                  11                      0.57000
                  12                      0.57000
                  13                      0.58000
                  14                      0.58000
                  15                      0.59000
                  16                      0.59000
                  17                      0.59000
                  18                      0.60000
                  19                      0.60000
                  20                      0.60000
                  21                      0.60000
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                    22                   0.60000
                    23                   0.60000
                    24                   0.60000
                    25                   0.60000
                    26                   0.60000
                    27                   0.60000
                    28                   0.60000
                    29                   0.60000

                   ******************
                   ****  RESULTS  ****
                   ******************



 ***   COMPONENT SPLIT FRACTIONS   ***

                     OUTLET STREAMS
                     --------------
               S-512       S-505
  COMPONENT:
  P-XYL      .79372E-01   .92063
  O-XYL      .32804E-01   .96720
  M-XYL      .70713E-01   .92929
  N-BUTANE    1.0000      0.0000
  N-PENT      1.0000      .36308E-14
  N-HEX       1.0000      .70792E-09
  WATER       1.0000      0.0000
  H2          1.0000      0.0000
  ETHYLBEN    .11302      .88698
  TOLUENE     .95549      .44512E-01
  BENZENE     1.0000      .70753E-06
  NAPTH      .95419E-05   .99999
  1:2:4-01   .60681E-03   .99939
  ISOPR-01   .10042E-01   .98996
  N-HEP-01    .99997      .31569E-04
  1-BUT-01    1.0000      0.0000
  1-PEN-01    1.0000      0.0000
  1-HEX-01    1.0000      .16512E-09
  1-HEP-01    .99999      .11951E-04


 ***    SUMMARY OF KEY RESULTS    ***
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```
   TOP STAGE TEMPERATURE          F                    209.002
   BOTTOM STAGE TEMPERATURE       F                    296.357
   TOP STAGE LIQUID FLOW          LBMOL/HR             2,021.01
   BOTTOM STAGE LIQUID FLOW       LBMOL/HR             1,271.21
   TOP STAGE VAPOR FLOW           LBMOL/HR             2,497.96
   BOILUP VAPOR FLOW              LBMOL/HR             4,599.15
   MOLAR REFLUX RATIO                                  0.80906
   MOLAR BOILUP RATIO                                  3.61793
   CONDENSER DUTY (W/O SUBCOOL)   BTU/HR               -0.306380+08
   REBOILER DUTY                  BTU/HR               0.754021+08

  ****   MAXIMUM FINAL RELATIVE ERRORS   ****

   DEW POINT                    0.66479E-06  STAGE= 16
   BUBBLE POINT                 0.35497E-06  STAGE= 17
   COMPONENT MASS BALANCE       0.72927E-06  STAGE= 30 COMP=NAPTH
   ENERGY BALANCE               0.13476E-06  STAGE=  2


  ****    PROFILES   ****

  **NOTE** REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE
FLOWS
         FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

                                  ENTHALPY
 STAGE TEMPERATURE   PRESSURE         BTU/LBMOL         HEAT DUTY
     F          PSIA         LIQUID      VAPOR       BTU/HR

   1   209.00       14.696      -429.49     -4577.9     -.30638+08
   2   221.14       14.696       3955.2      4057.3
  10   231.40       14.696       3428.8      5935.7
  11   232.48       14.696       3159.6      5820.2
  12   229.92       14.696       1569.8      5709.9
  13   242.19       14.696       5237.0      16521.
  14   246.46       14.696       6640.6      20753.
  15   248.25       14.696       7201.8      22398.
  16   249.27       14.696       7402.3      23073.
  17   250.10       14.696       7420.0      23327.
  29   283.89       14.696       1337.3      16874.
  30   296.36       14.696       4651.5      16816.      .75402+08
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 STAGE     FLOW RATE                 FEED RATE              PRODUCT RATE
           LBMOL/HR              LBMOL/HR             LBMOL/HR
      LIQUID     VAPOR      LIQUID    VAPOR    MIXED      LIQUID    VAPOR
   1  2021.      2498.                             2497.9640
   2  2034.      4519.
  10  1950.      4461.
  11  1975.      4448.               2.2144
  12  6052.      4471.      3766.9596
  13  6179.      4781.
  14  6217.      4908.
  15  6226.      4946.
  16  6226.      4955.
  17  6220.      4955.
  29  5870.      4723.
  30  1271.      4599.                          1271.2100

   ****  MASS FLOW PROFILES  ****

 STAGE     FLOW RATE                 FEED RATE              PRODUCT RATE
           LB/HR                  LB/HR               LB/HR
      LIQUID     VAPOR      LIQUID    VAPOR    MIXED      LIQUID    VAPOR
   1 0.1848E+06 0.2149E+06                              .21493+06
   2 0.1881E+06 0.3998E+06
  10 0.1868E+06 0.4020E+06
  11 0.1902E+06 0.4017E+06           145.4036
  12 0.5916E+06 0.4050E+06  .35807+06
  13 0.6082E+06 0.4484E+06
  14 0.6134E+06 0.4649E+06
  15 0.6153E+06 0.4701E+06
  16 0.6162E+06 0.4720E+06
  17 0.6169E+06 0.4729E+06
  29 0.6410E+06 0.5031E+06
  30 0.1433E+06 0.4977E+06                       .14328+06

                   ****   MOLE-X-PROFILE     ****
   STAGE     P-XYL        O-XYL        M-XYL        N-BUTANE      N-PENT
     1    0.37307E-01   0.10023E-02   0.32578E-02   0.17011E-02   0.19042E-01
     2    0.54109E-01   0.15527E-02   0.47695E-02   0.70336E-03   0.88759E-02
    10    0.16600       0.76331E-02   0.15566E-01   0.60103E-03   0.68752E-02
    11    0.17227       0.83923E-02   0.16265E-01   0.60093E-03   0.68530E-02
    12    0.16731       0.91587E-02   0.16009E-01   0.10045E-02   0.10841E-01
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  13    0.17282       0.93290E-02  0.16503E-01  0.11041E-03  0.24688E-02
  14    0.17793       0.94925E-02  0.16961E-01  0.11636E-04  0.53624E-03
  15    0.18383       0.96840E-02  0.17492E-01  0.11873E-05  0.11274E-03
  16    0.19116       0.99264E-02  0.18154E-01  0.12009E-06  0.23468E-04
  17    0.20054       0.10245E-01  0.19006E-01  0.12070E-07  0.48493E-05
  29    0.49183       0.27647E-01  0.47495E-01  0.23868E-20  0.72329E-14
  30    0.41543       0.26299E-01  0.40635E-01  0.10645E-21  0.63663E-15

                 ****   MOLE-X-PROFILE    ****
STAGE    N-HEX        WATER        H2          ETHYLBEN     TOLUENE
   1   0.58565E-01   0.72414E-02   0.11043E-06   0.84314E-03   0.82463
   2   0.33881E-01   0.33534E-02   0.45322E-07   0.11876E-02   0.85588
  10    0.23263E-01   0.25964E-02   0.45498E-07   0.30216E-02   0.70341
  11    0.23087E-01   0.25816E-02   0.45902E-07   0.30730E-02   0.68166
  12    0.32548E-01   0.41421E-02   0.37151E-07   0.28717E-02   0.60899
  13    0.14131E-01   0.86013E-03   0.47673E-10   0.29884E-02   0.64285
  14    0.58341E-02   0.17123E-03   0.60938E-13   0.30971E-02   0.65317
  15    0.23356E-02   0.33060E-04   0.76436E-16   0.32224E-02   0.65331
  16    0.92482E-03   0.63225E-05   0.95814E-19   0.33764E-02   0.64769
  17    0.36327E-03   0.11996E-05   0.70908E-22   0.35706E-02   0.63757
  29    0.10869E-08   0.44373E-15   0.26088E-59   0.81551E-02   0.11700
  30    0.18116E-09   0.34585E-16   0.20314E-62   0.65913E-02   0.57584E-01

                 ****   MOLE-X-PROFILE    ****
STAGE    BENZENE      NAPTH        1:2:4-01     ISOPR-01     N-HEP-01
   1   0.86395E-02   0.21431E-05   0.11894E-03   0.24509E-02   0.23302E-01
   2   0.60301E-02   0.52184E-05   0.23587E-03   0.41058E-02   0.18333E-01
  10    0.39933E-02   0.17177E-02   0.10139E-01   0.38271E-01   0.12030E-01
  11    0.39425E-02   0.34392E-02   0.15159E-01   0.45996E-01   0.11845E-01
  12    0.49632E-02   0.27589E-01   0.33993E-01   0.60303E-01   0.13546E-01
  13    0.30682E-02   0.27143E-01   0.33834E-01   0.60813E-01   0.10156E-01
  14    0.18159E-02   0.27032E-01   0.33887E-01   0.61393E-01   0.72508E-02
  15    0.10483E-02   0.27028E-01   0.34021E-01   0.62089E-01   0.50477E-02
  16    0.59926E-03   0.27065E-01   0.34211E-01   0.62971E-01   0.34763E-02
  17    0.33991E-03   0.27129E-01   0.34466E-01   0.64137E-01   0.23752E-02
  29    0.73374E-07   0.44086E-01   0.86163E-01   0.17762       0.54727E-05
  30    0.18215E-07   0.12471       0.13256       0.19619       0.16663E-05

                 ****   MOLE-X-PROFILE    ****
STAGE    1-BUT-01     1-PEN-01     1-HEX-01     1-HEP-01
   1   0.23329E-03   0.21103E-02   0.67518E-02   0.28057E-02
   2   0.95599E-04   0.96309E-03   0.37834E-02   0.21391E-02
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   10   0.82495E-04   0.75710E-03   0.26373E-02   0.13979E-02
   11   0.82502E-04   0.75494E-03   0.26188E-02   0.13774E-02
   12   0.13848E-03   0.12073E-02   0.37635E-02   0.16159E-02
   13   0.13786E-04   0.24989E-03   0.15141E-02   0.11552E-02
   14   0.13175E-05   0.49372E-04   0.57972E-03   0.78679E-03
   15   0.12194E-06   0.94412E-05   0.21521E-03   0.52231E-03
   16   0.11190E-07   0.17876E-05   0.79043E-04   0.34305E-03
   17   0.10206E-08   0.33602E-06   0.28801E-04   0.22351E-03
   29   0.39457E-22   0.16264E-15   0.34648E-10   0.28130E-06
   30   0.16066E-23   0.13078E-16   0.53454E-11   0.80776E-07

                    ****   MOLE-Y-PROFILE    ****
  STAGE     P-XYL        O-XYL        M-XYL        N-BUTANE      N-PENT
    1    0.18227E-01   0.45392E-03   0.15736E-02   0.17997E-01   0.89230E-01
    2    0.26760E-01   0.69918E-03   0.23268E-02   0.10709E-01   0.57840E-01
   10    0.79153E-01   0.32436E-02   0.72999E-02   0.10344E-01   0.53016E-01
   11    0.83018E-01   0.36016E-02   0.77085E-02   0.10370E-01   0.53122E-01
   12    0.86279E-01   0.39606E-02   0.80640E-02   0.10261E-01   0.52764E-01
   13    0.10134       0.46014E-02   0.94613E-02   0.12716E-02   0.13724E-01
   14    0.10997       0.49333E-02   0.10251E-01   0.13901E-03   0.31083E-02
   15    0.11688       0.51726E-02   0.10876E-01   0.14627E-04   0.67408E-03
   16    0.12441       0.54216E-02   0.11555E-01   0.14919E-05   0.14167E-03
   17    0.13361       0.57257E-02   0.12386E-01   0.15090E-06   0.29489E-04
   29    0.51114       0.26064E-01   0.48832E-01   0.60833E-19   0.57983E-13
   30    0.51294       0.28019E-01   0.49391E-01   0.30171E-20   0.90561E-14

                    ****   MOLE-Y-PROFILE    ****
  STAGE     N-HEX        WATER         H2          ETHYLBEN      TOLUENE
    1    0.13023       0.37971E-01   0.13747E-03   0.42741E-03   0.62905
    2    0.98177E-01   0.24228E-01   0.76040E-04   0.61334E-03   0.71652
   10    0.83276E-01   0.22418E-01   0.77000E-04   0.15214E-02   0.67144
   11    0.83329E-01   0.22461E-01   0.77219E-04   0.15648E-02   0.66165
   12    0.82886E-01   0.22298E-01   0.36444E-04   0.15962E-02   0.65252
   13    0.41202E-01   0.52434E-02   0.47029E-07   0.18828E-02   0.75560
   14    0.17791E-01   0.10829E-02   0.60021E-10   0.20551E-02   0.79445
   15    0.73336E-02   0.21524E-03   0.76602E-13   0.21989E-02   0.80626
   16    0.29348E-02   0.41541E-04   0.96045E-16   0.23581E-02   0.80614
   17    0.11621E-02   0.79447E-05   0.12040E-18   0.25515E-02   0.79909
   29    0.46874E-08   0.41332E-14   0.41844E-56   0.88080E-02   0.19299
   30    0.13373E-08   0.55682E-15   0.33293E-59   0.85874E-02   0.13343

                    ****   MOLE-Y-PROFILE    ****
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```
STAGE     BENZENE       NAPTH        1:2:4-01     ISOPR-01     N-HEP-01
   1    0.13101E-01   0.60558E-06   0.40960E-04   0.10128E-02   0.26861E-01
   2    0.11106E-01   0.12932E-05   0.75834E-04   0.16559E-02   0.25269E-01
  10    0.91216E-02   0.37286E-03   0.29565E-02   0.14295E-01   0.20427E-01
  11    0.91079E-02   0.75345E-03   0.44685E-02   0.17348E-01   0.20358E-01
  12    0.90569E-02   0.15195E-02   0.67190E-02   0.20883E-01   0.20234E-01
  13    0.62828E-02   0.17660E-02   0.77865E-02   0.24173E-01   0.17147E-01
  14    0.38630E-02   0.18710E-02   0.82610E-02   0.25747E-01   0.12786E-01
  15    0.22826E-02   0.19258E-02   0.85248E-02   0.26746E-01   0.91141E-02
  16    0.13172E-02   0.19683E-02   0.87422E-02   0.27687E-01   0.63422E-02
  17    0.75302E-03   0.20125E-02   0.89775E-02   0.28791E-01   0.43678E-02
  29    0.22349E-06   0.12506E-01   0.52808E-01   0.14684       0.13471E-04
  30    0.88620E-07   0.21801E-01   0.73340E-01   0.17248       0.65248E-05

                    ****   MOLE-Y-PROFILE    ****
STAGE     1-BUT-01      1-PEN-01      1-HEX-01      1-HEP-01
   1    0.27557E-02   0.11025E-01   0.16475E-01   0.34397E-02
   2    0.16276E-02   0.70380E-02   0.12126E-01   0.31561E-02
  10    0.15796E-02   0.65094E-02   0.10399E-01   0.25517E-02
  11    0.15837E-02   0.65231E-02   0.10408E-01   0.25445E-02
  12    0.15659E-02   0.64768E-02   0.10351E-01   0.25294E-02
  13    0.17530E-03   0.15283E-02   0.47642E-02   0.20455E-02
  14    0.17357E-04   0.31462E-03   0.19063E-02   0.14544E-02
  15    0.16561E-05   0.62062E-04   0.72873E-03   0.98900E-03
  16    0.15322E-06   0.11863E-04   0.27043E-03   0.65629E-03
  17    0.14061E-07   0.22463E-05   0.99324E-04   0.43104E-03
  29    0.11071E-20   0.14287E-14   0.16131E-09   0.73208E-06
  30    0.49919E-22   0.20397E-15   0.42747E-10   0.33673E-06

                    ****   K-VALUES          ****
STAGE     P-XYL         O-XYL         M-XYL        N-BUTANE      N-PENT
   1    0.30887       0.26061       0.30135       13.945        5.9813
   2    0.38465       0.32491       0.37566       15.753        6.9298
  10    0.45925       0.38957       0.44916       17.177        7.6996
  11    0.46776       0.39700       0.45756       17.325        7.7812
  12    0.44777       0.37967       0.43787       16.967        7.5835
  13    0.55024       0.46748       0.53865       18.945        8.6726
  14    0.58997       0.50144       0.57773       19.687        9.0836
  15    0.60733       0.51627       0.59480       20.007        9.2606
  16    0.61736       0.52489       0.60468       20.184        9.3584
  17    0.62559       0.53203       0.61280       20.317        9.4334
  29    1.0368        0.89563       1.0203        25.488        12.526
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   30    1.2347       1.0654       1.2155       28.342       14.225

                   ****   K-VALUES          ****
  STAGE     N-HEX        WATER        H2           ETHYLBEN      TOLUENE
    1     2.6536       6.7347       1681.9       0.33366      0.67948
    2     3.1571       7.6447       1681.9       0.41376      0.82402
   10     3.5780       8.6218       1688.7       0.49266      0.96504
   11     3.6228       8.7346       1689.3       0.50165      0.98102
   12     3.5127       8.4892       1720.0       0.48056      0.94377
   13     4.1155       9.5987       1700.0       0.58828       1.1316
   14     4.3475       9.9939       1697.3       0.62991       1.2032
   15     4.4488       10.162       1697.7       0.64808       1.2342
   16     4.5053       10.263       1698.1       0.65859       1.2522
   17     4.5487       10.352       1697.9       0.66723       1.2670
   29     6.3672       14.688       1604.0       1.0981       1.9888
   30     7.3821       16.100       1638.9       1.3028       2.3171

                   ****   K-VALUES          ****
  STAGE     BENZENE      NAPTH        1:2:4-01     ISOPR-01      N-HEP-01
    1     1.6979      0.30463E-01   0.11400      0.20702       1.2064
    2     1.9952      0.39677E-01   0.14631      0.26078       1.4741
   10     2.2868      0.49918E-01   0.17909      0.31332       1.7024
   11     2.3199      0.51146E-01   0.18288      0.31931       1.7269
   12     2.2465      0.48335E-01   0.17397      0.30514       1.6657
   13     2.6188      0.62262E-01   0.21998      0.37877       1.9994
   14     2.7575      0.67747E-01   0.23814      0.40759       2.1300
   15     2.8174      0.70158E-01   0.24613      0.42022       2.1872
   16     2.8523      0.71588E-01   0.25076      0.42750       2.2191
   17     2.8814      0.72812E-01   0.25458      0.43343       2.2436
   29     4.2714      0.14310      0.45402      0.73044      3.3077
   30     4.8653      0.17482      0.55326      0.87918      3.9156

                   ****   K-VALUES          ****
  STAGE     1-BUT-01     1-PEN-01     1-HEX-01     1-HEP-01
    1     15.612       6.7087       2.9460       1.3054
    2     17.565       7.7389       3.4849       1.5857
   10     19.111       8.5842       3.9403       1.8293
   11     19.272       8.6736       3.9891       1.8557
   12     18.883       8.4567       3.8703       1.7912
   13     21.012       9.6331       4.5135       2.1412
   14     21.805       10.077       4.7592       2.2769
   15     22.146       10.268       4.8659       2.3362
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  16    22.335       10.375       4.9255       2.3694
  17    22.478       10.457       4.9717       2.3953
  29    28.057       13.805       6.9371       3.5394
  30    31.071       15.596       7.9969       4.1686

                 ****   MASS-X-PROFILE    ****
STAGE    P-XYL        O-XYL        M-XYL        N-BUTANE     N-PENT
   1   0.43307E-01  0.11635E-02  0.37817E-02  0.10811E-02  0.15022E-01
   2   0.62106E-01  0.17822E-02  0.54745E-02  0.44198E-03  0.69235E-02
  10    0.18401     0.84613E-02  0.17255E-01  0.36474E-03  0.51792E-02
  11    0.18991     0.92515E-02  0.17931E-01  0.36267E-03  0.51341E-02
  12    0.18171     0.99467E-02  0.17387E-01  0.59725E-03  0.80016E-02
  13    0.18640     0.10062E-01  0.17800E-01  0.65199E-04  0.18097E-02
  14    0.19144     0.10214E-01  0.18250E-01  0.68545E-05  0.39211E-03
  15    0.19749     0.10404E-01  0.18792E-01  0.69833E-06  0.82312E-04
  16    0.20504     0.10647E-01  0.19473E-01  0.70520E-07  0.17107E-04
  17    0.21469     0.10968E-01  0.20347E-01  0.70742E-08  0.35281E-05
  29    0.47818     0.26880E-01  0.46178E-01  0.12704E-20  0.47790E-14
  30    0.39130     0.24771E-01  0.38275E-01  0.54894E-22  0.40751E-15

                 ****   MASS-X-PROFILE    ****
STAGE    N-HEX        WATER        H2           ETHYLBEN     TOLUENE
   1   0.55183E-01  0.14264E-02  0.24341E-08  0.97875E-03  0.83078
   2   0.31566E-01  0.65313E-03  0.98776E-09  0.13631E-02  0.85259
  10    0.20932E-01  0.48837E-03  0.95763E-09  0.33495E-02  0.67671
  11    0.20659E-01  0.48292E-03  0.96081E-09  0.33876E-02  0.65217
  12    0.28693E-01  0.76334E-03  0.76612E-09  0.31188E-02  0.57401
  13    0.12372E-01  0.15743E-03  0.97636E-12  0.32233E-02  0.60178
  14    0.50953E-02  0.31263E-04  0.12450E-14  0.33324E-02  0.60994
  15    0.20367E-02  0.60267E-05  0.15592E-17  0.34618E-02  0.60913
  16    0.80520E-03  0.11508E-05  0.19514E-20  0.36216E-02  0.60294
  17    0.31567E-03  0.21792E-06  0.14414E-23  0.38225E-02  0.59237
  29    0.85781E-09  0.73206E-16  0.48161E-61  0.79289E-02  0.98729E-01
  30    0.13850E-09  0.55277E-17  0.36331E-64  0.62084E-02  0.47073E-01

                 ****   MASS-X-PROFILE    ****
STAGE    BENZENE      NAPTH        1:2:4-01     ISOPR-01     N-HEP-01
   1   0.73789E-02  0.30035E-05  0.15631E-03  0.32210E-02  0.25530E-01
   2   0.50925E-02  0.72313E-05  0.30651E-03  0.53353E-02  0.19861E-01
  10    0.32568E-02  0.22987E-02  0.12724E-01  0.48028E-01  0.12586E-01
  11    0.31977E-02  0.45772E-02  0.18919E-01  0.57404E-01  0.12324E-01
  12    0.39659E-02  0.36173E-01  0.41796E-01  0.74144E-01  0.13885E-01
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   13   0.24350E-02  0.35346E-01  0.41315E-01  0.74260E-01  0.10339E-01
   14   0.14376E-02  0.35115E-01  0.41279E-01  0.74784E-01  0.73634E-02
   15   0.82861E-03  0.35055E-01  0.41378E-01  0.75516E-01  0.51181E-02
   16   0.47294E-03  0.35048E-01  0.41544E-01  0.76468E-01  0.35193E-02
   17   0.26773E-03  0.35063E-01  0.41772E-01  0.77734E-01  0.23999E-02
   29   0.52488E-07  0.51747E-01  0.94842E-01  0.19551      0.50220E-05
   30   0.12623E-07  0.14181      0.14135      0.20920      0.14814E-05

                **** MASS-X-PROFILE ****
  STAGE   1-BUT-01    1-PEN-01    1-HEX-01    1-HEP-01
    1   0.14312E-03  0.16183E-02  0.62132E-02  0.30121E-02
    2   0.57990E-04  0.73025E-03  0.34425E-02  0.22707E-02
   10   0.48327E-04  0.55440E-03  0.23175E-02  0.14331E-02
   11   0.48065E-04  0.54978E-03  0.22885E-02  0.14043E-02
   12   0.79481E-04  0.86617E-03  0.32402E-02  0.16230E-02
   13   0.78586E-05  0.17806E-03  0.12946E-02  0.11524E-02
   14   0.74916E-06  0.35093E-04  0.49447E-03  0.78294E-03
   15   0.69232E-07  0.67003E-05  0.18328E-03  0.51895E-03
   16   0.63433E-08  0.12667E-05  0.67210E-04  0.34031E-03
   17   0.57743E-09  0.23764E-06  0.24442E-04  0.22130E-03
   29   0.20274E-22  0.10446E-15  0.26704E-10  0.25294E-06
   30   0.79974E-24  0.81376E-17  0.39913E-11  0.70365E-07

                **** MASS-Y-PROFILE ****
  STAGE   P-XYL        O-XYL        M-XYL        N-BUTANE     N-PENT
    1   0.22491E-01  0.56010E-03  0.19416E-02  0.12157E-01  0.74825E-01
    2   0.32115E-01  0.83911E-03  0.27924E-02  0.70361E-02  0.47174E-01
   10   0.93258E-01  0.38217E-02  0.86008E-02  0.66719E-02  0.42450E-01
   11   0.97596E-01  0.42340E-02  0.90620E-02  0.66740E-02  0.42441E-01
   12   0.10112      0.46419E-02  0.94510E-02  0.65839E-02  0.42025E-01
   13   0.11473      0.52093E-02  0.10711E-01  0.78811E-03  0.10559E-01
   14   0.12325      0.55290E-02  0.11489E-01  0.85295E-04  0.23675E-02
   15   0.13053      0.57769E-02  0.12147E-01  0.89435E-05  0.51162E-03
   16   0.13865      0.60423E-02  0.12878E-01  0.91030E-06  0.10730E-03
   17   0.14861      0.63682E-02  0.13776E-01  0.91885E-07  0.22289E-04
   29   0.50937      0.25974E-01  0.48663E-01  0.33189E-19  0.39268E-13
   30   0.50320      0.27487E-01  0.48453E-01  0.16204E-20  0.60375E-14

                **** MASS-Y-PROFILE ****
  STAGE   N-HEX        WATER        H2           ETHYLBEN     TOLUENE
    1   0.13043      0.79503E-02  0.32209E-05  0.52739E-03  0.67364
    2   0.95639E-01  0.49339E-02  0.17328E-05  0.73608E-03  0.74630
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  10   0.79642E-01  0.44819E-02  0.17226E-05  0.17925E-02  0.68657
  11   0.79516E-01  0.44806E-02  0.17237E-05  0.18396E-02  0.67507
  12   0.78852E-01  0.44344E-02  0.81101E-06  0.18708E-02  0.66371
  13   0.37862E-01  0.10073E-02  0.10110E-08  0.21315E-02  0.74241
  14   0.16185E-01  0.20595E-03  0.12773E-11  0.23032E-02  0.77275
  15   0.66483E-02  0.40791E-04  0.16244E-14  0.24558E-02  0.78149
  16   0.26549E-02  0.78560E-05  0.20325E-17  0.26280E-02  0.77974
  17   0.10492E-02  0.14994E-05  0.25426E-20  0.28378E-02  0.77134
  29   0.37916E-08  0.69892E-15  0.79177E-58  0.87776E-02  0.16691
  30   0.10649E-08  0.92689E-16  0.62014E-61  0.84242E-02  0.11360

                 ****   MASS-Y-PROFILE    ****
STAGE    BENZENE      NAPTH       1:2:4-01     ISOPR-01     N-HEP-01
   1   0.11894E-01  0.90212E-06  0.57219E-04  0.14148E-02  0.31282E-01
   2   0.98065E-02  0.18737E-05  0.10304E-03  0.22499E-02  0.28623E-01
  10   0.79073E-02  0.53036E-03  0.39435E-02  0.19067E-01  0.22716E-01
  11   0.78779E-02  0.10693E-02  0.59472E-02  0.23089E-01  0.22589E-01
  12   0.78098E-02  0.21500E-02  0.89151E-02  0.27708E-01  0.22382E-01
  13   0.52333E-02  0.24137E-02  0.99798E-02  0.30983E-01  0.18322E-01
  14   0.31854E-02  0.25316E-02  0.10482E-01  0.32668E-01  0.13525E-01
  15   0.18757E-02  0.25965E-02  0.10779E-01  0.33817E-01  0.96072E-02
  16   0.10801E-02  0.26483E-02  0.11030E-01  0.34934E-01  0.66713E-02
  17   0.61621E-03  0.27023E-02  0.11304E-01  0.36253E-01  0.45851E-02
  29   0.16387E-06  0.15046E-01  0.59578E-01  0.16566      0.12671E-04
  30   0.63964E-07  0.25820E-01  0.81452E-01  0.19156      0.60413E-05

                 ****   MASS-Y-PROFILE    ****
STAGE    1-BUT-01     1-PEN-01     1-HEX-01     1-HEP-01
   1   0.17970E-02  0.89867E-02  0.16115E-01  0.39253E-02
   2   0.10323E-02  0.55798E-02  0.11537E-01  0.35031E-02
  10   0.98357E-03  0.50664E-02  0.97123E-02  0.27805E-02
  11   0.98391E-03  0.50658E-02  0.96992E-02  0.27664E-02
  12   0.96988E-03  0.50145E-02  0.96171E-02  0.27417E-02
  13   0.10488E-03  0.11430E-02  0.42756E-02  0.21417E-02
  14   0.10281E-04  0.23293E-03  0.16936E-02  0.15075E-02
  15   0.97748E-06  0.45788E-04  0.64517E-03  0.10215E-02
  16   0.90248E-07  0.87342E-05  0.23892E-03  0.67646E-03
  17   0.82652E-08  0.16504E-05  0.87572E-04  0.44339E-03
  29   0.58304E-21  0.94057E-15  0.12743E-09  0.67472E-06
  30   0.25880E-22  0.13219E-15  0.33242E-10  0.30550E-06

                 ****   MURPHREE EFF     ****
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 STAGE    P-XYL       O-XYL       M-XYL       N-BUTANE     N-PENT
    1   0.56000     0.56000     0.56000     0.56000     0.56000
    2   0.56000     0.56000     0.56000     0.56000     0.56000
   10   0.57000     0.57000     0.57000     0.57000     0.57000
   11   0.57000     0.57000     0.57000     0.57000     0.57000
   12   0.57000     0.57000     0.57000     0.57000     0.57000
   13   0.58000     0.58000     0.58000     0.58000     0.58000
   14   0.58000     0.58000     0.58000     0.58000     0.58000
   15   0.59000     0.59000     0.59000     0.59000     0.59000
   16   0.59000     0.59000     0.59000     0.59000     0.59000
   17   0.59000     0.59000     0.59000     0.59000     0.59000
   29   0.60000     0.60000     0.60000     0.60000     0.60000
   30   0.60000     0.60000     0.60000     0.60000     0.60000

                   ****   MURPHREE EFF      ****
 STAGE    N-HEX       WATER       H2          ETHYLBEN     TOLUENE
    1   0.56000     0.56000     0.56000     0.56000     0.56000
    2   0.56000     0.56000     0.56000     0.56000     0.56000
   10   0.57000     0.57000     0.57000     0.57000     0.57000
   11   0.57000     0.57000     0.57000     0.57000     0.57000
   12   0.57000     0.57000     0.57000     0.57000     0.57000
   13   0.58000     0.58000     0.58000     0.58000     0.58000
   14   0.58000     0.58000     0.58000     0.58000     0.58000
   15   0.59000     0.59000     0.59000     0.59000     0.59000
   16   0.59000     0.59000     0.59000     0.59000     0.59000
   17   0.59000     0.59000     0.59000     0.59000     0.59000
   29   0.60000     0.60000     0.60000     0.60000     0.60000
   30   0.60000     0.60000     0.60000     0.60000     0.60000

                   ****   MURPHREE EFF      ****
 STAGE    BENZENE     NAPTH       1:2:4-01    ISOPR-01     N-HEP-01
    1   0.56000     0.56000     0.56000     0.56000     0.56000
    2   0.56000     0.56000     0.56000     0.56000     0.56000
   10   0.57000     0.57000     0.57000     0.57000     0.57000
   11   0.57000     0.57000     0.57000     0.57000     0.57000
   12   0.57000     0.57000     0.57000     0.57000     0.57000
   13   0.58000     0.58000     0.58000     0.58000     0.58000
   14   0.58000     0.58000     0.58000     0.58000     0.58000
   15   0.59000     0.59000     0.59000     0.59000     0.59000
   16   0.59000     0.59000     0.59000     0.59000     0.59000
   17   0.59000     0.59000     0.59000     0.59000     0.59000
   29   0.60000     0.60000     0.60000     0.60000     0.60000
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  30   0.60000      0.60000      0.60000      0.60000      0.60000

                    ****   MURPHREE EFF       ****
 STAGE     1-BUT-01      1-PEN-01      1-HEX-01      1-HEP-01
    1    0.56000      0.56000      0.56000      0.56000
    2    0.56000      0.56000      0.56000      0.56000
   10    0.57000      0.57000      0.57000      0.57000
   11    0.57000      0.57000      0.57000      0.57000
   12    0.57000      0.57000      0.57000      0.57000
   13    0.58000      0.58000      0.58000      0.58000
   14    0.58000      0.58000      0.58000      0.58000
   15    0.59000      0.59000      0.59000      0.59000
   16    0.59000      0.59000      0.59000      0.59000
   17    0.59000      0.59000      0.59000      0.59000
   29    0.60000      0.60000      0.60000      0.60000
   30    0.60000      0.60000      0.60000      0.60000



                ********************************
                ***** HYDRAULIC PARAMETERS *****
                ********************************


    *** DEFINITIONS ***

     MARANGONI INDEX = SIGMA - SIGMATO
     FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
     QR = QV*SQRT(RHOV/(RHOL-RHOV))
     F FACTOR = QV*SQRT(RHOV)
       WHERE:
       SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
       SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
       ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
       MV IS THE MASS FLOW OF VAPOR TO THE STAGE
       RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
       RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
       QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE


                TEMPERATURE
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                    F
 STAGE      LIQUID FROM      VAPOR TO
   1        209.00           221.14
   2        221.14           224.21
  10         231.40           232.48
  11         232.48           229.90
  12         229.92           242.19
  13         242.19           246.46
  14         246.46           248.25
  15         248.25           249.27
  16         249.27           250.10
  17         250.10           251.00
  29         283.89           296.36
  30         296.36           296.36


           MASS FLOW               VOLUME FLOW        MOLECULAR WEIGHT
            LB/HR                  CUFT/HR
 STAGE LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR
TO
   1  0.18484E+06 0.39976E+06  3863.6     0.21722E+07  91.458      88.464
   2  0.18809E+06 0.40302E+06  3912.9     0.21882E+07  92.496      88.938
  10  0.18679E+06 0.40172E+06  3885.7     0.21744E+07  95.776      90.309
  11  0.19023E+06 0.40516E+06  3957.1     0.21772E+07  96.307      90.574
  12  0.59165E+06 0.44836E+06  12254.     0.23677E+07  97.756      93.778
  13  0.60817E+06 0.46489E+06  12587.     0.24451E+07  98.429      94.728
  14  0.61342E+06 0.47014E+06  12682.     0.24703E+07  98.671      95.061
  15  0.61531E+06 0.47203E+06  12713.     0.24787E+07  98.824      95.260
  16  0.61622E+06 0.47294E+06  12728.     0.24812E+07  98.979      95.455
  17  0.61689E+06 0.47360E+06  12742.     0.24816E+07  99.171      95.692
  29  0.64102E+06 0.49774E+06  13446.     0.24480E+07  109.20      108.22
  30  0.14328E+06  0.0000      2969.4      0.0000      112.72


            DENSITY                VISCOSITY        SURFACE TENSION
            LB/CUFT                CP               DYNE/CM
 STAGE LIQUID FROM  VAPOR TO     LIQUID FROM  VAPOR TO      LIQUID FROM
   1   47.841      0.18404      0.25600      0.88481E-02    18.824
   2   48.070      0.18418      0.24808      0.88812E-02    18.740
  10   48.072      0.18475      0.24473      0.89147E-02    18.716
  11   48.074      0.18609      0.24497      0.88717E-02    18.728
  12   48.280      0.18936      0.25370      0.89674E-02    19.214
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  13   48.317      0.19013      0.24434      0.90132E-02    18.861
  14   48.369      0.19031      0.24157      0.90346E-02    18.773
  15   48.402      0.19044      0.24061      0.90437E-02    18.753
  16   48.415      0.19061      0.24017      0.90466E-02    18.747
  17   48.414      0.19085      0.23986      0.90458E-02    18.742
  29   47.675      0.20332      0.23366      0.89552E-02    17.709
  30   48.254                 0.24342                   18.243


     MARANGONI INDEX   FLOW PARAM          QR          REDUCED F-FACTOR
STAGE    DYNE/CM                         CUFT/HR       (LB-CUFT)**.5/HR
   1                  0.28678E-01      0.13499E+06      0.93186E+06
   2   -.84704E-01      0.28889E-01      0.13571E+06      0.93910E+06
  10   0.32782E-02      0.28826E-01      0.13506E+06      0.93461E+06
  11   0.11486E-01      0.29212E-01      0.13572E+06      0.93922E+06
  12   -.95596          0.82641E-01      0.14858E+06      0.10303E+07
  13   -.35356          0.82065E-01      0.15368E+06      0.10662E+07
  14   -.87506E-01      0.81844E-01      0.15526E+06      0.10777E+07
  15   -.20246E-01      0.81766E-01      0.15578E+06      0.10817E+07
  16   -.56825E-02      0.81755E-01      0.15599E+06      0.10833E+07
  17   -.47522E-02      0.81781E-01      0.15611E+06      0.10841E+07
  29   -.80505E-01      0.84105E-01      0.16021E+06      0.11038E+07
  30   0.53402                         0.0000          0.0000



             ***********************************
             ***** TRAY SIZING CALCULATIONS *****
             ***********************************


   *******************
   *** SECTION   1 ***
   *******************

   STARTING STAGE NUMBER                               2
   ENDING STAGE NUMBER                               13
   FLOODING CALCULATION METHOD                             GLITSCH

   DESIGN PARAMETERS
   -----------------
```

```
PEAK CAPACITY FACTOR                          1.00000
SYSTEM FOAMING FACTOR                           1.00000
FLOODING FACTOR                           0.80000
MINIMUM COLUMN DIAMETER        FT                  1.00000
MINIMUM DC AREA/COLUMN AREA                          0.100000
HOLE AREA/ACTIVE AREA                          0.12000

TRAY SPECIFICATIONS
-------------------
TRAY TYPE                                 SIEVE
NUMBER OF PASSES                                    1
TRAY SPACING               FT                  2.00000


      ***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER                              13
COLUMN DIAMETER                FT                  16.0155
DC AREA/COLUMN AREA                                 0.100000
DOWNCOMER VELOCITY            FT/SEC                  0.17356
FLOW PATH LENGTH               FT                  11.0034
SIDE DOWNCOMER WIDTH           FT                  2.50603
SIDE WEIR LENGTH               FT                  11.6370
CENTER DOWNCOMER WIDTH         FT                   0.0
CENTER WEIR LENGTH             FT                  0.0
OFF-CENTER DOWNCOMER WIDTH      FT                  0.0
OFF-CENTER SHORT WEIR LENGTH    FT                  0.0
OFF-CENTER LONG WEIR LENGTH     FT                  0.0
TRAY CENTER TO OCDC CENTER      FT                  0.0


                **** SIZING PROFILES ****

  STAGE   DIAMETER    TOTAL AREA   ACTIVE AREA   SIDE DC AREA
           FT          SQFT        SQFT          SQFT
    2      13.535      143.89      115.11       14.389
    3      13.535      143.89      115.11       14.389
    4      13.531      143.79      115.03       14.379
    5      13.526      143.69      114.95       14.369
    6      13.522      143.60      114.88       14.360
    7      13.517      143.49      114.80       14.349
    8      13.512      143.39      114.71       14.339
```

```
     9     13.506      143.26     114.61      14.326
    10      13.500      143.13      114.51      14.313
    11      13.544      144.08      115.27      14.408
    12      15.722      194.15      155.32      19.415
    13      16.015      201.45      161.16      20.145

BLOCK:  F-300    MODEL: FLASH2
------------------------------
  INLET STREAM:          S-307
  OUTLET VAPOR STREAM:   S-310
  OUTLET LIQUID STREAM:  S-308
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                              IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           15947.6         15947.6         0.00000
      MASS(LB/HR   )           339324.         339324.        0.171540E-15
      ENTHALPY(BTU/HR  )      -0.155911E+10   -0.148209E+10   -0.493991E-01

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            93768.7      LB/HR
   PRODUCT STREAMS CO2E         93768.7      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        0.00000      LB/HR

                     ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE F                          359.600
  SPECIFIED PRESSURE    PSIA                     290.075
  MAXIMUM NO. ITERATIONS                           30
  CONVERGENCE TOLERANCE                              0.000100000

                      ***  RESULTS  ***
  OUTLET TEMPERATURE    F                          359.60
  OUTLET PRESSURE       PSIA                     290.08
  HEAT DUTY             BTU/HR                 0.77018E+08
  VAPOR FRACTION                               0.82624
```

```
  V-L PHASE EQUILIBRIUM :

    COMP           F(I)         X(I)         Y(I)         K(I)
    SORBITOL        0.14845E-01    0.85434E-01    0.15889E-06    0.18599E-05
    PROPANE         0.40088E-01    0.11061E-03    0.48495E-01     438.45
    CO2           0.13360       0.73119E-03    0.16154        220.93
    WATER          0.58063       0.91363       0.51060       0.55887
    H2           0.23084       0.97993E-04    0.27936        2850.8

 BLOCK:  HX-100   MODEL: HEATX
 -----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:         S-417
  OUTLET STREAM:        S-420
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE
  COLD SIDE:
  ----------
  INLET STREAM:         S-104
  OUTLET STREAM:        S-107
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

               ***  MASS AND ENERGY BALANCE  ***
                         IN            OUT       RELATIVE DIFF.
   TOTAL BALANCE
     MOLE(LBMOL/HR)          27662.9        27662.9        0.00000
     MASS(LB/HR   )          748975.        748975.       0.155433E-15
     ENTHALPY(BTU/HR  )      -0.337380E+10   -0.337380E+10   -0.424006E-15

               ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000      LB/HR
   PRODUCT STREAMS CO2E         0.00000      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION         0.00000      LB/HR

                 ***  INPUT DATA  ***

  FLASH SPECS FOR HOT SIDE:
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                              30
  CONVERGENCE TOLERANCE                                 0.000100000
```

```
FLASH SPECS FOR COLD SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                          30
CONVERGENCE TOLERANCE                            0.000100000

FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT   HEAT EXCHANGER
  SPECIFIED COLD OUTLET TEMP
  SPECIFIED VALUE              F                212.0000
  LMTD CORRECTION FACTOR                             1.00000

PRESSURE SPECIFICATION:
  HOT  SIDE PRESSURE DROP       PSI                  0.0000
  COLD SIDE PRESSURE DROP       PSI                  0.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:
  OVERALL COEFFICIENT          BTU/HR-SQFT-R        50.0000

                  ***  OVERALL RESULTS  ***

STREAMS:
              --------------------------------------
              |                                    |
S-417     ----->|              HOT              |-----> S-420
T=  6.9800D+02  |                               |      T=  5.0598D+02
P=  6.3970D+02  |                               |      P=  6.3970D+02
V=  1.0000D+00  |                               |      V=  1.0000D+00
              |                                    |
S-107     <-----|              COLD             |<----- S-104
T=  2.1200D+02  |                               |      T=  7.7042D+01
P=  4.2414D+01  |                               |      P=  4.2414D+01
V=  0.0000D+00  |                               |      V=  0.0000D+00
              --------------------------------------

DUTY AND AREA:
  CALCULATED HEAT DUTY          BTU/HR          36902766.2465
  CALCULATED (REQUIRED) AREA    SQFT                1615.4392
  ACTUAL EXCHANGER AREA         SQFT                1615.4392
  PER CENT OVER-DESIGN                                 0.0000

HEAT TRANSFER COEFFICIENT:
```

```
    AVERAGE COEFFICIENT (DIRTY)    BTU/HR-SQFT-R          50.0000
    UA (DIRTY)                 BTU/HR-R           80771.9596

  LOG-MEAN TEMPERATURE DIFFERENCE:
    LMTD CORRECTION FACTOR                             1.0000
    LMTD (CORRECTED)             F                  456.8760
    NUMBER OF SHELLS IN SERIES                          1

  PRESSURE DROP:
    HOTSIDE, TOTAL              PSI                  0.0000
    COLDSIDE, TOTAL              PSI                  0.0000

  PRESSURE DROP PARAMETER:
    HOT SIDE:                                0.0000
    COLD SIDE:                                0.0000

 BLOCK:  MIX-100  MODEL: MIXER
 -----------------------------
  INLET STREAMS:        S-115      S-114      S-113
  OUTLET STREAM:        S-119
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

              ***  MASS AND ENERGY BALANCE  ***
                       IN             OUT       RELATIVE DIFF.
   TOTAL BALANCE
     MOLE(LBMOL/HR)          36372.3        36372.3        0.00000
     MASS(LB/HR   )         0.124500E+07    0.124500E+07     0.00000
     ENTHALPY(BTU/HR  )      -0.583515E+10   -0.583515E+10     0.00000

              ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           0.00000      LB/HR
   PRODUCT STREAMS CO2E         0.00000      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        0.00000      LB/HR

                ***  INPUT DATA  ***
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                              30
  CONVERGENCE TOLERANCE                                0.000100000
  OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES
```

```
BLOCK:  P-000    MODEL: PUMP
----------------------------
 INLET STREAM:          S-000
 OUTLET STREAM:         S-100
 PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

              ***  MASS AND ENERGY BALANCE  ***
                         IN           OUT       RELATIVE DIFF.
  TOTAL BALANCE
    MOLE(LBMOL/HR)           36372.6        36372.6        0.00000
    MASS(LB/HR   )         0.124500E+07    0.124500E+07     0.00000
    ENTHALPY(BTU/HR  )      -0.573013E+10   -0.573012E+10   -0.132700E-05

              ***  CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E            0.00000      LB/HR
  PRODUCT STREAMS CO2E         0.00000      LB/HR
  NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
  UTILITIES CO2E PRODUCTION     0.00000      LB/HR
  TOTAL CO2E PRODUCTION         0.00000      LB/HR

                ***  INPUT DATA  ***
  PRESSURE CHANGE  PSI                          2.00000
  DRIVER EFFICIENCY                            1.00000

  FLASH SPECIFICATIONS:
  LIQUID PHASE CALCULATION
  NO FLASH PERFORMED
  MAXIMUM NUMBER OF ITERATIONS                        30
  TOLERANCE                                0.000100000

                 ***  RESULTS  ***
  VOLUMETRIC FLOW RATE  CUFT/HR                  16,830.2
  PRESSURE CHANGE  PSI                          2.00000
  NPSH AVAILABLE   FT-LBF/LB                     27.2010
  FLUID POWER  HP                              2.44803
  BRAKE POWER  HP                               2.98844
  ELECTRICITY  KW                              2.22848
  PUMP EFFICIENCY USED                          0.81917
  NET WORK REQUIRED  HP                          2.98844
  HEAD DEVELOPED FT-LBF/LB                       3.89325

BLOCK:  R-100    MODEL: RYIELD
```

```
 ------------------------------
   INLET STREAM:          S-107
   OUTLET STREAM:         S-110
   PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                          IN          OUT       GENERATION   RELATIVE DIFF.
   TOTAL BALANCE
   MOLE(LBMOL/HR)         12124.2       12124.1     -0.102851       0.00000
   MASS(LB/HR   )         415000.       415000.                     0.00000
   ENTHALPY(BTU/HR  )   -0.187310E+10 -0.194673E+10               0.378200E-01

                   ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E            0.00000      LB/HR
    PRODUCT STREAMS CO2E         0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                     ***  INPUT DATA  ***
   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE F                              212.000
   SPECIFIED PRESSURE    PSIA                           14.6959
   MAXIMUM NO. ITERATIONS                                  30
   CONVERGENCE TOLERANCE                                  0.000100000

    MASS-YIELD
     SUBSTREAM MIXED   :
     WATER     0.474        GLUCOSE   0.526

                      ***  RESULTS  ***
   OUTLET TEMPERATURE    F                               212.00
   OUTLET PRESSURE       PSIA                           14.696
   HEAT DUTY             BTU/HR                     -0.73625E+08
   VAPOR FRACTION                                   0.0000



   V-L PHASE EQUILIBRIUM :

     COMP            F(I)          X(I)          Y(I)          K(I)
     WATER           0.90000       0.90000       1.0000        1.0028
```

```
   GLUCOSE         0.99999E-01    0.99999E-01    0.23398E-06    0.21117E-05

BLOCK:  REF-500  MODEL: HEATER
------------------------------
  INLET STREAM:          S-521
  OUTLET STREAM:         S-508
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                 ***  MASS AND ENERGY BALANCE  ***
                              IN             OUT        RELATIVE DIFF.
   TOTAL BALANCE
     MOLE(LBMOL/HR)           705.706        705.706        0.00000
     MASS(LB/HR   )          74508.1        74508.1         0.00000
     ENTHALPY(BTU/HR  )      -0.681302E+07   -0.897628E+07    0.240998

                 ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000      LB/HR
   PRODUCT STREAMS CO2E         0.00000      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        0.00000      LB/HR

                    ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE               F                    -22.0000
  SPECIFIED PRESSURE                PSIA                   14.6959
  MAXIMUM NO. ITERATIONS                                    30
  CONVERGENCE TOLERANCE                                      0.000100000



                     ***  RESULTS  ***
  OUTLET TEMPERATURE    F                             -22.000
  OUTLET PRESSURE       PSIA                         14.696
  HEAT DUTY             BTU/HR                   -0.21633E+07
  OUTLET VAPOR FRACTION                               0.0000
  PRESSURE-DROP CORRELATION PARAMETER                        0.0000



  V-L PHASE EQUILIBRIUM :
```

```
    COMP            F(I)         X(I)         Y(I)         K(I)
    P-XYL          0.71989      0.71989      0.53386      0.26983E-03
    O-XYL          0.33233E-01  0.33233E-01  0.18416E-01  0.20163E-03
    M-XYL          0.69612E-01  0.69612E-01  0.47600E-01  0.24880E-03
    N-HEX          0.32632E-09  0.32632E-09  0.13004E-07  0.14500E-01
    ETHYLBEN       0.11709E-01  0.11709E-01  0.10614E-01  0.32981E-03
    TOLUENE        0.10373      0.10373      0.36554      0.12822E-02
    BENZENE        0.32811E-07  0.32811E-07  0.62054E-06  0.68814E-02
    NAPTH          0.38125E-06  0.38125E-06  0.47681E-08  0.45507E-05
    1:2:4-01       0.70387E-03  0.70387E-03  0.73988E-04  0.38248E-04
    ISOPR-01       0.61117E-01  0.61117E-01  0.23867E-01  0.14209E-03
    N-HEP-01       0.30016E-05  0.30016E-05  0.26459E-04  0.32074E-02
    1-HEX-01       0.96289E-11  0.96289E-11  0.46729E-09  0.17658E-01
    1-HEP-01       0.14550E-06  0.14550E-06  0.14170E-05  0.35434E-02

 BLOCK:  SEP-300  MODEL: SEP
 ---------------------------
   INLET STREAM:          S-323
   OUTLET STREAMS:        S-325      S-313
   PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                               IN            OUT        RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)          7810.82        7810.82        0.00000
       MASS(LB/HR   )          153817.        153817.        0.189210E-15
       ENTHALPY(BTU/HR  )     -0.526297E+09  -0.541065E+09   0.272937E-01

                  ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E            93678.2      LB/HR
    PRODUCT STREAMS CO2E         93678.2      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000     LB/HR
    UTILITIES CO2E PRODUCTION     0.00000     LB/HR
    TOTAL CO2E PRODUCTION         0.00000     LB/HR


                    ***  INPUT DATA  ***

   FLASH SPECS FOR STREAM S-325
   TWO    PHASE  TP  FLASH
   PRESSURE DROP        PSI                        0.0
   MAXIMUM NO. ITERATIONS                               30
```

```
 CONVERGENCE TOLERANCE                            0.000100000

 FLASH SPECS FOR STREAM S-313
 TWO    PHASE  TP  FLASH
 PRESSURE DROP        PSI                         0.0
 MAXIMUM NO. ITERATIONS                               30
 CONVERGENCE TOLERANCE                            0.000100000

 FRACTION OF FEED
   SUBSTREAM= MIXED
     STREAM= S-313     CPT= PROPANE   FRACTION=          1.00000
                         CO2                 1.00000
                         H2                 0.0


                        ***  RESULTS  ***

 HEAT DUTY            BTU/HR                      -0.14768E+08

 COMPONENT = PROPANE
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-313      MIXED             1.00000

 COMPONENT = CO2
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-313      MIXED             1.00000

 COMPONENT = WATER
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-313      MIXED             1.00000

 COMPONENT = H2
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-325      MIXED             1.00000

BLOCK:  SPT-100  MODEL: FSPLIT
------------------------------
 INLET STREAM:         S-100
 OUTLET STREAMS:       S-101       S-102       S-103
 PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
```

```
                             IN           OUT        RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            36372.6        36372.6        0.00000
       MASS(LB/HR   )         0.124500E+07    0.124500E+07     0.00000
       ENTHALPY(BTU/HR  )      -0.573012E+10   -0.573012E+10     0.00000

                  ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E            0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                     ***  INPUT DATA  ***

  FRACTION OF FLOW               STRM=S-101    FRAC=        0.33333
                            STRM=S-102    FRAC=        0.33333

                     ***  RESULTS  ***

  STREAM= S-101          SPLIT=          0.33333     KEY=  0    STREAM-ORDER=   1
          S-102                  0.33333          0                2
          S-103                  0.33333          0                3

 BLOCK:  VAL-200  MODEL: VALVE
 -----------------------------
   INLET STREAM:          S-224
   OUTLET STREAM:         S-225
   PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                             IN           OUT        RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            36374.4        36374.4        0.00000
       MASS(LB/HR   )         0.125242E+07    0.125242E+07     0.00000
       ENTHALPY(BTU/HR  )      -0.597601E+10   -0.597601E+10     0.00000

                  ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E            0.00000      LB/HR
    PRODUCT STREAMS CO2E          0.00000      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
```

```
TOTAL CO2E PRODUCTION         0.00000      LB/HR

                    ***  INPUT DATA  ***

VALVE OUTLET PRESSURE     PSIA                        741.696
VALVE FLOW COEF CALC.                                 NO

                    FLASH SPECIFICATIONS:
NPHASE                                        2
MAX NUMBER OF ITERATIONS                               30
CONVERGENCE TOLERANCE                                  0.000100000

                    ***  RESULTS  ***

VALVE PRESSURE DROP       PSI                        418.606
```