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CHEMICAL SPECIES *and* CHEMICAL REACTIONS *of importance in* NONEQUILIBRIUM PERFORMANCE CALCULATIONS

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TRW SYSTEMS Group

One Space Park • Redondo Beach, California

CHEMICAL SPECIES AND CHEMICAL REACTIONS OF IMPORTANCE IN NONEQUILIBRIUM PERFORMANCE CALCULATIONS

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CONTENTS

I. INTRODUCTION

This report contains the results of a study to determine the chemical species and chemical reactions of importance in nonequilibrium performance calculations. This study was performed by TRW Systems Group for NASA (MSC) under contract NAS 9-4358, Improvement of Analytical Predictions of Delivered Specific Impulse.

The objective of this contract was to develop a family of four computer programs to calculate inviscid, one-dimensional and axisymmetric nonequilibrium nozzle flow fields accounting for the nonequilibrium effects of finite rate chemical reactions between gaseous combustion products and velocity and thermal lags between gaseous and condensed combustion products.

The four programs developed under this contract are:

- A one-dimensional program which calculates the equilibrium, frozen and kinetic performance of propellant systems having gaseous exhaust products containing the elements carbon, hydrogen, oxygen, nitrogen, fluorine and chlorine.
- A one-dimensional program which calculates the equilibrium, frozen and kinetic performance of systems having gaseous and condensed exhaust products containing the elements carbon, hydrogen, oxygen, nitrogen, fluorine, chlorine and one metal element, either aluminum, beryllium, boron or lithium.
- An axisymmetric program which calculates the kinetic performance of propellant systems having gaseous exhaust products containing the elements carbon, hydrogen, oxygen, nitrogen, fluorine and chlorine. On option, this program considers either the expansion of a uniform mixture (the ideal engine case) or of a two-zoned mixture (the film cooled engine case).
- An axisymmetric program which calculates the kinetic performance of propellant systems having gaseous and condensed exhaust products containing the elements carbon, hydrogen, oxygen, nitrogen, fluorine, chlorine and one metal element, either aluminum, beryllium, boron or lithium. This program considers only the expansion of a uniform mixture (the ideal engine case).

These programs differ in a number of ways from previous programs developed to calculate nonequilibrium nozzle expansions.

In particular:

- The programs are completely self-contained requiring specification of only the propellant system (elemental composition and heat of formation), relaxation rates and nozzle geometry to run a case.
- The chemical species considered by the programs have been selected to allow accurate equilibrium, frozen and kinetic performance analyses of cryogenic, space storable, prepackaged, hybrid and solid propellant systems of current and projected operational use.
- All dissociation-recombination and binary exchange reactions between the gaseous species present in the exhaust are considered by the programs allowing complete kinetic expansion calculations.
- The programs utilize TRW Systems implicit integration method which allows rapid integration of the chemical and gas-particle relaxation equations from equilibrium chamber conditions. Typical run times are three minutes for the one-dimensional programs and ten minutes for the axisymmetric programs on an IBM 7094 Mod II computer.
- The programs allow analysis of the performance loss associated with film cooling in propellant systems having all gaseous exhaust products.
- The programs allow simultaneous consideration of both chemical and gas-particle relaxation losses in propellant systems having condensed exhaust products.
- The one-dimensional programs allow equilibrium, frozen and kinetic performance calculations to be performed during a single machine run.
- The programs are written in machine independent language (Fortran IV) allowing their use on all standard computers.

The study described in this report was performed to determine the significant chemical species and chemical reactions which need be considered in nonequilibrium performance calculations for typical propellant systems containing the elements: carbon, hydrogen, oxygen, nitrogen fluorine, chlorine; and one metal element, either aluminum, beryllium, boron or lithium. The significant chemical species were defined in contract NAS 9-4358 as those which must be considered to determine the equilibrium of the propellant systems under investigation to within 0.5 second of specific impulse at an area ratio of 40. The selection of the significant chemical species in typical propellant exhaust mixtures on the basis of equilibrium performance calculations does not, however, insure the validity of the selection for all nonequilibrium performance calculations. If the significant chemical species selection is valid for both equilibrium flow (infinite reaction rates) and frozen flow (zero reaction rates), however, the selection will also be valid for nonequilibrium flows having finite reaction rates. Thus, an additional restriction was imposed on the significant chemical species selection and the significant chemical species were defined as those which must be considered to determine both the equilibrium and frozen specific impulse of the propellant systems under investigation to within 0.5 second at an area ratio of 40.

After determining the significant species, all possible dissociation-recombination and binary exchange reactions between these species were studied. Those reactions having an energy barrier due to the fact that they cannot occur in the ground state (the so-called "spin forbidden" reactions) were identified, and those reactions, which while stoichiometrically possible were highly improbable due to structural or steric factors, were identified and eliminated from consideration. A literature rate survey was performed to determine the status of rate data for the chemical reactions of interest.

These studies are described in the following sections.

2. CHEMICAL SPECIES STUDY

A number of propellant systems containing the elements: carbon, hydrogen, oxygen, nitrogen, fluorine and chlorine, and one metal element, either aluminum, beryllium, boron or lithium, were selected as representative of typical liquid rocket cryogenic, space storable and prepackaged storable propellant systems, hybrid and solid rocket propellants. The propellant systems selected for study are given in Table I of Appendix A. These propellant systems are representative of current and projected operational propellant systems.

The number of chemical species in the exhaust mixtures of these propellants for which JANAF thermochemical data exists is over one hundred. The number of chemical reactions between these species which are stoichiometrically possible is naturally immense. It is clearly undesirable to attempt to account for all possible chemical species and chemical reactions in nonequilibrium performance calculations since it is known that relatively few of the total possible species and reactions are of engineering importance in nozzle and plume expansions.

The approach taken in this study to determine the minimum number of species which must be considered in nonequilibrium performance calculations was to consider equilibrium and frozen expansions as the limits of nonequilibrium expansions. Thus, by determining the significant species which must be considered to accurately calculate the equilibrium and frozen performance of these typical propellant systems, the significant species which must be considered in calculating the nonequilibrium performance of these and similar propellant systems can be determined. For the purpose of this study, the significant chemical species were thus defined as those which must be considered to determine both the equilibrium and frozen specific impulse of the propellant systems considered in the study to within 0.5 second at an area ratio of 40.

Equilibrium and frozen performance calculations were performed for the propellant systems listed in Table I, Appendix A, at two chamber pressures, 100 psia and 1000 psia, considering all species for which JANAF thermochemical data exist present in the exhaust mixtures. These calculations were used as the reference calculations for comparison with calculations performed considering fewer species. Those molecular species appearing in only trace amounts (less than approximately 10^{-3} mole percent) in the reference calculations were neglected and the calculations repeated to determine the effect of neglecting trace species on the calculated equilibrium and frozen performance of these propellant systems. After a series of such calculations considering different chemical species present in the various exhaust mixtures, it was determined that the significant species present in these exhaust mixtures are those given in Table II, Appendix A. Those significant species present in each propellant system studied are given in Table III, Appendix A. Comparisons of the equilibrium and frozen performance calculated considering all species present and only the significant species present is given in Tables IV through XXXVII in Appendix A for all propellant systems studied.

Examination of Tables IV through XXXVII, Appendix A, shows that for the nonmetallized propellant systems the maximum performance difference between the calculations considering all species present and only the significant species present is 0.49 second of specific impulse at an area ratio of 40. This difference occurs in the frozen performance calculation of the Chlorine Trifluoride/86% Monomethyl Hydrazine + 14% Hydrazine system at a mixture ratio of 3.2 and 100 psia chamber pressure. In the metallized systems, the maximum performance difference is 0.38 second of specific impulse at an area ratio of 40 which occurs in the frozen performance calculation of the double base-beryllium-ammonium perchlorate system for 100 psia chamber pressure. It is seen that the neglected chemical species have little effect on the calculated performance of the propellant systems studied. Thus, performance calculations performed considering only the significant chemical species given in Table II present in the exhaust mixture will allow the accurate determination of the equilibrium, frozen and nonequilibrium performance of these and similar propellant systems.

Although the significant chemical species given in Table II were determined from studying specific propellant systems, the utility of nonequilibrium performance programs based on this species selection is not limited to these specific propellant systems, but is equally valid for chemically similar propellant systems. In studying similar propellant systems, the applicability of the significant species selection can be simply established by comparing equilibrium and frozen performance calculations considering all species present and only the significant species present. For chemically nonsimilar systems, the above methods can be readily utilized to determine the significant chemical species in these systems.

3. CHEMICAL REACTION STUDY

Having identified the significant chemical species in the above propellant systems, all possible recombination-dissociation and binary exchange reactions between the significant species present in each propellant system were studied. Those reactions which, although stoichiometrically possible, were highly improbable on the basis of structural or steric factors were eliminated resulting in the identification of those reactions given in Tables I through VI, Appendix B, as those reactions of possible chemical significance in nonequilibrium expansions of the propellant systems studied.

Those reactions eliminated due to steric and structural arguments (listed in Table VII, Appendix B) involve the breaking and formation of a number of chemical bonds and molecular rearrangements which are highly improbable compared to other reactions which can occur between the same species.

Although arguments can be given that some of the reactions identified to be of possible chemical significance in the nonequilibrium expansion of the propellant systems studied can be of little significance due to concentration considerations or possible activation energy considerations, current lack of rate knowledge precludes their elimination at this time. This approach of retaining all possible chemical reactions in nonequilibrium calculations which cannot be eliminated due to steric consideration insures that future rate measurements which may change the relative importance of various chemical reactions will not affect the nonequilibrium computer programs developed by TRW for NASA.

4. CHEMICAL REACTION RATE STUDY

A literature survey was performed to determine the status of rate data for the chemical reactions given in Tables I through VI of Appendix B. Those reactions for which rates have been reported are given in Table IX of Appendix B. In addition, those reactions having an energy barrier due to the fact that they cannot occur in the ground state (the so-called "spin forbidden" reactions) were identified and are listed in Table VIII of Appendix B.

Order of magnitude rate estimates can be obtained by statistical mechanics and kinetic theory for those reactions for which rate data are not reported. When rate constants are represented by an Arrhenius equation, $k = AT^n \exp(-{}^{E}/RT)$, where T is the absolute temperature, R is the gas constant, A is the frequency factor, E is the activation energy, and n determines the pre-exponential temperature dependence, order of magnitude approximations can be made as follows:

A. Exothermic, trimolecular reactions

$$B + C + M \rightleftharpoons BC + M \quad , \quad k = 3x10^{16}\ T^{-0.5}$$

B. Exothermic, bimolecular reactions with triatomic transition states.

$B + CD \rightleftharpoons BC + D$, $k = 5 \times 10^{11} T^{0.5} \exp\left\{- E/RT\right\}$

where E = 5.5% of the CD bond energy (Hirschfelder Rule)

C. Exothermic, bimolecular reactions with transition states of more than three atoms

$BC + DE \rightleftharpoons BCD + E$, $k = 1 \times 10^{11} T^{0.5} \exp\left\{- E/RT\right\}$

where E = 5.5% of the DE bond energy

D. Exothermic, bimolecular, binary exchange reactions

$BC + DE \rightleftharpoons BD + CE$, $k = 1 \times 10^{10} T^{0.5} \exp\left\{- E/RT\right\}$

where E = 28% of the sum of the BC and DE bond energies

The reaction rates for the "spin forbidden" reactions can be similarly estimated if the rate constants are corrected by Boltzmann factors for the fact that these reactions do not occur in the ground state.

The above methods of estimating exothermic reaction rates are similar to those used by Tunder, et al. *

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* R. Tunder, S. Mayer, B. Cook, and L. Schieler, "Compilation of Reaction Rate Data for Nonequilibrium Performance and Re-entry Calculation Programs," Aerospace Corporation (1966).

APPENDIX A

Table I. Propellant Systems Studied at Chamber Pressures of 100 and 1000 psia to Identify Significant Chemical Species

	Oxidizer/Fuel	Mixture Ratios
1.	Oxygen/Hydrogen	MR = 2.0, 4.0, 5.0, 6.0, 10.0
2.	Fluorine/Hydrogen	MR = 3.0, 7.0, 10.0, 13.0, 20.0
3.	Oxygen/RP-1	MR = 1.0, 2.2, 2.6, 3.0, 5.0
4.	Nitrogen Tetroxide/Hydrazine	MR = 0.5, 0.9, 1.1, 1.3, 2.0
5.	Compound "A"/ Hydrazine	MR = 1.0, 2.3, 2.5, 2.7, 5.0
6.	Nitrogen Tetroxide/Monomethyl Hydrazine	MR = 0.5, 1.5, 1.8, 2.1, 3.5
7.	Oxygen Difluoride/Monomethyl Hydrazine	MR = 0.5, 1.5, 1.8, 2.1, 3.5
8.	Perchloryl Fluoride/Monomethyl Hydrazine	MR = 0.5, 1.5, 1.8, 2.1, 3.5
9.	Hydrazine/Diborane	MR = 1.15, 1.25, 1.35
10.	Oxygen Difluoride/Diborane	MR = 2.4, 3.2, 4.0
11.	Oxygen Difluoride/Lithium Hydride	MR = 2.5, 3.0, 3.5
12.	Chlorine Trifluoride/86% Monomethyl Hydrazine+14% Hydrazine	MR = 2.4, 2.8, 3.2
13.	Chlorine Trifluoride/49% Monomethyl Hydrazine+8% Hydrazine+ 43% Aluminum	MR = 2.5, 3.0, 3.5
14.	Chlorine Trifluoride/43% Monomethyl Hydrazine+7% Hydrazine+ 50% Boron	MR = 4.0, 5.0, 6.0
15.	Chlorine Trifluoride/43% Monomethyl Hydrazine+7% Hydrazine+ 50% Beryllium	MR = 3.5, 4.5, 5.5

Table 1 (Continued)

Oxidizer/Fuel	Composition		
16. Ammonium Perchlorate/PBAA— Aluminum	14	percent	Organic Fu
	16	"	Aluminum
	70	"	NH_4ClO_4
17. Ammonium Perchlorate/PBAA— Beryllium	16	"	Organic Fu
	13	"	Beryllium
	71	"	NH_4ClO_4
18. Ammonium Perchlorate/Double Base— Aluminum	69.4	"	Double Bas
	19.8	"	Aluminum
	10.8	"	NH_4ClO_4
19. Ammonium Perchlorate/Double Base— Beryllium	81	"	Double Bas
	10	"	Beryllium
	9	"	NH_4ClO_4

Table II. Species Selected for Use in the TRW/NASA Nonequilibrium Performance Programs

Basic Species for C, H, N, O, Cl, and F Propellant Systems Having Gaseous Combustion Products

C	Cl	F	H	N	O
CO	Cl_2	F_2	H_2	N_2	O_2
CO_2	ClF		H_2O	NO	OH
			HF		
			HCl		

Additional Species for Propellant Systems Having Condensed Carbon as a Combustion Product	Additional Species for Propellant Systems Containing Aluminum	Additional Species for Propellant Systems Containing Boron	Additional Species for Propellant Systems Containing Beryllium	Additional Species for Propellant Systems Containing Lithium
C(S)	Al	B	Be	Li
C_2	AlO	B(L)	BeOH	LiH
CH	Al_2O	B(S)	BeO_2H_2	LiOH
CH	Al_2O_3(L)	BO	BeO	LiO
CH_3	Al_2O_3(S)	BO_2	BeO(L)	Li_2O
CH_4	AlOCl	BF	BeO(S)	LiCl
C_2H_2	AlOF	BF_2	Be_2O	LiF
CF	AlCl	BF_3	BeCl	Li_2F_2
C_2F_2	$AlCl_2$	BCl	$BeCl_2$	
CN	$AlCl_3$	BCl_2	BeF	
ClCN	AlClF	BCl_3	BeF_2	
FCN	$AlClF_2$	BClF	BeClF	
HCN	$AlCl_2F$	BCl_2F		
	AlF	$BClF_2$		
	AlF_2	BOF		
	AlF_3	BOCl		
		BN		
		BN(S)		

Table III. Significant Species Considered in Each Propellant System

Propellant System (Table I)

O_2/H_2	F_2/H_2	$O_2/RP-1$	N_2O_4/H_2H_4	A/N_2H_4
		Species		
H	H	C	H	Cl
H_2	H_2	C(S)	H_2	Cl_2
H_2O	HF	CO	H_2O	ClF
O	F	CO_2	N	F
O_2	F_2	C_2	N_2	F_2
OH		CH	NO	H
		CH_2	O	H_2
		CH_3	O_2	HF
		CH_4	OH	HCl
		C_2H_2		N
		H		N_2
		H_2		
		H_2O		
		O		
		O_2		
		OH		
Total Number of Species Considered In Each Case				
6	5	15	9	11

Table III. (Continued)
Propellant System

N_2O_4/MMH	OF_2/MMH	ClO_3F/MMH	N_2H_4/B_2H_6	OF_2/B_2H_6
		Species		
C	C	C	B	B
C(S)	C(S)	C(S)	B(L)	B(L)
CO	CO	CO	B(S)	B(S)
CO_2	CO_2	CO_2	BN	BO
CN	CN	CN	BN(S)	BO_2
C_2	C_2	C_2	H	BF
CH	CH	CH	H_2	BF_2
CH_2	CH_2	CH_2	N	BF_3
CH_3	CH_3	CH_3	N_2	BOF
CH_4	CH_4	CH_4		F
C_2H_2	C_2H_2	C_2H_2		F_2
H	CF	CF		H
H_2	C_2F_2	C_2F_2		H_2
H_2O	F	Cl		H_2O
HCN	F_2	Cl_2		HF
N	FCN	ClCN		O
N_2	H	ClF		C_2
NO	H_2	F		OH
O	H_2O	F_2		
O_2	HF	FCN		
OH	HCN	H		
	N	H_2		
	N_2	H_2O		
	NO	HF		
	O	HCl		
	O_2	HCN		
	OH	N		
		N_2		
		NO		
		O		
		O_2		
		OH		
Total Number of Species Considered In Each System				
21	27	32	9	18

Table III. (Continued)
Propellant System

OF_2/LiH	CTF/86% MMH + 14% N_2H_4	CTF/49% MMH + 8% N_2H_4 + 43% Al	CTF/43% MMH + 7% N_2H_4 + 50% B	CTF/43% MMH + 7% N_2H_4 + 50% Be
		Species		
F	C	C	C	C
F_2	C(S)	C(S)	C(S)	C(S)
H	C_2	C_2	C_2	C_2
H_2	CN	CN	CN	CN
H_2O	CH	CH	CH	CH
HF	CH_2	CH_2	CH_2	CH_2
Li	CH_3	CH_3	CH_3	CH_3
LiH	CH_4	CH_4	CH_4	CH_4
LiOH	C_2H_2	C_2H_2	C_2H_2	C_2H_2
LiO	CF	CF	CF	CF
Li_2O	C_2F_2	C_2F_2	C_2F_2	C_2F_2
LiF	Cl	Cl	Cl	Cl
Li_2F_2	Cl_2	Cl_2	Cl_2	Cl_2
O	ClCN	ClCN	ClCN	ClCN
O_2	ClF	ClF	ClF	ClF
OH	F	F	F	F
	F_2	F_2	F_2	F_2
	FCN	FCN	FCN	FCN
	H	H	H	H
	H_2	H_2	H_2	H_2
	HF	HF	HF	HF
	HCl	HCl	HCl	HCl
	HCN	HCN	HCN	HCN
	N	N	N	N
	N_2	N_2	N_2	N_2
		Al	B	Be
		AlCl	B(L)	BeCl
		$AlCl_2$	B(S)	$BeCl_2$
		AlF	BF	BeF
		AlF_2	BF_2	BeF_2
		AlF_3	BF_3	BeClF
		$AlCl_3$	BN	
		AlClF	BN(S)	
		$AlClF_2$	BCl	
		$AlCl_2F$	BCl_2	
			BCl_3	
			BClF	
			BCl_2F	
			$BClF_2$	
Total Number of Species Considered In Each System				

Table III. (Continued)
Propellant System

AP/PBAA-Al	AP/PBAA-Be	AP/DB-Al	AP/DB-Be
	Species		
C	C	C	C
C(S)	C(S)	C(S)	C(S)
CO	CO	CO	CO
CO_2	CO_2	CO_2	CO_2
CN	CN	CN	CN
C_2	C_2	C_2	C_2
CH	CH	CH	CH
CH_2	CH_2	CH_2	CH_2
CH_3	CH_3	CH_3	CH_3
CH_4	CH_4	CH_4	CH_4
C_2H_2	C_2H_2	C_2H_2	C_2H_2
Cl	Cl	Cl	Cl
Cl_2	Cl_2	Cl_2	Cl_2
ClCN	ClCN	ClCN	ClCN
H	H	H	H
H_2	H_2	H_2	H_2
H_2O	H_2O	H_2O	H_2O
HCl	HCl	HCl	HCl
HCN	HCN	HCN	HCN
N	N	N	N
N_2	N_2	N_2	N_2
NO	NO	NO	NO
O	O	O	O
O_2	O_2	O_2	O_2
OH	OH	OH	OH
Al	Be	Al	Be
AlO	BeOH	AlO	BeOH
Al_2O	BeO_2H_2	Al_2O	BeO_2H_2
Al_2O_3(L)	BeO	Al_2O_3(L)	BeO
Al_2O_3(S)	BeO(L)	Al_2O_3(S)	BeO(L)
AlCl	BeO(S)	AlCl	BeO(S)
$AlCl_2$	BeCl	$AlCl_2$	BeCl
AlOCl	$BeCl_2$	AlOCl	$BeCl_2$
$AlCl_3$	Be_2O	$AlCl_3$	Be_2O
Total Number of Species Considered In Each System			
34	34	34	34

Table IV. Theoretical Specific Impulse of O_2/H_2 System
Chamber Pressure = 100 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	6 Significant Species	ΔI_{sp}	All Species	6 Significant Species	ΔI_{sp}
2.0	10.0	406.89	406.88	0.01	406.77	406.78	0.01
	20.0	419.36	419.36	0.00	419.25	419.25	0.00
	30.0	425.18	425.18	0.00	425.06	425.06	0.00
	40.0	428.76	428.76	0.00	428.64	428.65	0.01
4.0	10.0	425.99	425.99	0.00	415.04	415.04	0.00
	20.0	442.84	442.84	0.00	430.36	430.36	0.00
	30.0	450.70	450.70	0.00	437.48	437.48	0.00
	40.0	455.55	455.55	0.00	441.87	441.87	0.00
5.0	10.0	421.42	421.42	0.00	402.37	402.37	0.00
	20.0	440.51	440.51	0.00	418.04	418.04	0.00
	30.0	449.67	449.67	0.00	425.39	425.39	0.00
	40.0	455.40	455.40	0.00	429.93	429.93	0.00
6.0	10.0	412.08	412.08	0.00	387.58	387.58	0.00
	20.0	433.09	433.09	0.00	403.10	403.10	0.00
	30.0	443.41	443.41	0.00	410.43	410.43	0.00
	40.0	449.98	449.98	0.00	414.97	414.98	0.01
10.0	10.0	359.60	359.61	0.01	336.24	336.24	0.00
	20.0	379.67	379.68	0.01	349.97	349.97	0.00
	30.0	389.92	389.93	0.01	356.48	356.49	0.01
	40.0	396.60	396.60	0.00	360.54	360.55	0.01

Table V. Theoretical Specific Impulse of O_2/H_2 System
Chamber Pressure = 1000 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	6 Significant Species	ΔI_{sp}	All Species	Significant Species	ΔI_{sp}
2.0	10.0	406.89	406.87	0.02	406.85	406.85	0.00
	20.0	419.36	419.36	0.00	419.32	419.32	0.00
	30.0	425.18	425.18	0.00	425.14	425.14	0.00
	40.0	428.76	428.76	0.00	428.72	428.73	0.01
4.0	10.0	427.01	427.01	0.00	422.02	422.02	0.00
	20.0	443.60	443.60	0.00	437.95	437.95	0.00
	30.0	451.35	451.35	0.00	445.37	445.37	0.00
	40.0	456.13	456.13	0.00	449.95	449.95	0.00
5.0	10.0	424.36	424.36	0.00	413.55	413.55	0.00
	20.0	442.80	442.81	0.01	430.25	430.25	0.00
	30.0	451.66	451.66	0.00	438.15	438.15	0.00
	40.0	457.19	457.19	0.00	443.06	443.06	0.00
6.0	10.0	417.72	417.72	0.00	401.19	401.19	0.00
	20.0	437.68	437.68	0.00	417.96	417.97	0.01
	30.0	447.46	447.46	0.00	425.99	426.00	0.01
	40.0	453.68	453.68	0.00	431.01	431.02	0.01
10.0	10.0	366.60	366.61	0.01	348.49	348.52	0.03
	20.0	386.06	386.08	0.02	363.34	363.38	0.04
	30.0	395.86	395.87	0.01	370.50	370.53	0.03
	40.0	402.19	402.20	0.01	374.99	375.02	0.03

Table VI. Theoretical Performance of F_2/H_2 System

Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	5 Significant Species	ΔI_{sp}	All Species	5 Significant Species	ΔI_{sp}
3.0	10.0	425.46	425.46	0.00	423.31	423.31	0.00
	20.0	437.38	437.38	0.00	435.12	435.13	0.01
	30.0	442.87	442.88	0.01	440.57	440.57	0.00
	40.0	446.26	446.26	0.00	443.91	443.91	0.00
7.0	10.0	443.93	443.93	0.00	410.49	410.49	0.00
	20.0	460.76	460.76	0.00	421.97	421.97	0.00
	30.0	468.33	468.33	0.00	427.10	427.10	0.00
	40.0	472.87	472.87	0.00	430.22	430.22	0.00
10.0	10.0	439.15	439.15	0.00	397.12	397.12	0.00
	20.0	458.94	458.94	0.00	407.91	407.91	0.00
	30.0	468.23	468.23	0.00	412.68	412.68	0.00
	40.0	473.92	473.92	0.00	415.56	415.56	0.00
13.0	10.0	433.94	433.94	0.00	387.44	387.44	0.00
	20.0	454.89	454.89	0.00	397.75	397.75	0.00
	30.0	465.13	465.13	0.00	402.28	402.28	0.00
	40.0	471.57	471.57	0.00	405.00	405.00	0.00
20.0	10.0	416.55	416.56	0.01	363.45	363.45	0.00
	20.0	438.62	438.63	0.01	372.74	372.74	0.00
	30.0	449.49	449.49	0.00	376.81	376.81	0.00
	40.0	456.23	456.24	0.01	379.24	379.25	0.01

Table VII. Theoretical Performance of F_2/H_2 System
Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	5 Significant Species	ΔI_{sp}	All Species	5 Significant Species	ΔI_{sp}
3.0	10.0	425.51	425.51	0.00	424.77	424.77	0.00
	20.0	437.42	437.42	0.00	436.64	436.64	0.00
	30.0	442.91	442.91	0.00	442.12	442.12	0.00
	40.0	446.28	446.28	0.00	445.48	445.48	0.00
7.0	10.0	448.06	448.06	0.00	426.87	426.87	0.00
	20.0	463.74	463.74	0.00	439.46	439.46	0.00
	30.0	470.78	470.78	0.00	445.06	445.06	0.00
	40.0	475.01	475.01	0.00	448.45	448.45	0.00
10.0	10.0	447.25	447.25	0.00	416.27	416.27	0.00
	20.0	465.21	465.21	0.00	428.40	428.40	0.00
	30.0	473.51	473.51	0.00	433.75	433.76	0.01
	40.0	478.57	478.57	0.00	436.97	436.97	0.00
13.0	10.0	444.18	444.18	0.00	407.19	407.19	0.00
	20.0	463.58	463.58	0.00	418.88	418.88	0.00
	30.0	472.74	472.74	0.00	424.01	424.02	0.01
	40.0	478.41	478.41	0.00	427.08	427.10	0.02
20.0	10.0	428.82	428.82	0.00	383.44	383.44	0.00
	20.0	449.06	449.07	0.01	393.98	393.99	0.01
	30.0	458.41	458.42	0.01	398.59	398.59	0.00
	40.0	464.16	464.16	0.00	401.34	401.33	0.01

Table VIII. Theoretical Performance of O_2/RP-1 System

Chamber Pressure = 100 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	16 Significant Species	ΔI_{sp}	All Species	16 Significant Species	ΔI_{sp}
1.0	10.0	243.42	243.42	0.00	225.54	225.54	0.00
	20.0	256.28	256.28	0.00	232.46	232.46	0.00
	30.0	263.00	263.01	0.01	235.62	235.62	0.00
	40.0	267.48	267.48	0.00	237.51	237.51	0.00
2.2	10.0	320.10	320.10	0.00	301.61	301.62	0.01
	20.0	335.14	335.14	0.00	313.17	313.18	0.01
	30.0	342.49	342.49	0.00	318.61	318.62	0.01
	40.0	347.17	347.17	0.00	321.98	321.99	0.01
2.6	10.0	320.65	320.65	0.00	297.29	297.30	0.01
	20.0	338.29	338.29	0.00	309.03	309.04	0.01
	30.0	347.17	347.18	0.01	314.60	314.60	0.00
	40.0	352.91	352.91	0.00	318.06	318.07	0.01
3.0	10.0	315.06	315.07	0.01	291.40	291.40	0.00
	20.0	333.32	333.32	0.00	303.08	303.08	0.00
	30.0	342.84	342.84	0.00	308.65	308.65	0.00
	40.0	349.15	349.16	0.01	312.11	312.12	0.01
5.0	10.0	286.97	286.97	0.00	266.60	266.61	0.01
	20.0	303.36	303.37	0.01	277.51	277.53	0.02
	30.0	311.83	311.84	0.01	282.74	282.76	0.02
	40.0	317.40	317.41	0.01	286.03	286.03	0.00

Table IX. Theoretical Performance of O_2/RP-1 System
Chamber Pressure = 1000 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	16 Significant Species	ΔI_{sp}	All Species	16 Significant Species	ΔI_{sp}
1.0	10.0	250.41	250.42	0.01	232.73	232.74	0.01
	20.0	263.46	263.46	0.00	240.11	240.12	0.01
	30.0	270.24	270.24	0.00	243.52	243.53	0.01
	40.0	274.74	274.74	0.00	245.61	245.62	0.01
2.2	10.0	323.22	323.22	0.00	311.55	311.57	0.02
	20.0	337.63	337.63	0.00	323.94	323.96	0.02
	30.0	344.68	344.69	0.01	329.83	329.85	0.02
	40.0	349.18	349.18	0.00	333.49	333.52	0.03
2.6	10.0	327.31	327.32	0.01	309.12	309.14	0.02
	20.0	344.08	344.09	0.01	321.85	321.88	0.03
	30.0	352.41	352.41	0.00	327.97	328.00	0.03
	40.0	357.75	357.76	0.01	331.82	331.84	0.02
3.0	10.0	323.21	323.22	0.01	303.46	303.48	0.02
	20.0	341.38	341.39	0.01	316.16	316.18	0.02
	30.0	350.77	350.77	0.00	322.29	322.32	0.03
	40.0	356.94	356.94	0.00	326.16	326.18	0.02
5.0	10.0	293.24	293.25	0.01	276.55	276.58	0.03
	20.0	309.32	309.33	0.01	288.31	288.34	0.03
	30.0	317.51	317.52	0.01	294.01	294.04	0.03
	40.0	322.84	322.85	0.01	297.60	297.63	0.03

Table X. Theoretical Performance of N_2O_4/N_2H_4 System
Chamber Pressure = 100 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	9 Significant Species	ΔI_{sp}	All Species	9 Significant Species	ΔI_{sp}
0.5	10.0	288.09	288.09	0.00	287.46	287.46	0.00
	20.0	297.27	297.27	0.00	296.59	296.59	0.00
	30.0	301.54	301.53	0.01	300.83	300.83	0.00
	40.0	304.18	304.16	0.02	303.46	303.46	0.00
0.9	10.0	310.06	310.06	0.00	303.11	303.12	0.01
	20.0	321.77	321.77	0.00	314.00	314.00	0.00
	30.0	327.22	327.22	0.00	319.05	319.05	0.00
	40.0	330.58	330.58	0.00	322.16	322.17	0.01
1.1	10.0	314.68	314.68	0.00	302.44	302.44	0.00
	20.0	327.65	327.65	0.00	313.68	313.68	0.00
	30.0	333.76	333.76	0.00	318.91	318.92	0.01
	40.0	337.55	337.55	0.00	322.15	322.15	0.00
1.3	10.0	315.95	315.95	0.00	298.38	298.38	0.00
	20.0	330.24	330.24	0.00	309.65	309.65	0.00
	30.0	337.08	337.08	0.00	314.92	314.92	0.00
	40.0	341.35	341.35	0.00	318.18	318.18	0.00
2.0	10.0	290.92	290.93	0.01	276.98	276.99	0.01
	20.0	303.74	303.75	0.01	287.42	287.43	0.01
	30.0	309.84	309.84	0.00	292.31	292.32	0.01
	40.0	313.63	313.63	0.00	295.33	295.34	0.01

Table XI. Theoretical Performance of N_2O_4/N_2H_4 System
Chamber Pressure = 1000 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	9 Significant Species	ΔI_{sp}	All Species	9 Significant Species	I_{sp}
0.5	10.0	288.11	288.11	0.00	287.90	287.90	0.00
	20.0	297.31	297.28	0.03	297.06	297.06	0.00
	30.0	301.60	301.54	0.06	301.31	301.31	0.00
	40.0	304.29	304.17	0.12	303.94	303.94	0.00
0.9	10.0	310.57	310.58	0.01	307.54	307.55	0.01
	20.0	322.16	322.16	0.00	318.78	318.78	0.00
	30.0	327.55	327.55	0.00	324.00	324.00	0.00
	40.0	330.87	330.87	0.00	327.22	327.23	0.01
1.1	10.0	315.96	315.96	0.00	309.48	309.49	0.01
	20.0	328.62	328.62	0.00	321.31	321.31	0.00
	30.0	334.59	334.59	0.00	326.84	326.85	0.01
	40.0	338.29	338.29	0.00	330.27	330.28	0.01
1.3	10.0	318.45	318.44	0.01	307.01	307.01	0.00
	20.0	332.18	332.19	0.01	319.01	319.02	0.01
	30.0	338.75	338.75	0.00	324.66	324.67	0.01
	40.0	342.85	342.85	0.00	328.17	328.18	0.01
2.0	10.0	292.43	292.44	0.01	283.06	283.08	0.02
	20.0	304.91	304.92	0.01	294.02	294.04	0.02
	30.0	310.84	310.84	0.00	299.16	299.18	0.02
	40.0	314.53	314.53	0.00	302.36	302.38	0.02

Table XII. Theoretical Performance of Compound A/N_2H_4

Chamber Pressure = 100 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	11 Significant Species	ΔI_{sp}	All Species	11 Significant Species	ΔI_{sp}
1.0	10.0	312.43	312.43	0.00	304.68	304.69	0.01
	20.0	322.05	322.05	0.00	313.63	313.63	0.00
	30.0	326.41	326.41	0.00	317.70	317.70	0.00
	40.0	329.07	329.08	0.01	320.19	320.20	0.01
2.3	10.0	340.94	340.94	0.00	311.55	311.56	0.01
	20.0	355.27	355.27	0.00	320.42	320.43	0.01
	30.0	361.89	361.89	0.00	324.37	324.38	0.01
	40.0	365.92	365.92	0.00	326.76	326.77	0.01
2.5	10.0	341.63	341.63	0.00	312.42	312.43	0.01
	20.0	356.48	356.48	0.00	321.37	321.38	0.01
	30.0	363.42	363.42	0.00	325.36	325.37	0.01
	40.0	367.65	367.65	0.00	327.78	327.79	0.01
2.7	10.0	341.59	341.60	0.01	310.25	310.26	0.01
	20.0	356.86	356.86	0.00	319.02	319.04	0.02
	30.0	364.12	364.12	0.00	322.93	322.94	0.01
	40.0	368.60	368.60	0.00	325.29	325.30	0.01
5.0	10.0	263.30	263.30	0.00	238.27	238.27	0.00
	20.0	275.36	275.37	0.01	244.10	244.10	0.00
	30.0	281.01	281.01	0.00	246.72	246.72	0.00
	40.0	284.51	284.51	0.00	248.29	248.29	0.00

Table XIII Theoretical Performance of Compound A/N_2H_4

Chamber Pressure, 1000 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	11 Significant Species	ΔI_{sp}	All Species	11 Significant Species	ΔI_{sp}
1.0	10.0	312.84	312.84	0.00	309.46	309.47	0.01
	20.0	322.34	322.35	0.01	318.68	318.69	0.01
	30.0	326.66	326.66	0.00	322.87	322.88	0.01
	40.0	329.30	329.30	0.00	325.44	325.44	0.00
2.3	10.0	345.52	345.53	0.01	325.22	325.24	0.02
	20.0	358.71	358.71	0.00	335.06	335.08	0.02
	30.0	364.77	364.77	0.00	339.45	339.48	0.03
	40.0	368.46	368.46	0.00	342.11	342.14	0.03
2.5	10.0	346.79	346.79	0.00	324.51	324.53	0.03
	20.0	360.43	360.43	0.00	334.27	334.30	0.03
	30.0	366.73	366.74	0.01	338.63	338.66	0.03
	40.0	370.58	370.58	0.00	341.26	341.29	0.03
2.7	10.0	347.16	347.17	0.01	323.22	323.25	0.03
	20.0	361.31	361.31	0.00	332.87	332.91	0.04
	30.0	367.92	367.92	0.00	337.18	337.21	0.03
	40.0	371.96	371.97	0.01	339.78	339.81	0.03
5.0	10.0	269.48	269.49	0.01	247.86	247.86	0.00
	20.0	280.44	280.44	0.00	254.15	254.16	0.01
	30.0	285.69	285.70	0.01	257.00	257.00	0.00
	40.0	289.06	289.06	0.00	258.72	258.73	0.01

Table XIV. Theoretical Performance of N_2O_4/MMH System
Chamber Pressure ≈ 100 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	21 Significant Species	ΔI_{sp}	All Species	21 Significant Species	ΔI_{sp}
0.5	10.0	248.77	248.77	0.00	228.95	228.95	0.00
	20.0	261.37	261.37	0.00	235.58	235.57	0.01
	30.0	267.85	267.85	0.00	238.52	238.51	0.01
	40.0	272.11	272.11	0.00	240.24	240.24	0.00
1.5	10.0	304.66	304.66	0.00	295.75	295.76	0.01
	20.0	316.84	316.84	0.00	306.45	306.45	0.00
	30.0	322.68	322.68	0.00	311.42	311.43	0.01
	40.0	326.36	326.36	0.00	314.49	314.50	0.01
1.8	10.0	309.86	309.86	0.00	294.84	294.85	0.01
	20.0	323.42	323.42	0.00	305.92	305.92	0.00
	30.0	329.95	329.95	0.00	311.10	311.11	0.01
	40.0	334.07	334.07	0.00	314.31	314.31	0.00
2.1	10.0	310.76	310.76	0.00	290.57	290.57	0.00
	20.0	325.85	325.85	0.00	301.70	301.70	0.00
	30.0	333.18	333.18	0.00	306.92	306.93	0.01
	40.0	337.83	337.83	0.00	310.16	310.17	0.01
3.5	10.0	283.47	283.48	0.01	266.12	266.13	0.01
	20.0	297.25	297.25	0.00	276.42	276.43	0.01
	30.0	303.92	303.92	0.00	281.28	281.29	0.01
	40.0	308.13	308.14	0.01	284.30	284.31	0.01

Table XV. Theoretical Performance of N_2O_4/MMH System

Chamber Pressure = 1000 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	21 Significant Species	ΔI_{sp}	All Species	21 Significant Species	ΔI_{sp}
0.5	10.0	256.22	256.23	0.01	237.69	237.69	0.00
	20.0	268.83	268.84	0.01	244.82	244.82	0.00
	30.0	275.28	275.30	0.02	248.06	248.06	0.00
	40.0	279.51	279.52	0.01	250.01	250.00	0.01
1.5	10.0	305.33	305.38	0.00	300.95	300.96	0.01
	20.0	317.40	317.40	0.00	312.06	312.07	0.01
	30.0	323.17	323.17	0.00	317.24	317.25	0.01
	40.0	326.81	326.81	0.00	320.44	320.45	0.01
1.8	10.0	311.71	311.71	0.00	302.90	302.91	0.01
	20.0	324.86	324.87	0.01	314.64	314.66	0.02
	30.0	331.21	331.21	0.00	320.17	320.19	0.02
	40.0	335.21	335.21	0.00	323.60	323.62	0.02
2.1	10.0	314.28	314.28	0.00	300.03	300.04	0.01
	20.0	328.64	328.64	0.00	311.95	311.97	0.02
	30.0	335.63	335.63	0.00	317.61	317.62	0.01
	40.0	340.06	340.06	0.00	321.13	321.14	0.01
3.5	10.0	286.10	286.11	0.01	273.39	273.41	0.02
	20.0	299.34	299.34	0.00	284.31	284.33	0.02
	30.0	305.75	305.75	0.00	289.50	289.52	0.02
	40.0	309.79	309.79	0.00	292.74	292.75	0.01

Table XVI. Theoretical Performance of OF_2/MMH System
Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow: All Species	Equilibrium Flow: 27 Significant Species	Equilibrium Flow: ΔI_{sp}	Frozen Flow: All Species	Frozen Flow: 27 Significant Species	Frozen Flow: ΔI_{sp}
0.5	10.0	294.08	294.08	0.00	289.10	289.11	0.01
	20.0	305.56	305.56	0.00	298.20	298.20	0.00
	30.0	311.46	311.46	0.00	302.44	302.44	0.00
	40.0	315.34	315.34	0.00	305.06	305.07	0.01
1.5	10.0	357.82	357.82	0.00	333.68	333.68	0.00
	20.0	371.75	371.75	0.00	343.74	343.75	0.01
	30.0	378.16	378.16	0.00	348.27	348.28	0.01
	40.0	382.07	382.07	0.00	351.03	351.03	0.00
1.8	10.0	364.08	364.08	0.00	333.69	333.70	0.01
	20.0	379.97	379.98	0.01	343.78	343.79	0.01
	30.0	387.43	387.43	0.00	348.32	348.32	0.00
	40.0	392.03	392.03	0.00	351.07	351.07	0.00
2.1	10.0	366.18	366.19	0.01	331.65	331.65	0.00
	20.0	383.86	383.86	0.00	341.63	341.64	0.01
	30.0	392.34	392.34	0.00	346.10	346.11	0.01
	40.0	397.62	397.62	0.00	348.82	348.83	0.01
3.5	10.0	355.12	355.12	0.00	316.22	316.23	0.01
	20.0	374.07	374.08	0.01	325.35	325.36	0.01
	30.0	383.77	383.77	0.00	329.43	329.43	0.01
	40.0	390.11	390.11	0.00	331.89	331.89	0.00

Table XVII. Theoretical Performance of OF_2/MMH System
Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	27 Significant Species	ΔI_{sp}	All Species	27 Significant Species	ΔI_{sp}
0.5	10.0	296.12	296.13	0.01	289.65	289.67	0.02
	20.0	308.24	308.24	0.00	298.81	298.82	0.01
	30.0	314.41	314.42	0.01	303.07	303.09	0.02
	40.0	318.46	318.46	0.00	305.72	305.73	0.01
1.5	10.0	360.88	360.88	0.00	345.85	345.88	0.03
	20.0	374.01	374.02	0.01	356.83	356.83	0.00
	30.0	380.06	380.06	0.00	361.76	361.76	0.00
	40.0	383.76	383.76	0.00	364.75	364.75	0.00
1.8	10.0	369.15	369.15	0.00	347.86	347.89	0.03
	20.0	383.83	383.84	0.01	359.00	359.03	0.03
	30.0	390.71	390.72	0.01	364.03	364.06	0.03
	40.0	394.95	394.96	0.01	367.08	367.11	0.03
2.1	10.0	373.37	373.38	0.01	346.71	346.74	0.03
	20.0	389.59	389.59	0.00	357.82	357.85	0.03
	30.0	397.28	397.28	0.00	362.84	362.87	0.03
	40.0	402.06	402.07	0.01	365.88	365.91	0.03
3.5	10.0	363.75	363.75	0.00	330.31	330.33	0.02
	20.0	382.30	382.31	0.01	340.46	340.47	0.01
	30.0	391.64	391.64	0.00	345.00	345.02	0.02
	40.0	397.65	397.65	0.00	347.74	347.76	0.02

Table XVIII. Theoretical Performance of $ClOF_3$/MMH System

Chamber Pressure = 100 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	32 Significant Species	ΔI_{sp}	All Species	32 Significant Species	ΔI_{sp}
0.5	10.0	254.45	254.45	0.00	243.34	243.34	0.00
	20.0	266.45	266.45	0.00	250.69	250.69	0.00
	30.0	272.62	272.62	0.00	254.07	254.07	0.00
	40.0	276.67	276.67	0.00	256.12	256.11	0.01
1.5	10.0	306.02	306.03	0.01	294.32	294.32	0.00
	20.0	317.54	317.55	0.01	304.06	304.07	0.01
	30.0	322.99	322.99	0.00	308.52	308.51	0.01
	40.0	326.41	326.41	0.00	311.26	311.25	0.01
1.8	10.0	311.90	311.91	0.01	293.77	293.78	0.01
	20.0	324.93	324.93	0.00	303.77	303.78	0.01
	30.0	331.10	331.11	0.01	308.35	308.36	0.01
	40.0	334.96	334.97	0.01	311.17	311.18	0.01
2.1	10.0	313.63	313.63	0.00	290.35	290.36	0.01
	20.0	328.24	328.24	0.00	300.35	300.36	0.01
	30.0	335.25	335.25	0.00	304.95	304.96	0.01
	40.0	339.65	339.65	0.00	307.77	307.78	0.01
3.5	10.0	294.11	294.13	0.02	268.73	268.76	0.03
	20.0	309.53	309.55	0.02	277.92	277.95	0.03
	30.0	317.20	317.22	0.02	282.15	282.17	0.02
	40.0	322.11	322.12	0.01	284.75	284.77	0.02

Table XIX. Theoretical Performance of $ClOF_3$/MMH System
Chamber Pressure = 1000 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	32 Significant Species	ΔI_{sp}	All Species	32 Significant Species	ΔI_{sp}
0.5	10.0	259.96	259.97	0.01	246.91	246.91	0.00
	20.0	272.20	272.21	0.01	254.49	254.49	0.00
	30.0	278.45	278.46	0.01	257.99	257.99	0.00
	40.0	282.54	282.55	0.01	260.12	260.12	0.00
1.5	10.0	307.02	307.03	0.01	300.92	300.94	0.02
	20.0	318.29	318.31	0.02	311.15	311.17	0.02
	30.0	323.65	323.65	0.00	315.84	315.86	0.02
	40.0	327.01	327.00	0.01	318.72	318.74	0.02
1.8	10.0	314.18	314.19	0.01	303.09	303.12	0.03
	20.0	326.67	326.68	0.01	313.81	313.84	0.03
	30.0	332.61	332.61	0.00	318.76	318.79	0.03
	40.0	336.32	336.32	0.00	321.80	321.82	0.02
2.1	10.0	317.63	317.63	0.00	301.18	301.22	0.04
	20.0	331.37	331.38	0.01	312.05	312.09	0.04
	30.0	337.97	337.97	0.00	317.10	317.13	0.03
	40.0	342.10	342.10	0.00	320.19	320.23	0.04
3.5	10.0	299.59	299.63	0.04	278.90	278.98	0.08
	20.0	314.30	314.34	0.04	288.91	288.99	0.08
	30.0	321.52	321.55	0.03	293.56	293.63	0.07
	40.0	326.10	326.13	0.03	296.42	296.49	0.07

Table XX. Theoretical Performance of N_2H_4/B_2H_6 System

Chamber Pressure = 100 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	9 Significant Species	ΔI_{sp}	All Species	9 Significant Species	ΔI_{sp}
1.15	10.0	368.47	368.48	0.01	363.30	363.32	0.02
	20.0	385.60	385.60	0.00	379.82	379.84	0.02
	30.0	394.03	394.04	0.01	387.95	387.96	0.01
	40.0	399.43	399.43	0.00	393.14	393.15	0.01
1.25	10.0	365.63	365.63	0.00	362.80	362.85	0.05
	20.0	382.32	382.31	0.01	379.15	379.21	0.06
	30.0	390.50	390.50	0.00	387.18	387.24	0.06
	40.0	395.74	395.73	0.01	392.31	392.37	0.06
1.35	10.0	362.02	362.02	0.00	359.90	359.93	0.03
	20.0	378.26	378.26	0.00	375.90	375.94	0.04
	30.0	386.21	386.22	0.01	383.73	383.77	0.04
	40.0	391.28	391.28	0.00	388.72	388.76	0.04

Table XXI. Theoretical Performance of N_2H_4/B_2H_6 System
Chamber Pressure = 1000 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	9 Significant Species	ΔI_{sp}	All Species	Significant Species	ΔI_{sp}
1.15	10.0	368.81	368.84	0.03	366.59	366.71	0.12
	20.0	385.87	385.89	0.02	383.39	383.52	0.13
	30.0	394.28	394.29	0.01	391.67	391.80	0.13
	40.0	399.65	399.67	0.02	396.96	397.10	0.14
1.25	10.0	365.84	365.85	0.01	364.70	364.78	0.08
	20.0	382.48	382.48	0.00	381.21	381.29	0.08
	30.0	390.65	390.66	0.01	389.32	389.40	0.08
	40.0	395.87	395.87	0.00	394.50	394.58	0.08
1.35	10.0	362.18	362.18	0.00	361.38	361.42	0.04
	20.0	378.39	378.39	0.00	377.50	377.54	0.04
	30.0	386.33	386.33	0.00	385.39	385.44	0.05
	40.0	391.38	391.39	0.01	390.42	390.47	0.05

Table XXII. Theoretical Performance of OF_2/B_2H_6 System
Chamber Pressure = 100 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	18 Significant Species	ΔI_{sp}	All Species	Significant Species	ΔI_{sp}
2.4	10.0	380.05	380.16	0.11	351.00	351.13	0.13
	20.0	399.82	399.91	0.09	363.42	363.54	0.12
	30.0	409.90	409.98	0.08	369.21	369.32	0.11
	40.0	416.49	416.57	0.08	372.78	372.88	0.10
3.2	10.0	388.09	388.17	0.08	355.80	355.87	0.07
	20.0	408.71	408.78	0.07	368.17	368.24	0.07
	30.0	419.32	419.39	0.07	373.92	373.98	0.06
	40.0	426.31	426.37	0.06	377.46	377.52	0.06
4.0	10.0	390.36	390.37	0.01	355.15	355.12	0.03
	20.0	411.28	411.29	0.01	367.31	367.26	0.05
	30.0	422.03	422.04	0.01	372.94	372.89	0.05
	40.0	429.10	429.11	0.01	376.40	376.35	0.05

Table XXIII. Theoretical Performance of OF_2/B_2H_6
Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	18 Significant Species	ΔI_{sp}	All Species	18 Significant Species	ΔI_{sp}
2.4	10.0	387.64	387.87	0.23	364.44	364.76	0.32
	20.0	407.03	407.21	0.19	378.00	378.28	0.28
	30.0	416.96	417.14	0.18	384.38	384.65	0.27
	40.0	423.54	423.71	0.17	388.33	388.60	0.27
3.2	10.0	397.86	398.06	0.20	371.29	371.47	0.18
	20.0	418.35	418.52	0.17	384.94	385.10	0.16
	30.0	428.84	429.01	0.17	391.38	391.54	0.16
	40.0	435.75	435.90	0.15	395.38	395.52	0.14
4.0	10.0	400.50	400.57	0.07	371.13	371.10	0.03
	20.0	421.26	421.34	0.08	384.58	384.54	0.04
	30.0	431.81	431.89	0.07	390.93	390.87	0.06
	40.0	438.70	438.76	0.06	394.86	394.79	0.07

Table XXIV. Theoretical Performance of OF_2/LiH System
Chamber Pressure = 100 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	16 Significant Species	ΔI_{sp}	All Species	16 Significant Species	ΔI_{sp}
2.5	10.0	346.73	346.76	0.03	322.10	322.19	0.09
	20.0	364.06	364.09	0.03	333.44	333.54	0.10
	30.0	372.91	373.93	0.02	338.72	338.82	0.10
	40.0	378.72	378.74	0.02	341.99	342.09	0.10
3.0	10.0	352.67	352.72	0.05	322.46	322.58	0.12
	20.0	371.27	371.32	0.05	333.66	333.79	0.13
	30.0	380.68	380.72	0.04	338.86	338.99	0.13
	40.0	386.79	386.83	0.04	342.07	342.19	0.12
3.5	10.0	351.84	351.89	0.05	320.09	320.23	0.14
	20.0	370.89	370.94	0.05	330.97	331.12	0.15
	30.0	380.66	380.70	0.04	336.00	336.15	0.15
	40.0	387.06	387.10	0.04	339.09	339.24	0.15

Table XXV. Theoretical Performance of OF_2/LiH System
Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	16 Significant Species	ΔI_{sp}	All Species	16 Significant Species	ΔI_{sp}
2.5	10.0	354.00	354.04	0.04	335.21	335.35	0.14
	20.0	371.48	371.52	0.04	347.82	347.97	0.15
	30.0	380.41	380.45	0.04	353.78	353.93	0.15
	40.0	386.30	386.33	0.03	357.49	357.64	0.15
3.0	10.0	361.04	361.10	0.06	337.48	337.65	0.17
	20.0	379.22	379.26	0.04	350.01	350.18	0.17
	30.0	388.41	388.46	0.05	355.91	356.09	0.18
	40.0	394.42	394.47	0.05	359.58	359.76	0.18
3.5	10.0	361.02	361.09	0.07	335.49	335.67	0.18
	20.0	379.67	379.73	0.06	347.67	347.87	0.20
	30.0	389.14	389.20	0.06	353.40	353.60	0.20
	40.0	395.33	395.38	0.05	356.94	357.14	0.20

Table XXVI. Theoretical Performance of CTF/86% MMH+ +14% N_2H_4 System

Chamber Pressure = 100 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	25 Significant Species	ΔI_{sp}	All Species	25 Significant Species	ΔI_{sp}
2.4	10.0	305.43	305.45	0.02	283.35	283.56	0.21
	20.0	318.46	318.48	0.02	292.71	292.92	0.21
	30.0	324.54	324.55	0.01	296.99	297.21	0.22
	40.0	328.28	328.29	0.01	299.62	299.84	0.22
2.8	10.0	306.97	307.01	0.04	281.68	282.04	0.36
	20.0	320.78	320.81	0.03	290.82	291.20	0.38
	30.0	327.28	327.31	0.03	295.00	295.39	0.39
	40.0	331.29	331.32	0.03	297.55	297.95	0.40
3.2	10.0	304.26	304.32	0.06	278.46	278.92	0.46
	20.0	317.30	317.34	0.04	287.35	287.84	0.49
	30.0	323.65	323.66	0.01	291.41	291.90	0.49
	40.0	327.72	327.68	0.04	293.87	294.39	0.49

Table XXVII. Theoretical Performance of CTF/86% MMH + +14% N_2H_4 System

Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	25 Significant Species	ΔI_{sp}	All Species	25 Significant Species	ΔI_{sp}
2.4	10.0	307.49	307.52	0.03	289.38	289.58	0.20
	20.0	320.02	320.04	0.02	299.28	299.48	0.20
	30.0	325.86	325.87	0.01	303.82	304.03	0.21
	40.0	329.45	329.47	0.02	306.61	306.83	0.22
2.8	10.0	309.92	309.96	0.04	287.92	288.23	0.31
	20.0	323.05	323.09	0.04	297.66	297.99	0.33
	30.0	329.21	329.24	0.03	302.13	302.46	0.33
	40.0	333.01	333.04	0.03	304.87	305.21	0.34
3.2	10.0	306.57	306.62	0.05	284.89	285.04	0.15
	20.0	319.54	319.49	0.05	294.41	294.58	0.17
	30.0	325.91	325.74	0.17	298.77	298.95	0.16
	40.0	329.96	329.67	0.29	301.44	301.62	0.18

Table XXVIII. Theoretical Performance of CTF/49% MMH+8% N_2H_4+43% Al

Chamber Pressure = 100 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	35 Significant Species	ΔI_{sp}	All Species	35 Significant Species	ΔI_{sp}
2.5	10.0	295.19	295.52	0.33	267.94	268.09	0.15
	20.0	311.19	311.47	0.28	277.15	277.35	0.20
	30.0	319.41	319.68	0.27	281.41	281.64	0.23
	40.0	324.83	325.08	0.25	284.04	284.28	0.24
3.0	10.0	294.88	295.02	0.14	266.75	266.86	0.11
	20.0	310.96	311.08	0.12	275.73	275.87	0.14
	30.0	319.22	319.32	0.10	279.88	280.03	0.15
	40.0	324.64	324.74	0.10	282.42	282.59	0.17
3.5	10.0	292.48	292.56	0.08	264.69	264.83	0.14
	20.0	307.89	307.95	0.06	273.45	273.60	0.15
	30.0	315.45	315.51	0.06	277.49	277.65	0.16
	40.0	320.23	320.28	0.05	279.97	280.13	0.16

Table XXIX. Theoretical Performance of CTF/49% MMH+8% N_2H_4+43% Al

Chamber Pressure = 1000 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	35 Significant Species	ΔI_{sp}	All Species	35 Significant Species	ΔI_{sp}
2.5	10.0	302.13	302.24	0.11	280.35	280.47	0.12
	20.0	318.15	318.24	0.09	290.64	290.79	0.15
	30.0	326.33	326.41	0.08	295.49	295.64	0.15
	40.0	331.68	331.76	0.08	298.49	298.66	0.17
3.0	10.0	301.82	301.92	0.10	279.06	279.19	0.13
	20.0	317.88	317.96	0.08	289.06	289.22	0.16
	30.0	326.04	326.11	0.07	293.75	293.92	0.17
	40.0	331.36	331.43	0.07	296.66	296.82	0.16
3.5	10.0	298.45	298.54	0.09	276.56	276.74	0.18
	20.0	312.93	313.00	0.07	286.27	286.45	0.18
	30.0	320.00	320.06	0.06	290.80	290.99	0.19
	40.0	324.53	324.57	0.04	293.60	293.79	0.19

Table XXX. Theoretical Performance of CTF/43%MMH+ +7% N_2H_4+50% B

Chamber Pressure = 100 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	39 Significant Species	ΔI_{sp}	All Species	39 Significant Species	ΔI_{sp}
4.0	10.0	288.95	289.09	0.14	263.45	263.37	0.08
	20.0	305.12	305.24	0.12	273.00	272.95	0.05
	30.0	313.51	313.63	0.12	277.49	277.45	0.04
	40.0	319.07	319.18	0.11	280.28	280.24	0.04
5.0	10.0	291.82	291.89	0.07	264.37	264.35	0.02
	20.0	308.30	308.36	0.06	273.76	273.74	0.02
	30.0	316.82	316.89	0.07	278.15	278.14	0.01
	40.0	322.46	322.52	0.06	280.88	280.87	0.01
6.0	10.0	291.96	291.99	0.03	263.00	263.06	0.06
	20.0	308.50	308.55	0.05	272.17	272.23	0.05
	30.0	317.09	317.13	0.04	276.46	276.52	0.06
	40.0	322.75	322.79	0.04	279.11	279.17	0.06

Table XXXI. Theoretical Performance of CTF/43% MMH+ +7% N_2H_4+50% B

Chamber Pressure = 1000 psia

		Equilibrium Flow			Frozen Flow		
Mixture Ratio	Area Ratio	All Species	39 Significant Species	ΔI_{sp}	All Species	39 Significant Species	ΔI_{sp}
4.0	10.0	296.55	296.64	0.09	275.73	275.73	0.00
	20.0	312.87	312.95	0.08	286.35	286.37	0.02
	30.0	321.32	321.39	0.07	291.44	291.46	0.02
	40.0	326.91	326.98	0.07	294.62	294.65	0.03
5.0	10.0	299.71	299.77	0.06	276.87	276.94	0.07
	20.0	316.29	316.35	0.06	287.27	287.34	0.07
	30.0	324.86	324.92	0.06	292.23	292.30	0.07
	40.0	330.52	330.58	0.04	295.32	295.40	0.08
6.0	10.0	300.03	300.10	0.07	275.53	275.65	0.12
	20.0	316.29	316.37	0.08	285.64	285.78	0.14
	30.0	324.64	324.71	0.07	290.44	290.58	0.14
	40.0	330.07	330.13	0.06	293.44	293.57	0.13

Table XXXII. Theoretical Performance of CTF/45% MMH+ +7% N_2H_4+50% Be

Chamber Pressure = 100 psia

Mixture Ratio	Area Ratio	Equilibrium Flow All Species	Equilibrium Flow 31 Significant Species	Equilibrium Flow ΔI_{sp}	Frozen Flow All Species	Frozen Flow Significant Species	Frozen Flow ΔI_{sp}
3.5	10.0	309.82	309.98	0.16	283.86	283.77	0.09
	20.0	326.98	327.13	0.15	294.12	294.04	0.08
	30.0	335.88	336.02	0.14	298.95	298.88	0.07
	40.0	341.78	341.91	0.13	301.95	391.89	0.06
4.5	10.0	310.36	310.43	0.07	282.28	282.07	0.21
	20.0	327.39	327.47	0.08	292.16	291.94	0.22
	30.0	336.15	336.22	0.07	296.77	296.56	0.21
	40.0	341.92	341.99	0.07	299.64	299.42	0.22
5.5	10.0	306.16	306.22	0.06	277.60	277.57	0.03
	20.0	321.84	321.89	0.05	287.04	287.01	0.03
	30.0	329.47	329.52	0.05	291.42	291.41	0.01
	40.0	334.30	334.34	0.04	294.14	294.12	0.02

Table XXXIII. Theoretical Performance of CTF/45% MMH + +7% N_2H_4+50% Be

Chamber Pressure = 1000 psia

Mixture Ratio	Area Ratio	Equilibrium Flow All Species	Equilibrium Flow 31 Significant Species	Equilibrium Flow ΔI_{sp}	Frozen Flow All Species	Frozen Flow 31 Significant Species	Frozen Flow ΔI_{sp}
3.5	10.0	318.41	318.50	0.09	297.23	297.24	0.01
	20.0	335.57	335.66	0.09	308.51	308.54	0.03
	30.0	344.44	344.53	0.09	313.91	313.95	0.04
	40.0	350.30	350.38	0.08	317.29	317.33	0.04
4.5	10.0	318.50	318.56	0.06	295.31	295.25	0.06
	20.0	335.44	335.50	0.06	306.15	306.10	0.05
	30.0	344.10	344.16	0.06	311.29	311.24	0.05
	40.0	349.76	349.81	0.05	314.50	314.45	0.05
5.5	10.0	312.58	312.64	0.06	290.01	290.07	0.06
	20.0	327.15	327.21	0.06	300.32	300.39	0.07
	30.0	334.27	334.31	0.04	305.18	305.24	0.06
	40.0	338.84	338.86	0.02	308.19	308.26	0.07

Table XXXIV. Theoretical Performance of AP/PBAA-Al System

		Equilibrium Flow			Frozen Flow		
Chamber Pressure (psia)	Area Ratio	All Species	34 Significant Species	ΔI_{sp}	All Species	34 Significant Species	ΔI_{sp}
100	10.0	283.70	283.71	0.01	270.33	270.35	0.02
	20.0	299.29	299.29	0.00	282.14	282.16	0.02
	30.0	307.05	307.05	0.00	287.89	287.91	0.02
	40.0	312.03	312.04	0.01	291.52	291.55	0.03
1000	10.0	286.52	286.54	0.02	277.34	277.38	0.04
	20.0	301.70	301.70	0.00	289.74	289.78	0.04
	30.0	309.22	309.22	0.00	295.82	295.87	0.05
	40.0	314.04	314.04	0.00	299.70	299.74	0.04

Tablve XXXV. Theoretical Performance of AP/PBAA-Be System

Chamber Pressure (psia)	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	34 Significant Species	ΔI_{sp}	All Species	34 Significant Species	ΔI_{sp}
100	10.0	305.71	305.74	0.03	289.32	289.45	0.13
	20.0	324.00	324.03	0.03	303.10	303.25	0.15
	30.0	333.39	333.41	0.03	309.93	310.09	0.16
	40.0	339.56	339.57	0.01	314.32	314.48	0.16
1000	10.0	308.84	308.87	0.03	296.54	296.68	0.14
	20.0	327.15	327.18	0.03	311.01	311.16	0.15
	30.0	336.46	336.48	0.02	318.25	318.40	0.15
	40.0	342.53	342.55	0.02	322.91	323.07	0.16

Table XXXVI. Theoretical Performance of AP/DB-Al

Chamber Pressure (psia)	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	34 Significant Species	ΔI_{sp}	All Species	34 Significant Species	ΔI_{sp}
100	10.0	284.61	284.62	0.01	272.41	272.47	0.06
	20.0	300.70	300.73	0.03	284.76	284.83	0.07
	30.0	309.26	309.24	0.02	290.86	290.93	0.07
	40.0	314.82	314.78	0.04	294.76	294.83	0.07
1000	10.0	288.46	288.47	0.01	280.52	280.64	0.12
	20.0	304.20	304.20	0.00	293.53	293.67	0.14
	30.0	312.50	312.51	0.01	300.01	300.15	0.14
	40.0	317.87	317.89	0.02	304.18	304.32	0.14

Tablve XXXVII. Theoretical Performance of AP/DB-Be System

Chamber Pressure (psia)	Area Ratio	Equilibrium Flow			Frozen Flow		
		All Species	34 Significant Species	ΔI_{sp}	All Species	34 Significant Species	ΔI_{sp}
100	10.0	303.92	304.00	0.08	289.89	290.18	0.29
	20.0	322.16	322.23	0.07	303.67	304.00	0.33
	30.0	331.52	331.58	0.06	310.52	310.88	0.36
	40.0	337.66	337.72	0.06	314.92	315.30	0.38
1000	10.0	307.68	307.72	0.04	298.31	298.48	0.17
	20.0	325.93	325.97	0.04	312.87	313.06	0.19
	30.0	335.20	335.23	0.03	320.18	320.38	0.20
	40.0	341.24	341.27	0.03	324.90	325.10	0.20

APPENDIX B

Table 1. Chemical Reactions of Importance in Nonmetallized Propellant Systems Containing Carbon, Hydrogen, Oxygen, Nitrogen, Fluorine and Chlorine Having Gaseous Combustion Products

Chemical Reaction
$CO_2 + M \rightleftharpoons CO + O + M$
$H_2O + M \rightleftharpoons OH + H + M$
$CO + M \rightleftharpoons C + O + M$
$Cl_2 + M \rightleftharpoons 2Cl + M$
$F_2 + M \rightleftharpoons 2F + M$
$HCl + M \rightleftharpoons H + Cl + M$
$HF + M \rightleftharpoons H + F + M$
$H_2 + M \rightleftharpoons 2H + M$
$N_2 + M \rightleftharpoons 2H + M$
$NO + M \rightleftharpoons N + O + M$
$OH + M \rightleftharpoons O + H + M$
$O_2 + M \rightleftharpoons 2O + M$
$ClF + M \rightleftharpoons Cl + F + M$
$CO_2 + H \rightleftharpoons CO + OH$
$CO_2 + O \rightleftharpoons CO + O_2$
$H_2O + Cl \rightleftharpoons OH + HCl$
$H_2O + H \rightleftharpoons OH + H_2$
$H_2O + O \rightleftharpoons 2OH$
$CO + CO \rightleftharpoons CO_2 + C$
$CO + H \rightleftharpoons C + OH$
$CO + N \rightleftharpoons C + NO$
$CO + NO \rightleftharpoons CO_2 + N$
$CO + O \rightleftharpoons C + O_2$
$HCl + Cl \rightleftharpoons H + Cl_2$

Chemical Reaction
$HCl + HCl \rightleftharpoons H_2 + Cl_2$
$HCl + O \rightleftharpoons OH + Cl$
$HF + Cl \rightleftharpoons HCl + F$
$HF + F \rightleftharpoons H + F_2$
$HF + H \rightleftharpoons H_2 + F$
$HF + HF \rightleftharpoons H_2 + F_2$
$HF + O \rightleftharpoons OH + F$
$HF + OH \rightleftharpoons H_2O + F$
$H_2 + Cl \rightleftharpoons HCl + H$
$H_2 + O \rightleftharpoons OH + H$
$H_2 + O_2 \rightleftharpoons 2OH$
$N_2 + O \rightleftharpoons NO + N$
$N_2 + O_2 \rightleftharpoons 2NO$
$NO + H \rightleftharpoons N + OH$
$NO + O \rightleftharpoons N + O_2$
$O_2 + H \rightleftharpoons OH + O$
$Cl + ClF \rightleftharpoons Cl_2 + F$
$F + ClF \rightleftharpoons Cl + F_2$
$HF + Cl \rightleftharpoons ClF + H$
$HCl + F \rightleftharpoons ClF + H$
$HCl + HF \rightleftharpoons ClF + H_2$
$HF + ClF \rightleftharpoons F_2 + HCl$
$HF + Cl_2 \rightleftharpoons ClF + HCl$
$ClF + ClF \rightleftharpoons F_2 + Cl_2$

Table II. Additional Chemical Reactions of Importance in Propellant Systems Containing Condensed Carbon As a Combustion Product

Chemical Reaction	Chemical Reaction
$\mathrm{C_2 + M \rightleftharpoons C + C + M}$	$\mathrm{CO + F \rightleftharpoons CF + O}$
$\mathrm{CH + M \rightleftharpoons C + H + M}$	$\mathrm{CO + H \rightleftharpoons CH + O}$
$\mathrm{CH_2 + M \rightleftharpoons CH + H + M}$	$\mathrm{CO + H_2 \rightleftharpoons CH + OH}$
$\mathrm{CH_3 + M \rightleftharpoons CH_2 + H + M}$	$\mathrm{CO + HF \rightleftharpoons CF + OH}$
$\mathrm{CH_4 + M \rightleftharpoons CH_3 + H + M}$	$\mathrm{CO + N \rightleftharpoons CN + O}$
$\mathrm{C_2H_2 + M \rightleftharpoons CH + CH + M}$	$\mathrm{CO + N_2 \rightleftharpoons CN + NO}$
$\mathrm{CN + M \rightleftharpoons C + N + M}$	$\mathrm{CO + OH \rightleftharpoons CH + O_2}$
$\mathrm{HCN + M \rightleftharpoons CN + H + M}$	$\mathrm{C + CO \rightleftharpoons C_2 + O}$
$\mathrm{CNCl + M \rightleftharpoons CN + Cl + M}$	$\mathrm{CO + CO \rightleftharpoons C_2 + O_2}$
$\mathrm{CNF + M \rightleftharpoons F + CN + M}$	$\mathrm{F + CNCl \rightleftharpoons CN + ClF}$
$\mathrm{CF + M \rightleftharpoons C + F + M}$	$\mathrm{HCl + CNF \rightleftharpoons HCN + ClF}$
$\mathrm{C_2F_2 + M \rightleftharpoons CF + CF + M}$	$\mathrm{HF + CNCl \rightleftharpoons HCN + ClF}$
$\mathrm{HCN + M \rightleftharpoons CH + N + M}$	$\mathrm{ClF + CNF \rightleftharpoons CNCl + F_2}$
$\mathrm{CNF + M \rightleftharpoons CF + N + M}$	$\mathrm{Cl_2 + CNF \rightleftharpoons CNCl + ClF}$
$\mathrm{F + CF \rightleftharpoons F_2 + C}$	$\mathrm{C + HCN \rightleftharpoons CH + CN}$
$\mathrm{C + H_2 \rightleftharpoons CH + H}$	$\mathrm{C + CNF \rightleftharpoons CF + CN}$
$\mathrm{C + H_2O \rightleftharpoons CH + OH}$	$\mathrm{C + CH_3 \rightleftharpoons CH + CH_2}$
$\mathrm{C + HF \rightleftharpoons CH + F}$	$\mathrm{C + CH_2 \rightleftharpoons CH + CH}$
$\mathrm{C + HF \rightleftharpoons CF + H}$	$\mathrm{CH + HCN \rightleftharpoons CN + CH_2}$
$\mathrm{C + HCl \rightleftharpoons CH + Cl}$	$\mathrm{HCN + CF \rightleftharpoons CNF + CH}$
$\mathrm{C + N_2 \rightleftharpoons CN + N}$	$\mathrm{CH_4 + C \rightleftharpoons CH_3 + CH}$
$\mathrm{O + CN \rightleftharpoons NO + C}$	$\mathrm{HCN + CH_2 \rightleftharpoons CH_3 + CN}$
$\mathrm{C + OH \rightleftharpoons CH + O}$	$\mathrm{HCN + CH_3 \rightleftharpoons CH_4 + CN}$
$\mathrm{Cl + CF \rightleftharpoons ClF + C}$	$\mathrm{CH_3 + CH \rightleftharpoons CH_2 + CH_2}$

Table II. (continued)

$CH_4 + CH \rightleftharpoons CH_3 + CH_2$

$CH_3 + CH_3 \rightleftharpoons CH_2 + CH_4$

$Cl + HCN \rightleftharpoons CN + HCl$

$Cl + HCN \rightleftharpoons CNCl + H$

$Cl + CNF \rightleftharpoons CN + ClF$

$Cl + CNCl \rightleftharpoons CN + Cl_2$

$CF + CF \rightleftharpoons C_2 + F_2$

$HF + CNF \rightleftharpoons HCN + F_2$

$HCl + CNCl \rightleftharpoons HCN + Cl_2$

$H + C_2 \rightleftharpoons C + CH$

$H + CN \rightleftharpoons CH + N$

$H + CF \rightleftharpoons CH + F$

$H + HCN \rightleftharpoons CN + H_2$

$HF + CN \rightleftharpoons CNF + H$

$H + CNF \rightleftharpoons HCN + F$

$H + CNCl \rightleftharpoons CN + HCl$

$H_2 + CH \rightleftharpoons CH_2 + H$

$H + CH_3 \rightleftharpoons CH_2 + H_2$

$H_2 + CH_3 \rightleftharpoons CH_4 + H$

$H + C_2H_2 \rightleftharpoons CH + CH_2$

$F + C_2 \rightleftharpoons CF + C$

$F + CN \rightleftharpoons CF + N$

$HF + CN \rightleftharpoons HCN + F$

$F + CNF \rightleftharpoons CN + F_2$

$Cl + CNF \rightleftharpoons CNCl + F$

$HF + CH \rightleftharpoons CH_2 + F$

$HF + CH_2 \rightleftharpoons CH_3 + F$

$HF + CH_3 \rightleftharpoons CH_4 + F$

$H_2 + C_2 \rightleftharpoons CH + CH$

$H_2 + CF \rightleftharpoons CH + HF$

$HF + HCN \rightleftharpoons CNF + H_2$

$HCl + HCN \rightleftharpoons CNCl + H_2$

$H_2O + CH \rightleftharpoons CH_2 + OH$

$OH + HCN \rightleftharpoons CN + H_2O$

$H_2O + CH_2 \rightleftharpoons CH_3 + OH$

$H_2O + CH_3 \rightleftharpoons CH_4 + OH$

$HF + C_2 \rightleftharpoons CH + CF$

$HF + CF \rightleftharpoons CH + F_2$

$HF + CNCl \rightleftharpoons CNF + HCl$

$HCl + CH \rightleftharpoons CH_2 + Cl$

$HCl + CF \rightleftharpoons CH + ClF$

$Cl + CH_3 \rightleftharpoons CH_2 + HCl$

$HCl + CH_3 \rightleftharpoons CH_4 + Cl$

$C + CN \rightleftharpoons C_2 + N$

$N_2 + C_2 \rightleftharpoons CN + CN$

$CN + CO \rightleftharpoons C_2 + NO$

$OH + HCN \rightleftharpoons CH_2 + NO$

$N + CO \rightleftharpoons CN + O$

$O + HCN \rightleftharpoons CH + NO$

$O + HCN \rightleftharpoons CN + OH$

$O + CNF \rightleftharpoons CF + NO$

$OH + CH \rightleftharpoons CH_2 + O$

Table II. (continued)

$O + CH_3 \rightleftharpoons CH_2 + OH$

$OH + CH_3 \rightleftharpoons CH_4 + O$

$NO + CO \rightleftharpoons CN + O_2$

$CH + CO \rightleftharpoons C_2 + OH$

$OH + CN \rightleftharpoons CH + NO$

$OH + HCN \rightleftharpoons CH_2 + NO$

$H + HCN \rightleftharpoons CH_2 + N$

$N_2 + CH \rightleftharpoons HCN + N$

$N_2 + CF \rightleftharpoons CNF + N$

$N + C_2H_2 \rightleftharpoons CH + HCN$

$N + C_2F_2 \rightleftharpoons CF + CNF$

Table III. Additional Chemical Reactions of Importance in Aluminum Containing Propellant Systems

Chemical Reaction	Chemical Reaction
$\mathrm{AlO + M = Al + O + M}$	$\mathrm{Al + AlOCl = AlO + AlCl}$
$\mathrm{Al_2O + M = Al + AlO + M}$	$\mathrm{Al + AlOF = Al_2O + F}$
$\mathrm{AlCl + M = Al + Cl + M}$	$\mathrm{OH + AlF = HF + AlO}$
$\mathrm{AlCl_2 + M = AlCl + Cl + M}$	$\mathrm{O + AlF = F + AlO}$
$\mathrm{AlCl_3 + M = AlCl_2 + Cl + M}$	$\mathrm{AlO + H = Al + OH}$
$\mathrm{AlF + M = Al + F + M}$	$\mathrm{AlO + AlF = Al_2O + F}$
$\mathrm{AlF_2 + M = AlF + F + M}$	$\mathrm{AlOF + Al = AlF + AlO}$
$\mathrm{AlF_3 + M = AlF_2 + F + M}$	$\mathrm{Al_2O + Cl = AlO + AlCl}$
$\mathrm{AlOCl + M = AlO + Cl + M}$	$\mathrm{Al_2O + O = AlO + AlO}$
$\mathrm{AlOF + M = AlO + F + M}$	$\mathrm{AlCl + CO = AlOCl + C}$
$\mathrm{AlClF + M = AlF + Cl + M}$	$\mathrm{AlCl + HCl = AlCl_2 + H}$
$\mathrm{AlCl_2F + M = AlCl_2 + F + M}$	$\mathrm{AlCl + NO = AlOCl + N}$
$\mathrm{AlClF_2 + M = AlF_2 + Cl + M}$	$\mathrm{AlCl + OH = AlO + HCl}$
$\mathrm{AlOCl + M = AlCl + O + M}$	$\mathrm{AlCl + Cl = Al + Cl_2}$
$\mathrm{AlOF + M = AlF + O + M}$	$\mathrm{AlCl + H = Al + HCl}$
$\mathrm{AlClF + M = AlCl + F + M}$	$\mathrm{AlCl + O = AlO + Cl}$
$\mathrm{AlCl_2F + M = AlClF + Cl + M}$	$\mathrm{AlCl + AlCl = Al + AlCl_2}$
$\mathrm{AlClF_2 + M = AlClF + F + M}$	$\mathrm{AlCl + AlOCl = Al_2O + Cl_2}$
$\mathrm{Al + CO_2 = AlO + CO}$	$\mathrm{AlCl + AlOCl = AlO + AlCl_2}$
$\mathrm{Al + CO = AlO + C}$	$\mathrm{AlCl + AlOF = AlF + AlOCl}$
$\mathrm{Al + NO = AlO + N}$	$\mathrm{AlCl_2 + Cl = AlCl + Cl_2}$
$\mathrm{Al + O_2 = AlO + O}$	$\mathrm{AlOCl + CO = AlCl + CO_2}$
$\mathrm{Al + AlOCl = Al_2O + Cl}$	$\mathrm{AlOCl + HCl = AlCl_2 + OH}$

Table III. (continued)

$\mathrm{AlOCl + Cl \rightleftharpoons AlO + Cl_2}$

$\mathrm{AlOCl + Cl \rightleftharpoons AlCl_2 + O}$

$\mathrm{AlOCl + H \rightleftharpoons AlO + HCl}$

$\mathrm{AlOCl + H \rightleftharpoons AlCl + OH}$

$\mathrm{AlOCl + O \rightleftharpoons AlCl + O_2}$

$\mathrm{AlF + AlF \rightleftharpoons Al + AlF_2}$

$\mathrm{AlF + HCl \rightleftharpoons AlCl + HF}$

$\mathrm{AlF + HF \rightleftharpoons AlF_2 + H}$

$\mathrm{AlF + NO \rightleftharpoons AlOF + N}$

$\mathrm{AlF + Cl \rightleftharpoons AlCl + F}$

$\mathrm{AlF + F \rightleftharpoons Al + F_2}$

$\mathrm{AlF + H \rightleftharpoons Al + HF}$

$\mathrm{AlF + AlOF \rightleftharpoons AlO + AlF_2}$

$\mathrm{AlF_2 + F \rightleftharpoons AlF + F_2}$

$\mathrm{AlOF + HCl \rightleftharpoons AlOCl + HF}$

$\mathrm{AlOF + HF \rightleftharpoons AlF_2 + OH}$

$\mathrm{AlOF + Cl \rightleftharpoons AlOCl + F}$

$\mathrm{AlOF + F \rightleftharpoons AlO + F_2}$

$\mathrm{AlOF + F \rightleftharpoons AlF_2 + O}$

$\mathrm{AlOF + H \rightleftharpoons AlO + HF}$

$\mathrm{AlOF + H \rightleftharpoons AlF + OH}$

$\mathrm{AlOF + O \rightleftharpoons AlF + O_2}$

$\mathrm{Cl + AlF \rightleftharpoons ClF + Al}$

$\mathrm{F + AlCl \rightleftharpoons ClF + Al}$

$\mathrm{C + AlF \rightleftharpoons CF + Al}$

$\mathrm{CN + AlF \rightleftharpoons CNF + Al}$

$\mathrm{CN + AlCl \rightleftharpoons CNCl + Al}$

$\mathrm{AlF_2 + AlF \rightleftharpoons AlF_3 + Al}$

$\mathrm{AlClF + AlCl \rightleftharpoons AlCl_2F + Al}$

$\mathrm{AlF + AlCl_2 \rightleftharpoons AlCl_2F + Al}$

$\mathrm{AlF + AlClF \rightleftharpoons AlClF_2 + Al}$

$\mathrm{Cl + AlOF \rightleftharpoons ClF + AlO}$

$\mathrm{CO + AlF \rightleftharpoons CF + AlO}$

$\mathrm{C + AlOF \rightleftharpoons CF + AlO}$

$\mathrm{CN + AlOF \rightleftharpoons CNF + AlO}$

$\mathrm{CN + AlOCl \rightleftharpoons CNCl + AlO}$

$\mathrm{AlF_2 + AlOF \rightleftharpoons AlF_3 + AlO}$

$\mathrm{AlOCl + AlCl_2 \rightleftharpoons AlCl_3 + AlO}$

$\mathrm{AlOF + AlCl \rightleftharpoons AlClF + AlO}$

$\mathrm{AlF + AlOCl \rightleftharpoons AlClF + AlO}$

$\mathrm{AlOF + AlCl_2 \rightleftharpoons AlCl_2F + AlO}$

$\mathrm{AlClF + AlOCl \rightleftharpoons AlCl_2F + AlO}$

$\mathrm{AlCl_2 + AlOF \rightleftharpoons AlCl_2F + AlO}$

$\mathrm{AlF_2 + AlOCl \rightleftharpoons AlClF_2 + AlO}$

$\mathrm{AlClF + AlOF \rightleftharpoons AlClF_2 + AlO}$

$\mathrm{AlOCl + AlF \rightleftharpoons ClF + Al_2O}$

$\mathrm{AlCl + AlOF \rightleftharpoons ClF + Al_2O}$

$\mathrm{ClF + AlF \rightleftharpoons F_2 + AlCl}$

$\mathrm{F + AlClF \rightleftharpoons F_2 + AlCl}$

$\mathrm{AlCl + HF \rightleftharpoons AlClF + H}$

Table III. (continued)

$\mathrm{Cl_2 + AlF = ClF + AlCl}$

$\mathrm{Cl + AlClF = ClF + AlCl}$

$\mathrm{C + AlClF = CF + AlCl}$

$\mathrm{CNCl + AlF = CNF + AlCl}$

$\mathrm{AlCl + CNF = AlClF + CN}$

$\mathrm{AlCl + AlCl_2 = AlCl_3 + Al}$

$\mathrm{AlCl + AlF = Al + AlClF}$

$\mathrm{AlClF + AlF = AlF_2 + AlCl}$

$\mathrm{AlCl + AlF_3 = AlF_2 + AlClF}$

$\mathrm{AlCl + AlCl_3 = AlCl_2 + AlCl_2}$

$\mathrm{AlF + AlCl_2 = AlClF + AlCl}$

$\mathrm{AlCl + AlCl_2F = AlCl_2 + AlClF}$

$\mathrm{AlF + AlCl_3 = AlCl_2F + AlCl}$

$\mathrm{AlCl + AlClF_2 = AlCl_2 + AlF_2}$

$\mathrm{AlCl_2F + AlF = AlClF_2 + AlCl}$

$\mathrm{AlCl + AlClF_2 = AlClF + AlClF}$

$\mathrm{Cl + AlCl_3 = Cl_2 + AlCl_2}$

$\mathrm{AlCl_2 + F = AlCl + ClF}$

$\mathrm{Cl + AlClF = F + AlCl_2}$

$\mathrm{F + AlCl_2F = F_2 + AlCl_2}$

$\mathrm{Cl + AlClF_2 = F_2 + AlCl_2}$

$\mathrm{HCl + AlClF = HF + AlCl_2}$

$\mathrm{AlCl_2 + HF = AlCl_2F + H}$

$\mathrm{AlCl_2 + HCl = AlCl_3 + H}$

$\mathrm{F + AlCl_3 = ClF + AlCl_2}$

$\mathrm{Cl_2 + AlClF = ClF + AlCl_2}$

$\mathrm{Cl + AlCl_2F = ClF + AlCl_2}$

$\mathrm{C + AlCl_2F = CF + AlCl_2}$

$\mathrm{CN + AlCl_2F = CNF + AlCl_2}$

$\mathrm{CNCl + AlClF = CNF + AlCl_2}$

$\mathrm{AlCl_2 + CNCl = AlCl_3 + CN}$

$\mathrm{AlCl_2F + AlF = AlF_2 + AlCl_2}$

$\mathrm{AlCl_2 + AlF_2 = AlClF + AlClF}$

$\mathrm{AlCl_2 + AlOF = AlOCl + AlClF}$

$\mathrm{AlCl_2 + AlF_3 = AlF_2 + AlCl_2F}$

$\mathrm{AlCl_2 + AlF_3 = AlClF + AlClF_2}$

$\mathrm{AlCl_3 + AlF = AlClF + AlCl_2}$

$\mathrm{AlCl_2 + AlCl_2F = AlCl_3 + AlClF}$

$\mathrm{AlCl_2 + AlClF_2 = AlF_2 + AlCl_3}$

$\mathrm{AlCl_2 + AlClF_2 = AlClF + AlCl_2F}$

$\mathrm{AlOCl + F = AlO + ClF}$

$\mathrm{AlOCl + F = AlClF + O}$

$\mathrm{ClF + AlOF = F_2 + AlOCl}$

$\mathrm{AlOCl + HF = AlClF + OH}$

$\mathrm{Cl_2 + AlOF = ClF + AlOCl}$

$\mathrm{CO + AlClF = CF + AlOCl}$

$\mathrm{AlClF + AlOF = AlF_2 + AlOCl}$

$\mathrm{AlClF_2 + AlOF = AlF_3 + AlOCl}$

$\mathrm{AlCl_3 + AlOF = AlCl_2F + AlOCl}$

$\mathrm{AlCl_2F + AlOF = AlClF_2 + AlOCl}$

Table III. (continued)

$Cl \overset{0.26}{+} AlClF \rightleftharpoons Cl_2 + AlF$

$AlF + HCl \rightleftharpoons AlClF + H$

$Cl + AlF_2 \rightleftharpoons ClF + AlF$

$F + AlClF \rightleftharpoons ClF + AlF$

$CO + AlOF \rightleftharpoons CO_2 + AlF$

$AlF_2 + C \rightleftharpoons AlF + CF$

$AlF + CNF \rightleftharpoons AlF_2 + CN$

$CNCl + AlF \rightleftharpoons CN + AlClF$

$AlF + AlF_3 \rightleftharpoons AlF_2 + AlF_2$

$AlF + AlCl_2F \rightleftharpoons AlClF + AlClF$

$AlF + AlClF_2 \rightleftharpoons AlF_2 + AlClF$

$AlF_2 + Cl \rightleftharpoons AlClF + F$

$AlF_2 + Cl_2 \rightleftharpoons AlClF + ClF$

$F + AlCl_2F \rightleftharpoons Cl_2 + AlF_2$

$Cl + AlClF_2 \rightleftharpoons Cl_2 + AlF_2$

$F + AlF_3 \rightleftharpoons F_2 + AlF_2$

$H + AlF_3 \rightleftharpoons HF + AlF_2$

$AlF_2 + HCl \rightleftharpoons AlClF + HF$

$AlF_2 + HCl \rightleftharpoons AlClF_2 + H$

$F + AlClF_2 \rightleftharpoons ClF + AlF_2$

$C + AlF_3 \rightleftharpoons CF + AlF_2$

$CN + AlF_3 \rightleftharpoons CNF + AlF_2$

$AlF_2 + CNCl \rightleftharpoons AlClF_2 + CN$

$AlClF + AlCl_2F \rightleftharpoons AlCl_3 + AlF_2$

$AlF + AlClF_2 \rightleftharpoons AlClF + AlF_2$

$AlClF_2 + AlClF \rightleftharpoons AlCl_2F + AlF_2$

$AlF_3 + AlClF \rightleftharpoons AlClF_2 + AlF_2$

$AlOF + Cl \rightleftharpoons AlClF + O$

$AlOF + HCl \rightleftharpoons AlClF + OH$

$CO + AlF_2 \rightleftharpoons CF + AlOF$

$AlOF + CNCl \rightleftharpoons AlOCl + CNF$

$AlF_3 + Cl \rightleftharpoons AlF_2 + ClF$

$AlF_3 + Cl \rightleftharpoons AlClF_2 + F$

$AlF_3 + Cl_2 \rightleftharpoons AlClF_2 + ClF$

$AlF_3 + HCl \rightleftharpoons AlClF_2 + HF$

$AlF_3 + ClF \rightleftharpoons AlClF_2 + F_2$

$CNCl + AlF_3 \rightleftharpoons CNF + AlClF_2$

$AlF_3 + AlCl_3 \rightleftharpoons AlCl_2F + AlClF_2$

$AlClF_2 + AlClF_2 \rightleftharpoons AlCl_2F + AlF_3$

$Cl + AlCl_2F \rightleftharpoons F + AlCl_3$

$ClF + AlCl_2F \rightleftharpoons F_2 + AlCl_3$

$HCl + AlCl_2F \rightleftharpoons HF + AlCl_3$

$Cl_2 + AlCl_2F \rightleftharpoons ClF + AlCl_3$

$CNCl + AlCl_2F \rightleftharpoons CNF + AlCl_3$

$AlCl_3 + AlClF_2 \rightleftharpoons AlCl_2F + AlCl_2$

$Cl + AlCl_2F \rightleftharpoons Cl_2 + AlClF$

$ClF + AlF_2 \rightleftharpoons F_2 + AlClF$

$F + AlClF_2 \rightleftharpoons F_2 + AlClF$

$H + AlClF_2 \rightleftharpoons HF + AlClF$

$AlClF + HCl \rightleftharpoons AlCl_2F + H$

Table III. (continued)

$AlClF + ClF = AlCl_2 + F_2$

$F + AlCl_2F = ClF + AlClF$

$Cl + AlClF_2 = ClF + AlClF$

$C + AlClF_2 = CF + AlClF$

$CN + AlClF_2 = CNF + AlClF$

$CNCl + AlF_2 = CNF + AlClF$

$AlClF + CNCl = AlCl_2F + CN$

$AlClF_2 + Cl = AlCl_2F + F$

$AlClF_2 + Cl_2 = AlCl_2F + ClF$

$AlClF_2 + HCl = AlCl_2F + HF$

$AlClF_2 + ClF = AlCl_2F + F_2$

$AlClF_2 + CNCl = AlCl_2F + CNF$

$AlOCl + Cl_2 = AlCl_3 + O$

$O + AlClF_2 = F_2 + AlOCl$

$O + AlCl_2F = ClF + AlOCl$

$AlF + CO = AlOF + C$

Table IV. Additional Chemical Reactions of Importance in Beryllium Containing Propellant Systems

Chemical Reactions	Chemical Reactions
$BeOH + M \rightleftharpoons Be + OH + M$	$Be_2O + HF \rightleftharpoons BeF + BeOH$
$BeOHOH + M \rightleftharpoons BeOH + OH + M$	$Be_2O + OH \rightleftharpoons BeO + BeOH$
$BeO + M \rightleftharpoons Be + O + M$	$Be_2O + Cl \rightleftharpoons BeO + BeCl$
$Be_2O + M \rightleftharpoons Be + BeO + M$	$Be_2O + H \rightleftharpoons Be + BeOH$
$BeCl + M \rightleftharpoons Be + Cl + M$	$Be_2O + O \rightleftharpoons BeO + BeO$
$BeCl_2 + M \rightleftharpoons BeCl + Cl + M$	$BeOHOH + Be \rightleftharpoons BeOH + BeOH$
$BeF + M \rightleftharpoons Be + F + M$	$BeOH + Cl \rightleftharpoons BeO + HCl$
$BeF_2 + M \rightleftharpoons BeF + F + M$	$BeOH + Cl \rightleftharpoons BeCl + OH$
$BeOH + M \rightleftharpoons BeO + H + M$	$H_2O + Be \rightleftharpoons H + BEOH$
$BeClF + M \rightleftharpoons BeCl + F + M$	$BeOH + H \rightleftharpoons BeO + H_2$
$BeClF + M \rightleftharpoons BeF + Cl + M$	$BeOH + O \rightleftharpoons BeO + CH$
$Be + BeF_2 \rightleftharpoons BeF + BeF$	$Be + BeCl_2 \rightleftharpoons BeCl + BeCl$
$BeO + H_2O \rightleftharpoons BeOH + OH$	$BeCl + H_2O \rightleftharpoons BeOH + HCl$
$CO_2 + Be \rightleftharpoons CO + BeO$	$H + BeCl_2 \rightleftharpoons HCl + BeCl$
$BeO + HCl \rightleftharpoons BeCl + OH$	$BeCl + Cl \rightleftharpoons Be + Cl_2$
$BeO + HF \rightleftharpoons BeOH + F$	$BeCl + H \rightleftharpoons Be + HCl$
$CO + Be \rightleftharpoons C + BeO$	$BeF + H_2O \rightleftharpoons BeOH + HF$
$BeO + Cl \rightleftharpoons BeCl + O$	$BeF + HCl \rightleftharpoons BeCl + HF$
$BeO + H \rightleftharpoons Be + OH$	$BeF + OH \rightleftharpoons BeO + HF$
$NO + Be \rightleftharpoons N + BeO$	$BeF + OH \rightleftharpoons BeOH + F$
$O_2 + Be \rightleftharpoons O + BeO$	$BeF + Cl \rightleftharpoons BeCl + F$
$BeO + BeF \rightleftharpoons Be_2O + F$	$BeF + F \rightleftharpoons Be + F_2$
$Be_2O + H_2O \rightleftharpoons BeOH + BeOH$	$BeF + H \rightleftharpoons Be + HF$
$Be_2O + HCl \rightleftharpoons BeCl + BeOH$	$BeF + O \rightleftharpoons BeO + F$

Table IV. (continued)

$\mathrm{BeF_2 + H = BeF + HF}$
$\mathrm{BeOHOH + H = BeOH + H_2O}$
$\mathrm{Cl + BeF = ClF + Be}$
$\mathrm{C + BeF = CF + Be}$
$\mathrm{CN + BeF = CNF + Be}$
$\mathrm{Be + CNCl = BeCl + CN}$
$\mathrm{BeF + BeCl = BeClF + Be}$
$\mathrm{F + BeClF = F_2 + BeCl}$
$\mathrm{ClF + BeF = F_2 + BeCl}$
$\mathrm{H + BeClF = HF + BeCl}$
$\mathrm{Cl + BeClF = ClF + BeCl}$
$\mathrm{Cl_2 + BeF = ClF + BeCl}$
$\mathrm{C + BeClF = CF + BeCl}$
$\mathrm{CNCl + BeF = CNF + BeCl}$
$\mathrm{CN + BeCl_2 = CNCl + BeCl}$
$\mathrm{BeCl + BeF_2 = BeClF + BeF}$
$\mathrm{BeF + BeCl_2 = BeClF + BeCl}$
$\mathrm{BeOH + C = BeO + CH}$
$\mathrm{Cl + BeClF = F + BeCl_2}$

$\mathrm{ClF + BeClF = F_2 + BeCl_2}$
$\mathrm{BeCl_2 + HF = BeClF + HCl}$
$\mathrm{Cl_2 + BeClF = ClF + BeCl_2}$
$\mathrm{CNCl + BeClF = CNF + BeCl_2}$
$\mathrm{BeCl_2 + BeF_2 = BeClF + BeClF}$
$\mathrm{CO + BeF = CF + BeO}$
$\mathrm{Cl + BeClF = Cl_2 + BeF}$
$\mathrm{F + BeF_2 = F_2 + BeF}$
$\mathrm{H + BeClF = HCl + BeF}$
$\mathrm{Cl + BeF_2 = ClF + BeF}$
$\mathrm{F + BeClF = ClF + BeF}$
$\mathrm{C + BeF_2 = CF + BeF}$
$\mathrm{CN + BeF_2 = CNF + BeF}$
$\mathrm{BeF + CNCl = BeClF + CN}$
$\mathrm{BeF_2 + Cl = BeClF + F}$
$\mathrm{BeF_2 + Cl_2 = BeClF + ClF}$
$\mathrm{BeF_2 + HCl = BeClF + HF}$
$\mathrm{BeF_2 + ClF = BeClF + F_2}$
$\mathrm{BeF_2 + CNCl = BeClF + CNF}$

Table V. Additional Chemical Reactions of Importance in Boron Containing Propellant Systems

Chemical Reaction	Chemical Reaction
$BN + M = B + N + M$	$BO + BO = B + BO_2$
$BO + M = B + O + M$	$CO + BO_2 = CO_2 + BO$
$BO_2 + M = BO + O + M$	$BO + CO = B + CO_2$
$BCl + M = B + Cl + M$	$BO + CO = BO_2 + C$
$BCl_2 + M = BCl + Cl + M$	$BO + HCl = BCl + OH$
$BCl_3 + M = BCl_2 + Cl + M$	$BO + HF = BF + OH$
$BF + M = B + F + M$	$BO + NO = BN + O_2$
$BF_2 + M = BF + F + M$	$BO + NO = BO_2 + N$
$BF_3 + M = BF_2 + F + M$	$CO + B = C + BO$
$BOCl + M = BCl + O + M$	$BO + Cl = BCl + O$
$BOF + M = BO + F + M$	$BO + F = BF + O$
$BClF + M = BF + Cl + M$	$BO + H = B + OH$
$BCl_2F + M = BCl_2 + F + M$	$BO + N = BN + O$
$BOF + M = BF + O + M$	$BO + O = B + O_2$
$BOCl + M = BO + Cl + M$	$BO + BCl = B + BOCl$
$BClF + M = BCl + F + M$	$BO + BOCl = BO_2 + BCl$
$BCl_2F + M = BClF + Cl + M$	$BO + BF = B + BOF$
$BClF_2 + M = BF_2 + Cl + M$	$BOF + BF_2 = BF_3 + BO$
$BClF_2 + M = BClF + F + M$	$BO + BOF = BF + BO_2$
$B + N_2 = BN + N$	$BO_2 + HF = BOF + OH$
$B + NO = BN + O$	$BO_2 + Cl = BOCl + O$
$N + BO = NO + B$	$BO_2 + H = BO + OH$
$N_2 + BO = NO + BN$	$BO_2 + O = BO + O_2$

Table V. (continued)

<u>Chemical Reaction</u>

$BCl + BCl = B + BCl_2$

$BCl + Cl = B + Cl_2$

$BCl + H = B + HCl$

$BCl + N = BN + Cl$

$BCl + BOF = BOCl + BF$

$BCl_2 + Cl = BCl + Cl_2$

$BCl_3 + Cl = BCl_2 + Cl_2$

$BOCl + HCl = BCl_2 + OH$

$HCl + BO_2 = OH + BOCl$

$BOCl + Cl = BO + Cl_2$

$BOCl + Cl = BCl_2 + O$

$BOCl + H = BO + HCl$

$BOCl + H = BCl + OH$

$BOCl + N = BCl + NO$

$BOCl + O = BCl + O_2$

$BF + BF = B + BF_2$

$CO + BOF = CO_2 + BF$

$BF + CO = BOF + C$

$BF + HCl = BCl + HF$

$BF + HF = BF_2 + H$

$BF + Cl = BCl + F$

$BF + F = B + F_2$

$BF + H = B + HF$

$BF + N = BN + F$

<u>Chemical Reaction</u>

$BF + BF_2 = B + BF_3$

$BF + BOF = BO + BF_2$

$BF_2 + F = BF + F_2$

$BF_3 + F = BF_2 + F_2$

$BF_3 + H = BF_2 + HF$

$BOF + BOF = BO_2 + BF_2$

$BOF + HCl = BOCl + HF$

$BOF + HF = BF_2 + OH$

$BOF + Cl = BOCl + F$

$BOF + F = BO + F_2$

$BOF + F = BF_2 + O$

$BOF + H = BO + HF$

$BOF + H = BF + OH$

$BOF + O = BO_2 + F$

$F + BCl = ClF + B$

$B + CN = BN + C$

$C + BF = CF + B$

$B + HCN = BN + CH$

$CN + BF = CNF + B$

$B + CNF = BN + CF$

$CN + BCl = CNCl + B$

$BCl + BCl_2 = BCl_3 + B$

$BF + BCl = BCLF + B$

$BCl + BClF = BCl_2F + B$

Table V. (continued)

Chemical Reaction	Chemical Reaction
$BF + BCl_2 = BCl_2F + B$	$C + BF_2 = CF + BF$
$BCl + BF_2 = BClF_2 + B$	$BF + CNF = BF_2 + CN$
$CN + BO = CO + BN$	$BF + CNCl = BCl + CNF$
$CN + BF = CF + BN$	$BF + CNCl = BClF + CN$
$F + BOCl = ClF + BO$	$BF + BCl_2 = BClF + BCl$
$CO + BF = CF + BO$	$BF + BCl_3 = BCl_2 + BClF$
$C + BOF = CF + BO$	$BF + BClF = BCl + BF_2$
$CN + BOCl = CNCl + BO$	$BF + BCl_2F = BCl + BClF_2$
$BCl + BOCl = BCl_2 + BO$	$BF + BCl_2F = BCl_2 + BF_2$
$BCl_2 + BOCl = BCl_3 + BO$	$BF + BCl_2F = BClF + BClF$
$BF + BOCl = BClF + BO$	$BF + BClF_2 = BCl + BF_3$
$BCl + BOF = BClF + BO$	$BF + BClF_2 = BClF + BF_2$
$BCl_2 + BOF = BCl_2F + BO$	$BF_2 + Cl = BClF + F$
$BClF + BOCl = BCl_2F + BO$	$BF_2 + Cl_2 = BClF + ClF$
$BO + BClF_2 = BOCl + BF_2$	$Cl + BClF_2 = Cl_2 + BF_2$
$BClF + BOF = BClF_2 + BO$	$BF_2 + HCl = BClF + HF$
$CO + BOF = CF + BO_2$	$BClF_2 + H = HCl + BF_2$
$BOCl + BOCl = BCl_2 + BO_2$	$Cl + BF_3 = ClF + BF_2$
$BOF + BOCl = BClF + BO_2$	$BF_2 + ClF = F_2 + BClF$
$BF + Cl_2 = BCl + ClF$	$F + BClF_2 = ClF + BF_2$
$Cl + BClF = Cl_2 + BF$	$CO + BF_2 = CF + BOF$
$BF + HCl = BClF + H$	$BF_2 + CNCl = BClF + CNF$
$F + BClF = ClF + BF$	$C + BF_3 = CF + BF_2$
$BF + ClF = BCl + F_2$	$CN + BF_3 = CNF + BF_2$

Table V. (continued)

Chemical Reaction	Chemical Reaction
$CN + BClF_2 = CNCl + BF_2$	$BOF + BCl_2 = BOCl + BClF$
$BClF_2 + BCl = BCl_2 + BF_2$	$BOF + BCl_3 = BOCl + BCl_2F$
$BF_2 + BCl_2 = BClF + BClF$	$BOF + BCl_2F = BOCl + BClF_2$
$BClF_2 + BCl_2 = BCl_3 + BF_2$	$F + BClF = F_2 + BCl$
$BCl_2F + BClF = BF_2 + BCl_3$	$BCl + HF = BClF + H$
$BClF + BOF = BOCl + BF_2$	$BCl + HCl = BCl_2 + H$
$BF_3 + BCl = BClF + BF_2$	$F + BCl_2 = ClF + BCl$
$BF_3 + BCl_2 = BCl_2F + BF_2$	$Cl + BClF = ClF + BCl$
$BClF_2 + BClF = BCl_2F + BF_2$	$CO + BOCl = CO_2 + BCl$
$BF_3 + BClF = BClF_2 + BF_2$	$C + BClF = CF + BCl$
$BF_3 + Cl = BClF_2 + F$	$BCl + CNF = BClF + CN$
$BF_3 + Cl_2 = BClF_2 + ClF$	$BCl + CNCl = BCl_2 + CN$
$BF_3 + HCl = BClF_2 + HF$	$BCl + BCl_3 = BCl_2 + BCl_2$
$BF_3 + ClF = BClF_2 + F_2$	$BCl + BCl_2F = BCl_2 + BClF$
$BF_3 + CNCl \quad BClF_2 + CNF$	$BCl + BClF_2 = BClF + BClF$
$BF_3 + BCl_2 = BClF + BClF_2$	$Cl + BClF = F + BCl_2$
$BF_3 + BCl_3 = BCl_2F + BClF_2$	$ClF + BClF = F_2 + BCl_2$
$BClF_2 + BOF = BOCl + BF_3$	$F + BCl_2F = F_2 + BCl_2$
$BF_3 + BCl_2F = BClF_2 + BClF_2$	$Cl + BClF_2 = F_2 + BCl_2$
$BOF + Cl = BClF + O$	$HCl + BClF = HF + BCl_2$
$BOF + Cl_2 = BOCl + ClF$	$H + BCl_2F = HF + BCl_2$
$BOF + HCl = BClF + OH$	$H + BCl_3 = HCl + BCl_2$
$BOF + ClF = BOCl + F_2$	$F + BCl_3 = ClF + BCl_2$
$BOF + CNCl = BOCl + CNF$	$Cl_2 + BClF = ClF + BCl_2$

Table V. (continued)

Chemical Reaction

$Cl + BCl_2F = ClF + BCl_2$

$C + BCl_2F = CF + BCl_2$

$CNCl + BClF = CNF + BCl_2$

$CN + BCl_2F = CNF + BCl_2$

$BCl_2 + CNCl = BCl_3 + CN$

$BCl_2 + BClF_2 = BClF + BCl_2F$

$Cl + BCl_2F = F + BCl_3$

$ClF + BCl_2F = F_2 + BCl_3$

$BCl_2 + BCl_2F = BCl_3 + BClF$

$HCl + BCl_2F = HF + BCl_3$

$Cl_2 + BCl_2F = ClF + BCl_3$

$CNCl + BCl_2F = CNF + BCl_3$

$BCl_2F + BCl_2F = BClF_2 + BCl_3$

$BOCl + F = BClF + O$

$BOCl + HF = BClF + OH$

$CO + BClF = CF + BOCl$

Chemical Reaction

$Cl + BCl_2F = Cl_2 + BClF$

$F + BClF_2 = F_2 + BClF$

$H + BClF_2 = HF + BClF$

$H + BCl_2F = HCl + BClF$

$F + BCl_2F = ClF + BClF$

$Cl + BClF_2 = ClF + BClF$

$C + BClF_2 = CF + BClF$

$CN + BClF_2 = CNF + BClF$

$CN + BCl_2F = CNCl + BClF$

$Cl + BClF_2 = F + BCl_2F$

$HCl + BClF_2 = HF + BCl_2F$

$Cl_2 + BClF_2 = ClF + BCl_2F$

$CNCl + BClF_2 = CNF + BCl_2F$

$ClF + BClF_2 = F_2 + BCl_2F$

$BCl + CO = BOCl + C$

Table VI. Additional Chemical Reactions of Importance in Lithium Containing Propellant Systems

Chemical Reaction	Chemical Reaction
$LiH + M = Li + H + M$	$LiO + OH = LiH + O_2$
$LiOH + M = Li + OH + M$	$NO + Li = N + LiO$
$LiO + M = Li + O + M$	$LiO + LiOH = Li_2O + OH$
$Li_2O + M = Li + LiO + M$	$LiO + LiF = Li_2O + F$
$LiCl + M = Li + Cl + M$	$LiOH + LiOH = H_2O + Li_2O$
$Li_2Cl_2 + M = LiCl + LiCl + M$	$LiF + LiOH = HF + Li_2O$
$LiF + M = Li + F + M$	$Li_2O + H_2 = LiH + LiOH$
$Li_2F_2 + M = LiF + LiF + M$	$Li_2O + H = LiH + LiO$
$LiOH + M = LiO + H + M$	$Li_2O + O = LiO + LiO$
$Li + H_2O = LiH + OH$	$H_2O + LiCl = HCl + LiOH$
$Li + H_2O = LiOH + H$	$LiOH + H_2 = LiH + H_2O$
$Li + CO = LiO + C$	$LiOH + OH = LiO + H_2O$
$Li + HF = LiH + F$	$OH + LiCl = Cl + LiOH$
$Li + H_2 = LiH + H$	$LiOH + H = LiH + OH$
$Li + OH = LiH + O$	$LiOH + H = LiO + H_2$
$Li + OH = LiO + H$	$LiOH + O = LiO + OH$
$Li + O_2 = LiO + O$	$LiOH + LiCl = Li_2O + HCl$
$Li + LiOH = LiH + LiO$	$LiF + H_2O = LiOH + HF$
$Li + LiOH = Li_2O + H$	$LiF + HF = LiH + F_2$
$HCl + Li = Cl + LiH$	$LiF + H_2 = LiH + HF$
$CO_2 + Li = CO + LiO$	$LiF + OH = LiOH + F$
$Cl + LiOH = HCl + LiO$	$LiF + OH = LiO + HF$
$LiO + HF = LiOH + F$	$LiF + Cl = LiCl + F$
$LiO + H_2 = LiH + OH$	$LiF + F = Li + F_2$

Table VI. (continued)

$\mathrm{LiF + H = Li + HF}$

$\mathrm{LiF + H = LiH + F}$

$\mathrm{LiF + O = LiO + F}$

$\mathrm{LiCl + HCl = LiH + Cl_2}$

$\mathrm{LiCl + HF = LiF + HCl}$

$\mathrm{LiCl + H_2 = LiH + HCl}$

$\mathrm{LiCl + OH = LiO + HCl}$

$\mathrm{LiCl + Cl = Li + Cl_2}$

$\mathrm{LiCl + H = Li + HCl}$

$\mathrm{LiCl + H = LiH + Cl}$

$\mathrm{LiCl + O = LiO + Cl}$

$\mathrm{LiCl + LiO = Li_2O + Cl}$

$\mathrm{F + LiCl = ClF + Li}$

$\mathrm{Cl + LiF = ClF + Li}$

$\mathrm{Li + CH = LiH + C}$

$\mathrm{C + LiF = CF + Li}$

$\mathrm{Li + HCN = LiH + CN}$

$\mathrm{CN + LiF = CNF + Li}$

$\mathrm{CN + LiCl = CNCl + Li}$

$\mathrm{Li + CH_2 = LiH + CH}$

$\mathrm{Li + CH_3 = LiH + CH_2}$

$\mathrm{Li + CH_4 = LiH + CH_3}$

$\mathrm{HF + LiCl = ClF + LiH}$

$\mathrm{CO + LiF = CF + LiO}$

$\mathrm{HCl + LiF = ClF + LiH}$

$\mathrm{CH + LiF = CF + LiH}$

$\mathrm{HCN + LiF = CNF + LiH}$

$\mathrm{HCN + LiCl = CNCl + LiH}$

$\mathrm{LiH + CO = LiO + CH}$

$\mathrm{LiOH + C = LiO + CH}$

$\mathrm{LiOH + CH = LiO + CH_2}$

$\mathrm{LiOH + CN = LiO + HCN}$

$\mathrm{LiOH + CH_2 = LiO + CH_3}$

$\mathrm{LiOH + CH_3 = LiO + CH_4}$

$\mathrm{LiF + Cl_2 = LiCl + ClF}$

$\mathrm{LiF + ClF = LiCl + F_2}$

$\mathrm{CNF + LiCl = CNCl + LiF}$

Table VII. Chemical Reactions Eliminated Due to Steric Considerations

Chemical Reactions Involving No Metallized Species

$C + H_2O = CO + H_2$

$C + O_2 + M = CO_2 + M$

$CO + H_2O = CO_2 + H_2$

$H_2 + NO = H_2O + N$

$H_2 + O + M = H_2O + M$

$H_2 + O_2 = H_2O + O$

$H_2O + N = H_2 + NO$

$CH_2 + M = C + H_2 + M$

$CH_2 + O = C + H_2O$

$CO + H_2 = CH_2 + O$

$CO + H_2O = CH_2 + O_2$

$CO_2 + F = CF + O_2$

$CO_2 + H = CH + O_2$

$CO_2 + H_2 = CH_2 + O_2$

$CO_2 + N = CN + O_2$

$C + CO_2 = C_2 + O_2$

$C + CH_4 = 2CH_2$

$C + C_2H_2 = C_2 + CH_2$

$CO_2 + CH_2 = C_2H_2 + O_2$

$CH + C_2H_2 = C_2 + CH_3$

$CH_2 + C_2H_2 = C_2 + CH_4$

$C_2H_2 + M = CH_2 + C + M$

$C_2F_2 + M = C_2 + F_2 + M$

$C_2F_2 + H_2 = F_2 + C_2H_2$

Chemical Reactions Involving No Metallized Species

$H + C_2H_2 = C + CH_3$

$CF + H_2 = F + CH_2$

$F + C_2H_2 = CF + CH_2$

$H_2 + C_2 = C + CH_2$

$C_2H_2 + M = H_2 + C_2 + M$

$CH_3 + M = H_2 + CH + M$

$H_2 + CN = CH_2 + N$

$H_2 + HCN = CH_3 + N$

$CH_4 + M = H_2 + CH_2 + M$

$H_2 + C_2H_2 = 2CH_2$

$H_2 + C_2H_2 = CH_4 + C$

$H_2 + C_2H_2 = CH_3 + CH$

$CO + CH_2 = H_2O + C_2$

$C_2H_2 + O = H_2O + C_2$

$H_2O + CN = CH_2 + NO$

$H_2O + HCN = CH_3 + NO$

$H_2O + CH_2 = CH_4 + O$

$CH_4 + CO = H_2O + C_2H_2$

$HF + C_2H_2 = CF + CH_3$

$N + C_2H_2 = CN + CH_2$

$CO + CH_2 = O + C_2H_2$

$CH_3 + CO = OH + C_2H_2$

$H_2O + CH = CH_3 + O$

Table VII. (continued) Chemical Reactions Eliminated Due to Steric Considerations

Chemical Reactions Involving Boron Species

$CO_2 + B = BO_2 + C$

$F_2 + B + M = BF_2 + M$

$H_2 + B + M = BH_2 + M$

$H_2O + B = BO + H_2$

$H_2O + B = BH_2 + O$

$O_2 + B + M = BO_2 + M$

$F_2 + BN = BF_2 + N$

$H_2 + BN = BH_2 + N$

$H_2O + BN = BH_2 + NO$

$O_2 + BN = BO_2 + N$

$F_2 + BO = BF_2 + O$

$H_2 + BO = BH_2 + O$

$H_2O + BO = BO_2 + H_2$

$H_2O + BO = BH_2 + O_2$

$F + BO_2 = BF + O_2$

$F_2 + BO_2 = BF_2 + O_2$

$H_2 + BO_2 = BO + H_2O$

$H_2 + BO_2 = BH_2 + O_2$

$N + BO_2 = BN + O_2$

$F + BH_2 = BF + H_2$

$F_2 + BH_2 = BF_2 + H_2$

Chemical Reactions Involving Boron Species (continued)

$N + BH_2 = BN + H_2$

$NO + BH_2 = BN + H_2O$

$F_2 + BF + M = BF_3 + M$

$H_2O + BF = BOF + H_2$

$O + BF_3 = BOF + F_2$

$BClF + M = B + ClF + M$

$BH_2 + C = B + CH_2$

$B + CH_3 = BH_2 + CH$

$B + CH_4 = BH_2 + CH_2$

$B + C_2H_2 = BH_2 + C_2$

$BF_2 + C_2 = B + C_2F_2$

$BClF + N = BN + ClF$

$BO_2 + CN = BN + CO_2$

$BH_2 + CN = BN + CH_2$

$BH_2 + HCN = BN + CH_3$

$BClF + O = BO + ClF$

$BH_2 + CO = BO + CH_2$

$BClF + O_2 = BO_2 + ClF$

$BF + CO_2 = BO_2 + CF$

$BH_2 + CO_2 = BO_2 + CH_2$

$BClF + H_2 = BH_2 + ClF$

Table VII. (continued) Chemical Reactions Eliminated Due to Steric Considerations

Chemical Reactions Involving Boron Species (Continued)

$BF + CH_2 = BH_2 + CF$

$BF_2 + C_2H_2 = BH_2 + C_2F_2$

$BCl_2F + M = BF + Cl_2$

$BF + C_2F_2 = BF_3 + C_2$

$BF + BCl_3 = BCl_2F + BCl$

$BCl_2F + F = BF_2 + Cl_2$

$BF_3 + Cl = BClF + F_2$

$BCl_2F + F_2 = BF_3 + Cl_2$

$BOF + Cl_2 = BCl_2F + O$

$BClF_2 + O = BOF + ClF$

$BClF_2 + M = BCl + F_2 + M$

$BOCl + H_2 = BCl + H_2O$

$BCl_2F + M = BCl + ClF + M$

$BCl_3 + F = BClF + Cl_2$

$BClF_2 + Cl_2 = BCl_3 + F_2$

$BCl_2F + O = BOCl + ClF$

Chemical Reactions Involving Lithium Species

$H_2O + Li = LiO + H_2$

$CO + LiH = LiOH + C$

$CO_2 + LiH = LiOH + CO$

$NO + LiH = LiOH + N$

$O + LiH + M = LiOH + M$

$O_2 + LiH = LiOH + O$

Chemical Reactions Involving Lithium Species (continued)

$C + LiOH = LiH + CO$

$F_2 + Li_2O = Li_2F_2 + O$

$Li_2F_2 + Cl_2 = Li_2Cl_2 + F_2$

Chemical Reactions Involving Aluminum Species

$Cl_2 + Al + M = AlCl_2 + M$

$H_2O + Al = AlO + H_2$

$Cl_2 + AlO = AlCl_2 + O$

$CO_2 + Al_2O = Al_2O_3 + C$

$Cl_2 + Al_2O = AlO + AlCl_2$

$O_2 + Al_2O + M = Al_2O_3 + M$

$H_2O + AlCl = AlOCl + H_2$

$AlClF + M = Al + ClF + M$

$Al + C_2F_2 = AlF_2 + C_2$

$AlCl + AlF_2 = Al + AlClF_2$

$AlClF + O = AlO + ClF$

$AlClF + AlO = Al_2O + ClF$

$AlCl_3 + M = AlCl + Cl_2 + M$

$AlCl_2F + M = AlCl + ClF + M$

$AlCl + C_2F_2 = AlClF_2 + C_2$

$AlCl_2F + M = AlF + Cl_2 + M$

$AlF_3 + M = AlF + F_2 + M$

$AlF + AlClF_2 = AlCl + AlF_3$

$AlClF_2 + M = AlF + ClF + M$

Table VII. (continued) Chemical Reactions Eliminated Due to Steric Considerations

Chemical Reactions Involving Aluminum Species (continued)

$AlF_3 + C_2 = AlF + C_2F_2$

$AlOF + Cl_2 = AlCl_2F + O$

$AlF_3 + O = AlOF + F_2$

$AlClF_2 + O = AlOF + ClF$

$AlF_3 + Cl = AlClF + F_2$

$AlF_3 + Cl_2 = AlCl_2F + F_2$

$AlCl_3 + F = AlClF + Cl_2$

$AlCl_3 + F_2 = AlClF_2 + Cl_2$

$AlClF_2 + M = AlCl + F_2 + M$

Chemical Reactions Involving Beryllium Species

$Cl_2 + Be + M = BeCl_2 + M$

$H_2O + Be = BeO + H_2$

$BeO_2H_2 + Be = Be_2O + H_2O$

$Cl_2 + BeOH = BeCl_2 + OH$

$Cl_2 + BeO = BeCl_2 + O$

$H_2O + BeO + M = BeO_2H_2 + M$

$BeCl_2 + BeO = Be_2O + Cl_2$

$BeClF + M = Be + ClF + M$

$Be + C_2F_2 = BeF_2 + C_2$

$BeClF + OH = BeOH + ClF$

$BeClF + O = BeO + ClF$

$BeO + BeClF = Be_2O + ClF$

Table VIII. Spin Forbidden Chemical Reactions Which Do Not Occur In the Ground State

$CO_2 + M = CO + O + M$

$FCN + M = CF + N + M$

$H + HCN = CH_2 + N$

$HCN + M = N + CH + M$

$CH + N_2 = N + HCN$

$CF + N_2 = N + FCN$

$N + C_2H_2 = CH + HCN$

$CF + FCN = N + C_2F_2$

$CO + AlCl = AlOCl + C$

$NO + AlCl = AlOCl + N$

$AlOCl + M = AlCl + O + M$

$AlOCl + Cl_2 = AlCl_3 + O$

$AlClF_2 + O = AlOCl + F_2$

$AlCl_2F + O = AlOCl + ClF$

$AlF + CO = AlOF + C$

$BOF + M = BF + O + M$

$BF + BOF = BO + F_2$

$BCl + CO = BOCl + C$

$C + BeO = Be + CO$

$N + BeO = Be + NO$

$BeO + M = Be + O + M$

$Be_2O + O = 2BeO$

Table IX. Chemical Reactions for Which Rate Constants Have Been Determined

Chemical Reaction	Exothermic Rate Constant•	Reference
$CO_2 + M \rightleftharpoons CO + O + M$	$3 \times 10^{20} T^{-1.0} \exp -\left(\frac{31391}{T}\right)$	Avramenko, L. I. and Kolesnikova, R. V., Izvest. Akad. Nauk. S.S.S.R., Otdel. Khim. Nauk., 1562 (1959).
$H_2O + M \rightleftharpoons OH + H + M$	$3 \times 10^{19} T^{-1.0}$	Mayer, S. W., Cook, E. A., Schieler, L., "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 18 Sept. 1964.
$CO + M \rightleftharpoons C + O + M$	$2 \times 10^{18} T^{-1.0}$	Wray, K. L., Avco Research Report 95 (1961).
$HF + M \rightleftharpoons H + F + M$	$1 \times 10^{19} \times T^{-0.5}$	S. W. Mayer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 19 Sept. 1964.
$H_2 + M \rightleftharpoons 2H + M$	$10^{19} T^{-1.0}$	W. E. Kaskan and W. G. Browne, "Kinetics of the $H_2/CO/O_2$ System," General Electric Document No. 63SD848, 14 February 1964.
$N_2 + M \rightleftharpoons 2N + M$	$2 \times 10^{18} T^{-1.0}$	K. L. Wray, Avco Research Report 104 (1961).
$NO + M \rightleftharpoons N + O + M$	$2 \times 10^{18} T^{-1.0}$	K. L. Wray, Avco Research Report 95 (1961).
$OH + M \rightleftharpoons O + H + M$	$2 \times 10^{18} T^{-1.0}$	S. W. Mayer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 19 Sept. 1964.
$O_2 + M \rightleftharpoons 2O + M$	$1 \times 10^{16} T^{-0.5}$	S. W. Mayer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 19 Sept. 1964.
$CO_2 + H \rightleftharpoons CO + OH$	$3.2 \times 10^{12} \exp -\left(\frac{6300}{RT}\right)$	W. E. Kaskan and W. G. Browne, "Kinetics of the $H_2/CO/O_2$ System," General Electric Document No. 63SD848, 14 Feb. 1964.
$CO_2 + O \rightleftharpoons CO + O_2$	$3.58 \times 10^{15} T^{-1.0}$	L. I. Avramenko and R. V. Kolesnikova, Izvest. Akad. Nauk. S.S.S.R., Otdel. Khim. Nauk., 1562 (1959).
$H_2O + H \rightleftharpoons OH + H_2$	$7 \times 10^{13} \exp -\left(\frac{6100}{RT}\right)$	S. W. Mayer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 19 Sept. 1964.
$H_2O + O \rightleftharpoons 2OH$	$2.5 \times 10^{14} \exp -\left(\frac{10000}{RT}\right)$	S. W. Mayer, E. A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139, Aerospace Corporation, Los Angeles, California, 19 Sept. 1964.

• Three body recombination rates have the units $cm^6/gmole^2$-sec.
Bimolecular reaction rates have the units $cm^3/gmole$-sec.

Table IX. Chemical Reactions for Which Rate Constants Have Been Determined (Continued)

Chemical Reaction	Exothermic Rate Constant	Reference
$2CO \rightleftharpoons CO_2 + C$	$2.11 \times 10^{16} T^{-1.0}$	L.L. Avramenko, R.V. Lorentso, Zhur. Fiz. Khim., 24, 207 (1950).
$CO + H \rightleftharpoons C + OH$	$1 \times 10^{14} \exp -\left(\frac{13000}{T}\right)$	F. Kaufman and J.P. Kelso, J. Chem. Phys., 23, 1072 (1955).
$CO + N \rightleftharpoons C + NO$	$1.44 \times 10^{16} T^{-1.0}$	L.L. Avramenki and R.V. Lorentso, Zhur. FIZ. Khim., 24, 207 (1950).
$CO + NO \rightleftharpoons CO_2 + N$	$2.47 \times 10^{15} T^{-1.0}$	L.I. Avramenko and R.V. Kilesnikova, Izvest. Akad. Nauk. S.S.S.R., Otdel. Khim. Nauk., 1562 (1959).
$CO + O \rightleftharpoons C + O_2$	$2.48 \times 10^{13} \exp -\left(\frac{990}{T}\right)$	L.I. Avramenko and R. V. Lorentso, Zhur, Fiz, Khim., 20, 207 (1950)
$HF + H \rightleftharpoons H_2 + F$	$5 \times 10^{12} \exp -\left(\frac{5700}{RT}\right)$	S W. Mayer, E A Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139 Aerospace Corporation, Los Angeles, California, 18 Sept 1964.
$HF + O \rightleftharpoons OH + F$	$5 \times 10^{11} T^{0.5} \exp -\left(\frac{6000}{RT}\right)$	S.W. Mayer, E.A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139 Aerospace Corporation, Los Angeles, California, 18 Sept. 1964.
$HF + OH \rightleftharpoons H_2O + F$	$5 \times 10^{11} T^{0.5} \exp -\left(\frac{7000}{RT}\right)$	S.W. Mayer, E.A. Cook, and L. Schieler, "Nonequilibrium Recombination in Nozzles," SSD-TDR-64-139. Aerospace Corporation, Los Angeles, California, 18 Sept. 1964.
$H_2 + O \rightleftharpoons OH + H$	$1.4 \times 10^{12} \exp -\left(\frac{5190}{RT}\right)$	W.E. Kaskan and W.G. Browne, "Kinetics of the $H_2/CO/O_2$ System," General Electric Document No. [illegible], 16 February 1964.
$H_2 + O_2 \rightleftharpoons 2OH$	$2.7 \times 10^{16} \exp -\left(\frac{53000}{T}\right)$	F. Kaufman and J.P. Kelso, J. Chem. Phys., 23, 1072 (1955).
$N_2 + O \rightleftharpoons NO + N$	$1.5 \times 10^{16} T^{-1}$	L.F. Phillips and H I. Schiff, J. Chem. Phys., 36, 1509 (1962)
$N_2 + O_2 \rightleftharpoons 2NO$	$9 \times 10^{23} T^{-5/2} \exp -\left(\frac{43000}{T}\right)$	E. Freedman and J. W. Daiber, J. Chem. Phys., 34, 1271 (1961).
$NO + O \rightleftharpoons N + O_2$	$1.011 \times 10^{11} T^{0.5} \exp -\left(\frac{3120}{T}\right)$	W.G. Vincenti, Stanford Univ. Dept. Aeronaut. Engr. Rept. 101 (1961).
$O_2 + H \rightleftharpoons OH + O$	$3.2 \times 10^{11} T^{-0.47} \exp -\left(\frac{100}{RT}\right)$	W.E. Kaskan and W.G. Browne, "Kinetics of the $H_2/CO/O_2$ System," General Electric Document No. [illegible], 16 Feb. 1964.