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AN INVESTIGATION OF CHEMICAL IDENTITY THINKING

A Dissertation Presented

by

COURTNEY L. NGAI

Submitted to the Office of Graduate Studies,
University of Massachusetts Boston,
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

May 2017

Chemistry PhD Program – Biological Chemistry Track

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ABSTRACT

AN INVESTIGATION OF CHEMICAL IDENTITY THINKING

May 2017

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Directed by Professor Hannah Sevian

Chemical identity is a foundational crosscutting concept in chemistry and encompasses the knowledge, reasoning, and practices relevant for the classification and differentiation of substances. Substances are found everywhere – from the chemistry classroom to the kitchen at home – so classification and differentiation of substances is important for everyday decisions as well as challenges that are solved using chemistry. An understanding of chemical identity, then, is essential for scientifically literate citizens in addition to students training to be chemists. A better understanding of how chemical identity thinking develops could be used to inform instruction and education research, with the intent of producing students and citizens who can use their chemical knowledge to reason with in order to practice chemical identity thinking.

This thesis characterizes chemical identity thinking from the perspective of chemical identity knowledge and chemical identity practices, both of which contribute to chemical identity thinking. First, the literature is examined for existing research on how students perceive substances and chemical identity, and a hypothetical learning progression for chemical identity thinking is proposed. This is followed by the design of a qualitative instrument, the CSI Survey, to capture the chemical identity practices exhibited by students at a range of education levels (8th grade – 4th year university). The data collected using the CSI Survey are analyzed using content analysis. Eight unique themes corresponding to chemical identity practices (the application of chemical identity knowledge and reasoning) are revealed by this analysis (*change, class, composition and structure, function, organism effect, sensory information, source, tests and experimental values*). The application of chemical identity knowledge in biochemical contexts by both expert biochemists and biochemistry students is investigated in the final chapter, and the chemical identity knowledge observed in the biochemical contexts is characterized using the eight themes of chemical identity practices. Suggestions are offered on how the products of the research on chemical identity thinking can be used to inform decisions in both instruction and research.

DEDICATION

I would like to dedicate this work to my family – past, present, and future.

ACKNOWLEDGMENTS

I would like to begin my acknowledgements with the woman who made this adventure not only possible, but a tremendous experience: my advisor, Hannah Sevian. I knew from the moment I met her that I wanted to work for Hannah. Hannah is filled with passion for her work, and has an incredible ability to motivate others in both research and instruction. I am still learning to appreciate the impact she has left on me, and I know that her influence on the way I investigate any problem and the way I teach any subject will have a lasting positive effect. Thank you for believing in me, supporting me, and helping me to learn so much more than I ever could have imagined.

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ABBREVIATIONS

AAAS	American Association for the Advancement of Science
CE	creative exercise
CER	chemistry education research
CI	chemical identity
CT	chemical thinking
CSI Survey	chemical substance identification survey
LP	learning progression
NRC	National Research Council
OECD	Organisation for Economic Cooperation and Development
PCAST	President's Council of Advisors on Science and Technology

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CHAPTER 1

INTRODUCTION

“All of us have a stake, as individuals and as a society, in scientific literacy... Scientific literacy enables people to use scientific principles and processes in making personal decisions and to participate in discussions of scientific issues that affect society. A sound grounding in science strengthens many of the skills that people use every day, like solving problems creatively, thinking critically, working cooperatively in teams, using technology effectively, and valuing life-long learning. And the economic productivity of our society is tightly linked to the scientific and technological skills of our work force.” (NRC, 1996, page ix)

As noted in the report published by the National Research Council, society stands to gain immensely from science. Science education promotes more than scientific knowledge; problem-solving, critical thinking, and creativity are all skills students can develop as part of their science education. The ability to apply these skills and scientific knowledge to societal concerns has been called scientific literacy (Bybee, 1997).

Recent international surveys have shown that the U.S. ranks below other countries in terms of scientific literacy (OECD, 2016). These findings, along with the results of nationwide reports on education, have prompted calls for targeted efforts to increase enrollment and retention in STEM fields (AAAS, 2011; NRC, 2009; PCAST, 2012). These reports call for research to better understand learning and retention in STEM fields and encourage educational reform driven by empirical research (PCAST, 2012). This has

resulted in an increase of discipline-based education research with the goal of understanding and improving education in STEM fields. Physics, chemistry, biology, and math have all experienced a growth in research focused on education within these disciplines (Talanquer, 2013).

Chemistry education research seeks to improve learning in chemistry. Chemistry education research identifies learning issues in chemistry education, some of which are general education issues (e.g. writing heuristics for science lab reports (Greenbowe, Poock, Burke, & Hand, 2007)) but many of which are issues specific to learning chemistry (e.g. strategies to improve students' interpretations of NMR spectra (Flynn, 2012)). Part of chemistry education research involves exploring the relationship between learning issues and the specific chemistry content in which these issues are observed. Because chemistry education research is dependent on both chemistry and learning sciences, it is necessary to apply expertise from both of these fields in order to engage in effective chemistry education research.

Learning theories

The work presented in this thesis is grounded in the current understanding of how people learn. Research in the constructivist tradition has provided evidence that students actively construct their ways of knowing through trying to reconcile what they are learning with their prior understanding (Cobb, 1994). This work is also guided by sociocultural tenets. Research guided by sociocultural activity theory has shown that learning is not an individual activity, and that student thinking is influenced by cultural

practices both within and outside the context of school (Cobb, 1994). Cultural and social interactions students experience shape how students integrate and apply what they are learning. Both of these traditions have influenced the Chemical Thinking framework that guides the research presented in this thesis.

Chemical Thinking framework

If the aim of science courses, including chemistry, is to produce students who are able to apply their scientific knowledge and reasoning to make informed decisions within today's society, then the curriculum, instruction, and assessment approaches must all coherently prepare students for these types of situations. The existing educational system and pedagogical approaches do not support the development of scientifically literate citizens (Fischer et al., 2005; Hofstein, Eilks, & Bybee, 2011; J. Osborne & Dillon, 2008). Traditional chemistry courses and curricula focus on covering concepts, resulting in a breadth of chemistry knowledge being transmitted to students taking chemistry courses. In order to accommodate the vast number of concepts they are expected to learn, students often sacrifice applicable understanding for rote memorization (Cooper, 2015). Studies have shown that many students do not use the concepts they have learned to develop a robust, explanatory framework of their chemistry knowledge, let alone apply it to contexts outside of the chemistry classroom (Eilks & Hofstein, 2015).

Recent reform efforts in K-12 science education have emphasized the need to focus student learning on the development, analysis, discussion, and application of central ideas in the different scientific disciplines (NRC, 2011, 2012; George et al., 2001).

They also highlight the importance of using crosscutting concepts, such as scale, structure, and energy, to analyze the properties of diverse systems and to build meaningful connections among those systems. These new K-12 standards and framework make a case for the use of crosscutting concepts to organize curricula, which allows teachers to focus students' attention on the search for answers to essential questions in science and introduces unifying ideas to guide student thinking (NRC, 2011; Sevian & Talanquer, 2014; Talanquer, 2013).

Conventional approaches to chemistry education at both K-12 and higher education levels typically present the discipline as a set of loosely related topics: chemical nomenclature, stoichiometry, atomic structure, etc. (Van Berkel, De Vos, Verdonk, & Pilot, 2000). Instruction in chemistry often involves helping students develop sets of isolated skills to solve academic problems (e.g. balancing chemical equations, drawing Lewis structures). This 'toolbox' approach to the teaching and learning of chemistry has had limited success in fostering meaningful understandings among diverse students (Gabel & Bunce, 1994; Kind, 2004). A disconnect exists between the traditional view of chemistry as comprised of concepts and skills and the ultimate aims of chemistry: synthesis, analysis, and transformation of substances (Chamizo, 2013). Frequently, students do not infer connections between the concepts and aims of chemistry without support from instructors. In response to the misalignment of chemistry education and the practice of chemistry, the Chemical Thinking framework presents a disciplinary nature of science approach that organizes knowledge, reasoning, and problem solving in the discipline of chemistry. The Chemical Thinking framework organizes the discipline of

chemistry by its crosscutting disciplinary practices. These disciplinary practices are what chemists do, and it is through these practices that they solve challenges using chemical knowledge. The six crosscutting concepts can direct the attention of teachers and students toward fundamental ways of thinking in chemistry that cut across a variety of topics. These six crosscutting disciplinary concepts are deemed essential to the practice of chemistry because these concepts comprise the questions that chemistry allows us to answer:

1. Chemical identity addresses “What is this substance?”
2. Structure–property relationships address “What properties does the substance have?”
3. Chemical causality addresses “What causes this substance to change?”
4. Chemical mechanism addresses “How does the substance change?”
5. Chemical control addresses “How can we control change?”
6. Benefits-costs-risks addresses “What are the consequences of changing matter?”

Authentic problems in chemistry involve several crosscutting disciplinary concepts. For example, a chemist may face the challenge of designing a novel method of producing acetaminophen. Doing so may require analyzing the relative merits and shortcomings of current production methods and economic costs, environmental factors, and societal and ethical consequences associated with alternatives (benefits-costs-risks thinking), identifying other reaction mechanisms that could be used (chemical mechanism thinking), designing a method for separating the desired product from the process

(structure-property relationships thinking) and for characterizing products (chemical identity thinking), and testing conditions that maximize yield while minimizing resources (chemical control thinking). Chemical identity thinking does not occur only in authentic problems in chemistry, but also occurs in exercises and problems in approaches to teaching chemistry that do not involve authentic problems. For example, many chemical nomenclature questions in general chemistry depend on a student first discerning whether a compound is molecular or ionic – a categorization activity that depends on chemical identity thinking.

The Chemical Thinking framework regards student understanding in chemistry as a dynamic cognitive landscape that constantly interacts with the environment (Sevian & Talanquer, 2014). Within this cognitive landscape are semi-stable attractors where the chemical understanding of students tends to be more robust. Attractors are both dynamic and context-dependent. These attractors can be characterized by the assumptions that guide and constrain students' chemical thinking, and the Chemical Thinking framework commits to investigating these assumptions. Assumptions are a form of cognitive construct, similar to constructs defined by other researchers, such as pre-suppositions (Vosniadou, 2013), core beliefs (Chi, 2008), or phenomenological primitives (p-prims) (diSessa, 1993). Assumptions are believed to direct student thinking in both productive and nonproductive ways, and are not characterized by degrees of correctness. Rather, students build new assumptions in a cumulative manner, and develop the capacity for qualifying when to rely on different assumptions as their chemistry expertise grows. By investigating assumptions, it is possible to explain why students come to certain

conclusions when reasoning in chemistry. The Chemical Thinking framework commits to identifying assumptions associated with each crosscutting disciplinary concept and hypothesizes that a progression comprised of these assumptions can be constructed as students move from novice toward advanced chemical thinking.

Two types of assumptions have been characterized by the Chemical Thinking framework: conceptual sophistication and modes of reasoning (Sevian & Talanquer, 2014). Conceptual sophistication is tied to the sophistication of the expressed content knowledge or the concepts of chemistry. It is a measure that typically proceeds from more novice to more expert, and although there are degrees of sophistication, they are not considered to be hierarchical levels through which students pass during their chemistry education. Modes of reasoning are a measure of the type of reasoning or argument a student chooses to apply to solving a problem. This type of assumption is domain general, and not necessarily linked to the conceptual sophistication of the argument. In empirical studies, these two variables have been shown to be relatively independent in characterizing how students reason about chemical problems (Banks et al., 2015).

Chemical identity

The concept of ‘chemical identity’ encompasses the most basic idea of chemistry: *What is this stuff?* The identification of substances has been core to chemistry throughout the history of the discipline (Schummer, 2002). Analysis with the intent of identifying a sample is, at heart, a problem of classification or differentiation. Such activity depends on the assumption that each chemical substance has at least one differentiating property that

makes it unique (Enke, 2001). Discriminating among substances requires the use of properties of matter to assign to ‘types of matter’ categories. However, decisions about which properties may be used as differentiating characteristics are not easy to make. Research suggests that ideas and decisions about identity and assignments to categories are constrained by what individuals perceive as surface features of items being classified (Talanquer, 2009; Vosniadou & Ortony, 1989) and the history of a sample of the material (Johnson, 2000). Substance (e.g., polybutadiene rubber) and object (e.g., bouncy ball) are often confused or conflated, as are extensive (e.g., volume) and intensive (e.g., density) differentiating properties (Wiser & Smith, 2008).

The concept of chemical identity (CI) provokes two major questions:

- Core question 1: What types of substances are there?
- Core question 2: How can substances be differentiated?

The first is a question of classification (Van Brakel, 2014). The second asks whether two substances are the same or not the same (Hoffmann, 1995).

Importance of chemical identity for the general public

One goal of science education is to prepare students to be scientifically literate citizens. This entails that citizens should be able to apply their scientific knowledge and skills in their everyday lives; there are many intersections of science and technology in society, and the general public should be prepared for these interactions (Hofstein et al., 2011).

Situations involving chemical identity occur frequently in daily life. Substances are encountered everywhere – from the lab to the grocery store to our homes. The chemical identity associated with a substance is often used to make decisions about substances. Box 1 below presents an example of a situation in which questions of chemical identity might be encountered outside of the chemistry classroom or lab.

Box 1: Chemical Identity in Daily Life

Imagine you are a citizen whose last chemistry class was in high school. You are shopping for jewelry, and a salesperson shows you a pair of lab-synthesized diamonds. She explains that these diamonds are a fraction of the cost of naturally mined diamonds. You start to wonder: What is the difference between these and naturally mined diamonds? Why would a lab-synthesized diamond be less expensive? Do the processes in the lab affect the diamond? Does the original source of the diamond have an impact? What are the essential features I am looking for in a diamond?

In this scenario, questions arise that are related to classifying the diamond (What are the essential features I am looking for in a diamond?) and to differentiating one diamond from another (Do the processes in the lab affect the diamond? Does the original source of the diamond have an impact?). Decisions such as this one that are based on chemical identity are context-dependent. Someone in this situation might only care about chemical identity on the macroscopic level (e.g. appearance or brilliance of the diamond), whereas someone else might care about the chemical identity on the microscopic level (e.g. purity of the diamond). In this scenario, how the chemical identity of the diamond is defined has an impact on its value as well – a real-world manifestation of attaching importance to chemical identity.

Importance of chemical identity for chemists

Chemical identity is relevant to the work of chemists as well. An important task in the discipline of chemistry is the differentiation of the entities relevant to chemistry

(Schummer, 2002). For chemistry, this entails substances and their many forms.

Determining whether substances are the same or not the same (Hoffmann, 1995) helps to establish the ways in which substances can be classified and the features that enable differentiation.

When solving problems with chemistry, chemists frequently ask questions of chemical identity. Knowledge of a substance's chemical identity is essential before attempting to transform it, a central aim of chemistry. Real-world challenges (e.g. fuel storage) that involve other disciplinary crosscutting concepts (e.g. chemical control of storing the fuel and then releasing it for consumption) often rest on the knowledge of chemical identity. The following box presents an example where a chemist might encounter a situation involving chemical identity.

Box 2. Chemical Identity in the Work of a Chemist

Imagine you are a chemist, and you are investigating new substances for use as semiconductors. You are interested in experimenting with diamond as a wide-band gap semiconductor. You know you can get naturally mined diamonds or lab synthesized diamonds, and question which would be better for your research. What level of purity can be achieved with the synthesized diamonds? How does the composition compare to mined diamonds? What type of doping is possible without compromising the diamonds? Are diamonds that are produced using chemical vapor deposition different than those produced using high-temperature, high-pressure reactors?

Situations like this one rely on chemical identity thinking, as they include the reasoning, knowledge, and practices chemists use to determine if substances are the same or not the same.

Importance of chemical identity for teaching and learning chemistry

Answering questions of chemical identity is typically a foundational aspect of solving problems using chemistry. Authentic problems are complex; discriminating

substances based on relevant types and knowing how to differentiate them is important before reasoning about other aspects of the problem that chemistry can address. Whether or not students plan to pursue a career in chemistry, chemical identity is relevant in daily contexts; thus, students at all levels should have a basic understanding of chemical identity. In order to become proficient at chemical identity thinking, students need exposure to the types of questions and situations where chemical identity is applicable.

Organization of chemical identity research

The Chemical Thinking framework guided the investigation of students' chemical identity thinking. This research is driven by the desire to uncover the assumptions guiding students' chemical identity thinking and to determine how training in chemistry influences the types of assumptions students hold and their application of assumptions in different contexts. Thus, the overarching research question for this doctoral work is:

What are the ways in which students think about chemical identity?

This work ultimately contributes to the development of a learning progression for chemical identity thinking. Learning progressions are educational models that describe pathways of expertise development in given domains (Duschl, Maeng, & Sezen, 2011). Learning progressions can guide curriculum development as well as instructional and assessment practices to foment more meaningful learning, clearer standards of learning progress, and more useful formative feedback (Alonzo & Gotwals, 2012). The development of these educational models demands a solid understanding of the ideas students have and their likely changes with instructional interventions. A learning

progression for chemical identity can be used to guide instructional decisions for teaching chemical identity practice and as a foundation for future research in chemistry education.

The path of this work is first grounded in a literature review investigating students' conceptions of substances and their chemical identity thinking. The ways in which students classify and differentiate substances are influenced by their conceptions of substance, for the views students hold of substances affect the cues students choose to pay attention to when reasoning about chemical identity. Thus, this literature review investigated existing research on philosophy of substance in addition to students' conceptions of chemical identity. This review provided the foundation for a hypothetical learning progression for chemical identity thinking, which included knowledge and assumptions related to chemical identity.

The need for empirical evidence of chemical identity thinking led to the development of a survey to elicit chemical identity thinking. The survey captured how students classify and differentiate substances, which is the practice of chemical identity. Practices of chemical identity are one facet of chemical identity thinking, and knowledge and reasoning associated with chemical identity thinking are typically evident in the practices of chemical identity. Finally, the relevance of chemical identity thinking in another discipline is explored. In this extension, chemical identity knowledge applied to biochemical contexts is analyzed. The knowledge associated with chemical identity thinking is another facet of chemical identity thinking. Implications for instruction and future research based on the studies in this thesis are also discussed.

CHAPTER 2

FOUNDATIONS OF CHEMICAL IDENTITY THINKING: A LITERATURE REVIEW

Conceptions of substance

Chemical identity thinking involves the knowledge, reasoning, and skills associated with the classification and differentiation of substances. How someone approaches classification and differentiation of substances, or chemical identity, rests on his/her conception(s) of substance. In order to classify or differentiate substances, one must have an understanding of what a substance *is*. Conceptions of substance have the potential to influence a person's chemical identity thinking. Thus, a person's chemical identity thinking can only be as sophisticated as his or her understanding of substances. Although this work does not attempt to suggest alternative perspectives on the concept of substance, it is worth outlining the current views and their merits in order to have an understanding of the different conceptions of substance that might ground chemical identity thinking. Students' conceptions of substance are unlikely to be as sophisticated as the ones presented here, but may contain components of these views.

Conceptions of substance have evolved throughout the history of chemistry, and the definition of substance is still debated today. At the core of this debate is the question:

what is the true essence of a substance? (Needham, 2012). Philosophers differ on whether to focus on the macroscopic level or the microscopic level to define substance identity (i.e. chemical kinds). Previously, Empedocles' classification of classical elements (earth, air, fire, water) was used to characterize substances (Ball, 2004). At this time, substances were viewed as ratios of these classical elements. Aristotle added qualities to the understanding of elements in order to explain their behavior; each element has an associated quality (heat, cold, wetness, dryness) that allows us to experience the substance, and account for the transformation of one substance into another (Ball, 2004). These classical elements, along with their qualities, were believed to determine the behavior of substances. In recent years, this four-element classification system has been modernized to a new argument of essentialism. Ellis (2002) has outlined essential properties that dictate both the nature and behavior of substances, and this "essence" can be used to group natural kinds. In his exposition on essentialism, Ellis claims that,

the chemical elements and compounds constitute the most readily accessible system of natural kinds of substances, their properties are mostly their essential properties, and the processes they undergo in chemical interactions are all natural kinds of processes that display the essential properties of the substances involved.

(2002, p. 139)

In short, there are defining features (essential properties) of a substance that are tied back to their elements, and these dictate both a substance's behavior and properties. By reducing the notion of a substance to the scale of atoms and molecules, it is possible to

identify the essential properties that define a substance, such as molecular shape, atomic weight, atomic number, etc.

Others, however, claim that substances should be approached from the manifest (macroscopic) perspective rather than the scientific (submicroscopic) perspective and the microstructure. A key feature of the argument against the microstructure perspective is that there are many assumptions and flaws in reducing the concept of substance from its macroscopic image to single molecules comprising the substance (which is the basis of the microstructure perspective). For example, VandeWall and van Brakel argue that the concept of a molecule itself is an idealization; molecules are not stable kinds, and are constantly changing bond lengths and shape, so although it serves well as a theoretical concept it cannot be said that each substance only has ONE definitive microstructure (van Brakel, 2000; VandeWall, 2007). Furthermore, van Brakel argues that the ultimate goal of chemists is the transformation of substances, which is grounded in the manifest perspective of the substance (van Brakel, 2000). Additionally, it is only the manifest perspective of substance, or collection of molecules, that can hold thermodynamic properties. These emergent properties (Luisi, 2002) are frequently used by chemists to identify and differentiate substances. Van Brakel and others (Needham, 2008; VandeWall, 2007) argue that the reduction of a substance to its molecular level changes the accepted understanding of a substance, and the theoretical notions of substance begin to break down.

Bursten (2014) combines these views, and argues for a united definition where both macroscopic and microscopic levels are considered. She draws from the manifest

perspective and uses reactivity patterns observed on a macroscopic level for the classification of substances, but argues that the rule of “all the same chemical reactions” that is used to identify and distinguish substances can be informed and improved by microstructural arguments. She provides phosphorous allotropes as one example (Bursten, 2014, p. 641-642) and explains that one allotrope manifests as a white solid capable of spontaneous combustion in warm air, while the other allotrope appears as a white crystal incapable of spontaneous combustion (and is insoluble in most solvents). Although the “all the same chemical reactions” rule differentiates these allotropes due to their differing behavior, the microstructure of these allotropes (tetrahedral vs. rectangular prisms in crystal lattice) explains their behavior. Bursten argues that differentiation using the microstructure provides valuable information for chemists, and that microstructure is often used in practice. Although few other philosophers of chemistry hold this intermediary view, it is likely that students will be more aligned with Bursten’s perspective and hold conceptions of substances at both the macro and micro level.

Despite the differing opinions, there is agreement that how a substance is defined is discipline-specific. As Hendry notes, “the classificatory practices of a scientific discipline reflect its particular theoretical and explanatory interests” (Hendry, 2006, p. 874). These viewpoints of substance all involve that which is most important to chemists: atoms, molecules, elements, chemical reactivity, purity, etc. Outside of chemistry, substances may be recognized by different classifications; for example, water and jade are not necessarily named as chemical substances, as these names represent the manifest substances encountered in daily life. Additionally, many philosophers contend that

substance identity is context-specific: time, scale, size, etc. All can influence the concept of substance (VandeWall, 2007; Weininger, 2000). How a chemist chooses to define and classify substances is dependent on the nature of the context; can a substance be identified by its boiling point, in which case the substance is considered as a collection of molecules, or is the context a question of radioactive decay, in which case the specific atoms and their submicroscopic configuration are essential to the identity? It is perhaps better, as Needham points out, to be specific when regarding substances and their properties, and to say that a specific substance has a specific property at a certain point in time (Needham, 2012).

Chemical Identity: A Core Chemistry Concept

All scientific disciplines focus a significant part of their efforts on differentiating the types of entities that are relevant in their domain. This is particularly important in disciplines such as chemistry that rely on classification not only for organizational purposes, but also as a powerful tool for predicting properties (Schummer, 1998). The search for proper cues to differentiate the diverse and increasing number of chemical substances in our world has been one of the core goals of the chemical enterprise throughout its history (Schummer, 2002). Modern chemical thought and practice have come to rely on the fundamental assumption that each material kind has at least one measurable differentiating characteristic that makes it unique and that can be used to identify it (Enke, 2001). Understanding chemical identity and the conditions and processes in which it is lost or preserved is a core goal of chemistry with major

implications for modern societies (e.g. detecting pollutants, tracking metabolites, purifying drinking water; Hoffmann, 1995). Consequently, understanding the ideas students hold about this crosscutting disciplinary concept should be considered of central importance in chemistry education.

The concept of chemical identity is not trivial and its meaning has changed several times in the history of chemistry as a discipline (Schummer, 2002). Processes that nowadays are conceived as conserving chemical identity, such as the transformation of ice into liquid water or the vaporization of this substance, were conceptualized as leading to the formation of new entities in the Aristotelian tradition (Toulmin & Goodfield, 1962). Elementary substances such as nickel and cobalt were thought of as mixtures of several metals by mineralogists in the eighteenth century (Llana, 1985). In part, these conceptions of chemical identity are related back to the conceptions of substance at that time. When the Aristotelian view dominated the understanding of substances, for example, the chemical identity of a substance was linked to the presence and ratios of the natural kinds within the substances. Changing the presence or quantity of the natural kinds was thought to constitute producing a new substance. Thus, substances were classified and differentiated based on their inherent natural kinds, which in turn were believed to define the behavior of a substance.

The current understanding of substances at the macroscopic (behavior of a collection of molecules) level and submicroscopic (molecular composition and structure) level has led to the classification and differentiation of substances based on their properties. Although chemical scientists have identified sets of properties that facilitate

the identification of chemical substances, the answer to the question of which properties count as chemically essential has changed with the development of new theoretical frameworks and experimental techniques. Historically, substances were characterized by a short set of factors: method of preparation, elemental analysis, melting or boiling point, visual characteristics, solubility in various solvents, and exemplary reactivities. Only in the past 50 years has chemical structure been added as a major and dominant differentiating characteristic (Schummer, 2002). The introduction of spectroscopic methods in chemical analysis has led to a radical reconceptualization of the concept of chemical identity, from a construct that depended on the characterization of the chemical composition and properties of pure macroscopic samples to a concept which now critically relies on the determination of the molecular structure of the submicroscopic components of the substance under analysis.

Given the long and complex historical evolution of the concept of chemical identity, one may suspect that many students will struggle to develop a meaningful understanding of this construct. Existing research in science education suggests that changes in student understanding of some core scientific concepts often resemble stages in the history of the concept's development (Wandersee, 1986). In fact, the different considerations of chemical identity (the short set of factors listed above, now with spectroscopic properties added to isolate chemical structure) remain present in how chemists continue to characterize substances today. Despite the complexity of the concept, at the bare minimum, scientifically literate individuals must come to understand that the chemical identity of substances in their surroundings is determined by their

submicroscopic composition and structure. Students should be given opportunities to identify the costs and benefits of applying chemical thinking to determining and changing the identity of materials. At more advanced levels, students should be able to recognize the emergent nature of chemical identity and the diversity of approaches that can be used to characterize it.

Although chemical identity is not a concept explicitly addressed by traditional chemistry curricula, its understanding can be expected to evolve as students are asked to recognize different types of substances, explore their properties, and identify their chemical composition and structure at the submicroscopic level. Thus, analysis of students' ideas in all of these areas should provide insights into common conceptualizations of chemical identity at different educational stages. In particular, understanding the underlying assumptions that support but also constrain student reasoning about chemical identity may help us devise strategies to effectively engage students in authentic chemistry practices and ways of thinking (Sevian & Talanquer, 2014).

Research Question and Goals

This literature review was guided by the following research question:

What major assumptions about chemical identity guide students' reasoning about chemical substances as they progress from less to more conceptual sophistication?

The specific goal was to characterize the common evolution of students' ideas about chemical identity as inferred from the analysis of existing research findings in the areas of students' alternative conceptions in science education. Ultimately, this literature review will build a knowledge base that can aid and support the construction of a learning progression on chemical identity thinking. Major components of this chapter have previously been published (Ngai, Sevian, & Talanquer, 2014). This chapter expands on the concept of substance and also incorporates newly published research that was not available when this literature review was initially conducted. These new findings are primarily discussed in the implications for teaching section.

Methodology

This study was based on the review and analysis of existing findings in science and chemistry education. In particular, existing research literature was analyzed to identify study participants' underlying assumptions about the answers to two major questions related to the concept of chemical identity (Sevian & Talanquer, 2014):

- What types of matter are there?
- What cues are used to differentiate matter types?

Research findings were carefully analyzed to infer assumptions about chemical identity that may have guided student thinking in the identified studies. Core inferences were often informed by the chemistry knowledge of the researchers, and by studies on the

history and philosophy of chemistry that refer to the concept of chemical identity. The analytical work consisted of several phases.

Phase 1: Initial resource collection – A list of search terms and concepts believed to be relevant to chemical identity was compiled (e.g. chemical substance, properties, composition). The resulting list of terms was then applied to complete thorough searches using three major online databases: Web of Science, SciFinder, and Google Scholar. If the search produced more than 500 results, additional search parameters were included (such as the phrase “chemistry education”) to reduce the number of results. If the pool of results exceeded 500, it was considered too broad for further examination. Initial evaluation of search results was based on the analysis of work titles and abstracts, focusing on those manuscripts that reported results on students’ abilities to identify or differentiate among various chemical substances (either as a main part of the study or as one of its components). There were no restrictions on publication date for the resources collected, type of research methodology employed, country of origin, or age of the research subjects. Thus, the identified studies involved diverse participants from a wide span of educational levels and regions of the world, from pre-school to graduate levels. This initial stage of analysis resulted in a collection of 170 works, which included articles published in journals, book chapters, online white papers, conference abstracts and papers, and doctoral theses.

Phase 2: Resource evaluation – The initial collection of resources was divided into two major categories after careful analysis of different study abstracts. The first group, or primary collection, included research on the approaches students take when classifying

objects and materials, the beliefs of learners about changes in chemical identity during physical or chemical changes, alternative conceptions about different types of matter, etc. The second collection included manuscripts not written in English, lacking a detailed description of findings, or indirectly related to the concept of chemical identity, such as studies focused on the analysis of the general ideas students have about different models of matter. Some of these resources were moved to the primary collection during Phase 3 of the analysis.

Phase 3: Additional references – Careful reading of all of the resources in the primary collection allowed for the identification of additional cited papers relevant to the investigation, which were included in either the primary or secondary collections. Adding these articles to the collection provided a method to check that the most relevant research available was gathered and brought the search closer to saturation. This resulted in a collection of 26 papers for analysis.

Phase 4: Analysis and synthesis – Findings from each research paper in the primary collection were summarized and analyzed to elucidate student thinking. Particular attention was paid to patterns of reasoning consistently elicited by several studies. Initial hypotheses about underlying assumptions guiding student reasoning were made by the author, and then discussed until consensus was reached among different researchers. For those studies involving instructional interventions, efforts were made to identify both initial assumptions (held by students prior to the intervention) and targeted assumptions (seen as the desirable outcome of the intervention). The results of these analyses were used to build hypotheses about a potential evolution in student assumptions about core

aspects of chemical identity. These hypotheses were also informed by prior disciplinary knowledge and teaching experience.

Existing data allowed for the development of a rather complete picture of the lower anchor for a learning progression on chemical identity. The lower anchor in a learning progression describes the initial ideas that many novice learners hold about a targeted concept before instruction (Duschl et al., 2011). The characterization of how these initial ideas evolve with training in the discipline was less complete, as major gaps were found in the analysis of students' ideas about substances at different educational levels. Data analysis led to the identification of various ways of thinking about chemical identity that could correspond to different degrees of conceptual sophistication. Such patterns of thinking were labeled (e.g. objectivization, principlism, compositionism), and their underlying assumptions (e.g. historicity, additivity, substantialism), using words that sought to capture the essence of student thinking and that had been used by prior authors in science education or in the history and philosophy of science to represent specific forms of reasoning. As part of the analysis, reconceptualizations were also identified in the learning progression (Wiser, Frazier, & Fox, 2013), which are similar to threshold concepts (Meyer & Land, 2006), representing productive ways of thinking that may support the transition to more sophisticated thinking with proper instruction.

Although the literature review was thorough, there may be relevant studies that were missed in the analysis. Nevertheless, the strong consistency in core findings across the different studies included in the review substantiates the major claims made in the following section.

Findings

The analysis of existing research findings revealed that students' ideas about chemical identity do progress with training in the discipline, but the development of canonical understandings is not straightforward. Figure 2-1 summarizes the major assumptions that emerged from the analysis that seem to guide the reasoning of a significant proportion of students at different degrees of conceptual sophistication. Assumptions are arranged into three major threads related to (from top to bottom): (a) how students conceptualize matter types, (b) what types of properties learners use in making decisions about chemical identity, and (c) what major reasoning patterns apply in making such judgments. In the following sections the existing evidence supporting the progression of assumptions represented in the figure is described.

Figure 2-1. Hypothetical progression of major assumptions about chemical identity

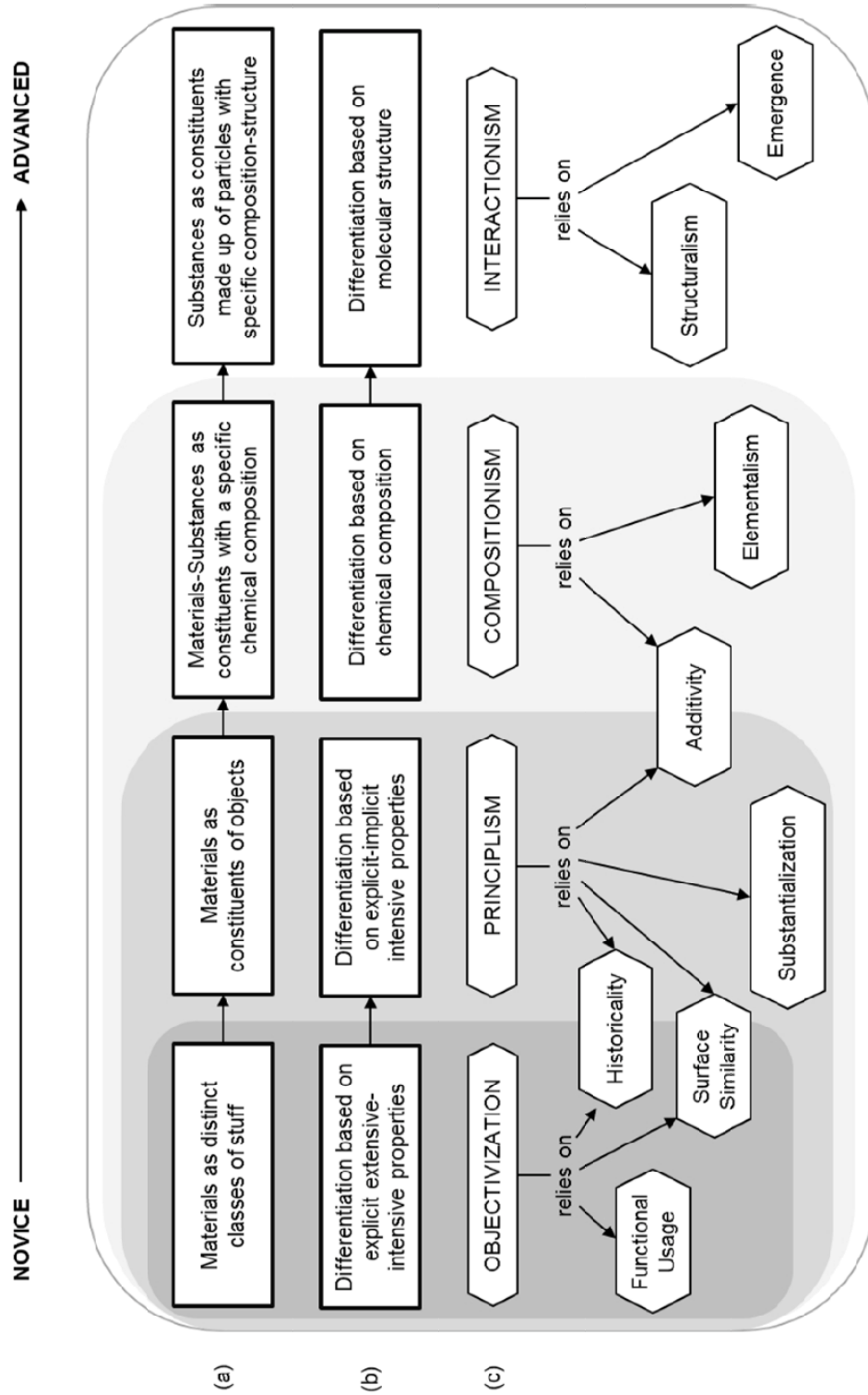


Figure 2.1. Hypothetical progression of major assumptions about chemical identity: (a) conceptualization of matter types, (b) types of properties used in making decisions about chemical identity, and (c) major reasoning patterns applied in making such judgments. Four major ways of thinking are highlighted that influence students' reasoning about chemical identity at different degrees of conceptual sophistication: 1. Objectivization: The tendency to use object-relevant properties to differentiate materials; 2. Principlism: The tendency to explain the properties of matter by reference to the presence (or absence) of 'principles' that carry such properties; 3. Compositionism: The tendency to think of substances as mixtures of atoms-elements with characteristic properties; 4. Interactionism: The tendency to view the properties of matter as emerging from the dynamic interactions among components

Novice Learners (Lower Anchor)

Although humans interact with a wide variety of materials from a very young age, existing research studies indicate that young children struggle to differentiate between the concepts of object and material, using object-relevant properties (e.g. size, shape) to classify different kinds of substances (Au, 1994; Dickinson, 1987; Johnson, 2000; Krnel, Watson, & Glažar, 1998, 2005; Smith, Carey, & Wisner, 1985; Vogelezang, 1987; Wisner & Smith, 2008). In reality, very few materials that learners meet in everyday life are single substances, i.e. most are mixtures. Novice learners typically do not distinguish between mixtures and pure substances. Although most children in preschool or early elementary school can distinguish an object from the material from which it is made (Au, 1994; Johnson, 2000), there is evidence that many students continue to use a mixture of object-relevant and substance-relevant properties to classify materials in secondary school (Krnel, Glažar, & Watson, 2003; Krnel, Watson, & Glažar, 1998, 2005). This tendency to ‘objectivize’ materials (objectivization) seems to have a strong influence on how students begin to think and make decisions about chemical identity.

Analysis of core results from different studies suggests that novice students’ reasoning about the identity of materials is influenced by three major categories of factors: (a) appearance, (b) usage, and (c) history. These types of factors are similar to those that guide people’s reasoning about object identity (e.g. deciding whether a perceived object is a chair or a table), and their application in differentiating kinds of substances is indicative of major assumptions about chemical identity described in the following paragraphs.

Surface similarity. Novice learners use perceptual cues to distinguish among different types of materials. They pay attention to perceivable properties of materials such as shape, color, texture, and smell to make judgments about category membership (Liu & Lesniak, 2006; Smith et al., 1985). What cues are used in differentiating substance may vary from one context to another, and may depend on the specific types of materials under consideration. For example, the liquidity of a set of materials often leads learners to classify them as ‘like water,’ or containing water, independently of differences in color, taste, or smell (Solominodou & Stavridou, 2000). Differences in the granularity of two samples of the same material (e.g. a solid piece versus a powdered sample) may lead children to classify them into two different groups, despite many apparent similarities (Dickinson, 1987). Abstraction of salient features shared by several materials may result in the development of a ‘prototype’ used to represent a particular type of matter. For example, gases are thought of as some type of ‘air;’ liquid materials are often seen as some type of ‘water;’ shiny solids are generically classified as ‘metal;’ while crystalline powders are said to be like ‘salt’ (Krnel, Watson, & Glažar, 1998, 2005).

The central role that ‘surface similarity’ plays in the categorization decisions of novice learners has been described and analyzed by a variety of authors (Vosniadou & Ortony, 1989; Wiser & Smith, 2008). When dealing with natural kinds, people often tacitly assume that surface similarity is likely indicative of common inner structures or essences (Gelman, 2003). This assumption is a powerful cognitive guide given that surface similarity may be revealing of deeper structural properties. Unfortunately, this assumption acts as a cognitive roadblock when making decisions about chemical identity

because perceivable commonalities are often misleading (e.g. not all crystalline white solids are sweet, or soluble in water, or edible). Surface features used to differentiate materials may vary not only when judging different entities, but also as attention shifts from one salient feature to another during the analysis of a given material (Stains & Talanquer, 2007).

Functional usage. Combinations of actions seem to help children differentiate matter types (Krnel, Watson, & Glažar, 1998). For example, solids can be held and broken, liquids can be poured and spilled, and gases can be blown. The actions with and uses of particular substances support the identification of different classes of materials. Thus, young children also create conceptual categories for kinds of substances based on functional usage in daily life (similarly to how objects are classified (Lynch & Jones, 1995; Stavy, 1991)). For example, Liu and Lesniak (2006) indicated that students of various ages often described substances in terms of their benefits and common use (e.g. water for drinking; baking soda for baking). Bretz and Emenike (2012) described the strong association that some elementary school children built between the concept of ‘chemicals,’ conceived as a special class of stuff, and materials used for practical purposes, such as cleaning products. Materials known to have similar functions (e.g. glues, oils) were often assumed to share the same intrinsic nature.

Historicality. Novice learners rely on their knowledge about the origin and history of a material to make decisions about both chemical identity and conservation of chemical identity during a process (Johnson, 2000; Krnel, Watson, & Glažar, 2005; Talanquer, 2006). The term ‘historicality’ is used to refer to the influence of knowledge

of origin and past history on current thought about entities of interest (Wandersee, 1992). Existing research suggests that samples of a given substance are often judged to be different if they come from distinct sources or result from different processes. For example, people are known to think differently about natural versus synthetic samples of the same substance (Rozin, 2005). The ability to trace the history of a material influences how learners make decisions about conservation of identity during physical or chemical changes (Krnel, Watson, & Glažar, 2005; Van Driel, 2002). Students often assume that changes that occur naturally, without external intervention, have little or no impact on chemical identity, particularly if modifications in appearance are gradual (i.e. traceable) and somewhat subtle (e.g. as when a piece of metal corrodes; Nieswandt, 2001). On the other hand, novice learners can be expected to make claims about change of identity when processes dramatically alter the appearance or functional usage of the materials under consideration, making them look like members of a different material class (Rahayu & Tytler, 1999; Tytler, 2000). This often occurs in processes involving gases (e.g. evaporating a liquid, burning a paper into ashes), which many novice learners conceive as immaterial entities (Wiser & Smith, 2008).

Surface similarity, functional usage, and historicity play a central role in the ideas novice learners have about what types of matter are there and what cues can be used to differentiate them. Initial views of materials are not compositional in nature, in the sense of thinking of materials as the constituents of things. Rather, materials are seen as distinct classes of stuff (e.g. metals, plastics, salts) with different perceivable properties, usages, or origins (Dickinson, 1987; Smith et al., 1985; Vogelesang, 1987). There is no

or little recognition of the wide diversity of substances within a class (Solominodou & Stavridou, 2000). At this level, students are likely to use a mixture of extensive (i.e. dependent on size) and intensive (i.e. independent of size) properties to classify materials (Krnel, Watson, & Glazar, 1998, 2005); these cues are likely to be explicit rather than implicit. Which specific cues are used to make judgments about the identity of a material depends on what cues are more salient in a given context, prior knowledge, and personal experience with different materials.

Initial progress

Novice learners' reasoning about the identity of materials, as described in the previous section, is quite different from established ways of thinking in modern chemistry. The notion of 'substance' as conceptualized by chemical scientists is difficult to interpret or conceive when students' thinking is constrained by the intuitive assumptions described above, as are the intellectual and experimental strategies used by chemical scientists to infer chemical identity. Existing educational research suggests that the development of these ideas likely takes a long time and it may occur in rather patchy ways, with more sophisticated understandings of some types of materials developing sooner than for others (e.g. solid versus gaseous materials; molecular versus ionic compounds; Dickinson, 1987; Johnson, 2000; Krnel, Glazar, & Watson, 2003). The road toward chemical thinking in this area seems to demand the following shifts in the ways students reason about materials and their properties:

- Students assume that materials or substances are the underlying 'constituents' of objects in their surroundings, rather than simple labels for classes of stuff with

common usages, history, or perceptual features (Smith, Carey, & Wiser, 1985; Wiser & Smith, 2008);

- Students differentiate the properties of a material from those of an object, and start paying increasing attention to implicit intensive properties of materials to categorize them (Krnjel, Watson, & Glažar, 1998, 2005; Krnel, Glažar, & Watson, 2003).
- Students recognize the limitations of perception in identifying or distinguishing materials and understand the need for experimental testing of selected differentiating properties (e.g. melting points) of substances that are acknowledged as unknown (Johnson, 2000).

Such shifts in thinking may be considered as ‘reconceptualizations’, conceived by Wiser and collaborators as a ‘deep and fundamental reorganization of the large network of knowledge relevant to understanding’ (Wiser et al., 2013, p. 96). Reconceptualizations in this sense are like ‘threshold concepts’ as conceptualized by Meyer and Land (2006), opening up new and previously inaccessible ways of thinking about something.

These changes in student reasoning are critical for supporting the development of core chemistry concepts such as substance, mixture, chemical change, and chemical analysis. Nevertheless, it is important to acknowledge that such changes may also trigger additional conceptual roadblocks. For example, assuming that materials are the underlying constituents of things may support essentialist views of matter in which core essences are seen as unchangeable (De Vos & Verdonk, 1987; Talanquer, 2006).

Materials may be thus conceived as enduring entities whose identity survives through most types of changes (Renström, Andersson, & Marton, 1990). This latter way of thinking has been elicited in a variety of studies involving secondary school science students in various countries (Johnson, 2000; Nieswandt, 2001; Rahayu & Tytler, 1999). Many students in these investigations did not seem to have a mental model that would allow them to explain how substances may change their identity. Thus, in trying to account for observed changes in matter, these types of learners often invoke processes that involve displacement of entities from one location to another, or the mixing or separation of existing components (Andersson, 1986).

Analysis of students' ideas about the properties of materials suggests that many learners may see some properties (e.g. color, taste, smell) as separable from the actual substances (Sanmartí, Izquierdo, & Watson, 1995; Scheffel, Brockmeier, & Parchmann, 2009). They may think of such properties as quasi-material entities that may be added, removed, or become exposed as a result of a process without change in a substance's identity. This tendency to substantialize some properties of matter (substantialization) has been described by various authors (Reiner, Slotta, & Chi, 2000; Taber & García-Franco, 2010). This way of thinking shares similarities with a dominant way of knowing in pre-modern chemistry referred to as principlism (Chang, 2011). In this framework, properties of matter were explained by the presence (or absence) of 'principles' that conferred substances the properties observed experimentally (if substance A had the important characteristic C, then it was assumed that A contained the principle P, which was responsible for C; Langley, Simon, Brandshaw, & Zytlow, 1987). For example, the

caloric principle was related to temperature, while the phlogiston principle was linked to a substance's combustibility. The transformation of substances was many times explained by the application (or withdrawal) of such principles, without reference to changes in chemical identity.

Students' 'principlist' ideas about the properties of materials can be expected to affect their thinking about chemical identity. For example, these views are likely to hinder their ability to differentiate between single substances and mixtures of substances, particularly when dealing with homogeneous materials (De Vos & Verdonk, 1987; Johnson, 2000; Wisner & Smith, 2008). Learners at this stage may think of a homogeneous entity as a single substance under some circumstances, but as a mixture of several components when trying to explain changes in perceivable properties. Students who think this way are also likely to assume that such perceivable properties are the result of the weighted average of the properties of individual components (additivity), rather than emerging from their dynamic interactions (Taber & García-Franco, 2010; Talanquer, 2008). In consequence, they may be misguided during identification or differentiation tasks by the presence of properties that they attribute to particular components (Andersson, 1986; Talanquer, 2013). With proper interventions, students can learn to recognize that single substances exhibit behaviors that differ from those of homogeneously mixed materials (e.g. constant versus varying melting temperatures; Johnson, 2000), and that new properties may emerge from interactions among components (Solominodou & Stavridou, 2000).

Chemical identity thinking in the traditional chemistry classroom

During their secondary school years, many students around the world are introduced to the particulate model of matter in their chemistry courses. The model is commonly used to explain the physical properties of generic forms of matter represented as collections of de-identified particles. Research on student learning in this area, although vast, provides little insight into the evolution of students' ideas about chemical identity. Nevertheless, at this stage most learners also learn about the existence of chemical elements and compounds, and are introduced to the symbols [e.g. $\text{NaHCO}_3(\text{s})$, $\text{CH}_3\text{COO}_2(\text{aq})$, and $\text{Cl}_2(\text{g})$] and icons (e.g. small circles in boxes as two-dimensional visualizations of molecule arrangements in different phases) used to represent their composition and structure at the submicroscopic level (atomic-molecular model of matter). Typically, the introduction of these topics involves a major shift in educational focus, from having students analyze real materials to having them interpret chemical representations, and from focusing the attention on measurable properties as differentiating characteristics to learning to rely on explicit and implicit cues conveyed by symbolic and iconic representations.

Most existing research on students' ideas about the atomic-molecular model of matter related to issues of chemical identity has focused on the analysis of the ability of students to identify or differentiate among major types of matter such as: elements, compounds, and mixtures (Briggs & Holding, 1986; Kind, 2004; Sanger, 2000; Stains & Talanquer, 2007); molecular (covalent) and ionic compounds (Taber, 2002); polar and non-polar substances (Furió, Calatayud, Bárcenas, & Padilla, 2000); or acids and bases

(Furió-Más, Calatayud, & Bárcenas, 2007; Ross & Munby, 1991). Despite the existence of different topic-specific challenges in the analysis of these various types of substances, research findings elicit common trends in student reasoning when facing identification or classification tasks using chemical representations. In particular, many students tend to reduce the complexity of the tasks by using a single cue or attribute to differentiate among represented substances. Most salient cues to novice learners tend to be explicit attributes (e.g. differences in the number of atoms present in chemical formulas) rather than implicit features (e.g. type of chemical bonding). The selected cues are more likely to be compositional than structural in nature, and their selection is often guided by strong mental associations between certain representational features and specific properties or types of materials. For example, many students associate the words element-atom and compound-molecule, and thus they tend to think of all chemical elements as atomic and of all chemical compounds as molecular (Stains & Talanquer, 2007; Taber, 2002). Other students have built strong associations between the presence of an H (or OH) symbol and acidic (or basic) behaviors (Furió-Más et al., 2007). Additionally, many learners fail to differentiate between some concepts, such as compound and homogeneous mixtures (Sanger, 2000), or bond polarity and molecular polarity (Furió, Calatayud, Bárcenas, & Padilla, 2000), which leads them to make inaccurate and inconsistent categorization decisions.

The difficulties students encounter in selecting proper and productive cues for the identification and differentiation of chemical substances have been elicited at different educational levels, and seem to persist with training in the discipline. Challenges in

differentiating between elements and compounds (Kind, 2004; Stains & Talanquer, 2007) or between substances with different acid–base properties (Cartrette & Mayo, 2011; McClary & Talanquer, 2011) have been reported in studies involving secondary school, undergraduate, and graduate students in chemistry. Research findings indicate that the critical attributes used by many students to make categorization decisions are not necessarily stable, and may change depending on the types of substances under analysis or the nature of the chemical representations. Learners struggle to discriminate relevant from irrelevant features, and their reasoning is highly influenced by the content being discussed in the classroom. For example, organic chemistry students have been found to rely on more explicit features, such as atom connectivity or the presence of certain functional groups, when classifying represented compounds, but these same students increase their reliance on implicit features such as stereochemistry as such topics become relevant in the curriculum (Domin, Al-Masum, & Mensah, 2008). Students' reasoning about chemical substances at the submicroscopic level is highly influenced by the same types of assumptions that learners make about properties and behaviors at the macroscopic level (Talanquer, 2006). For many students, the different types of atoms that make up a substance are ultimate carriers of the properties that are observed (elementalism). In this view, the atoms-elements become the 'principles' responsible for observed behaviors. Students tend thus to think of substances as mixtures of atoms-elements with characteristic properties (compositionism) that get added in a simple fashion (additivity) to generate the observed macroscopic features (Taber & García-Franco, 2010; Talanquer, 2008).

Research on teaching the concepts of substance and chemical identity

Researchers have also investigated instructional practices that influence student learning about the concepts of substance and chemical identity. One study (Vogelezang, van Berkel, & Verdonk, 2015) used the theory of van Hiele levels to model a curriculum for the concept of substance. Van Hiele levels were originally developed for mathematics education (Van Hiele, 1957), and propose a series of discontinuous levels within mathematics learning that are characterized by changes in language. In order to reach the highest van Hiele level (and thus the highest level of understanding) students must pass through all lower levels (Van Hiele, 1980; Wirszup, 1976). As a result of their study, Vogelezang et al. (2015) were able to characterize van Hiele levels for the progression of student understanding of the concepts of substance, element, and composition. As the study progressed, students moved from relying on a classification scheme based on previous observations to developing their own theoretical constructs of substance, element, and composition, as they worked to understand the results of different reactions they observed as part of their chemistry curriculum.

Other researchers (Canac & Kermen, 2016) focused on the role of language in building student understanding of substances. Canac and Kermen argue that chemistry is a language, and like all languages, involves interpretation based on context (e.g. “C” could represent a carbon atom or the chemical species). Canac and Kermen investigated the meanings students associated with the names of substances and how students used the names for classification tasks. This study revealed that students rarely used the names of substances to distinguish pure substances from mixtures, had difficulty transitioning

between micro and macro levels of understanding based on the provided name or representation of the substance, and did not consistently maintain an understanding of “molecule” across contexts. Canac and Kermen interpreted the results of their investigation as an indication that students have trouble overall with the language of chemistry, and the lack of emphasis on chemical language and its meanings leads to misinterpretations or missed opportunities when students encounter these chemical representations.

Discussion and Implications

The core results of the analysis from the literature review are summarized in Figure 2-1. This figure intends to represent what has been identified as major cognitive attractors for how students conceptualize materials and think about the factors that affect their identity. The figure seeks to highlight likely overlapping assumptions about chemical identity, some of which become less or more dominant as learners progress in their studies. These findings suggest that students’ ideas about chemical identity evolve with training in the discipline, but developing normative understandings may require considerable scaffolding. Specific suggestions in this regard are introduced and discussed below.

While Figure 2-1 represents a map that summarizes the analysis of the landscape of conceptual sophistication in thinking about chemical identity, it is important to point out that there are limits on interpreting this representation. The map does not imply, for example, that students’ reasoning progresses in a linear fashion from the less to the more

sophisticated assumptions highlighted in the figure, nor that progression occurs at the same pace along each of the three threads. It is also not contended that individual assumptions (e.g. historicity, functional usage) that are represented as clustered around a major pattern of reasoning (e.g. objectivization) do not influence student thinking as students' ideas about materials become more sophisticated. In fact, existing evidence suggests that historicity and surface similarity play a central role in how many individuals who have principlist or compositionist views of substances make judgments about conservation of chemical identity during a process. Similarly, students may hold principlist assumptions about some properties of materials, such as color, when expressing interactionist assumptions about other properties, such as melting point.

A detailed description of a hypothetical progression of students' ideas about chemical identity is difficult to build for a variety of reasons. First, learners do not seem to have a monolithic view about the nature, composition, and properties of the various types of materials they encounter in their daily lives. Thus, ideas about different classes of substances may evolve in different manners depending on prior knowledge and personal experiences with particular types of matter. Second, existing research on students' ideas related to chemical identity is somewhat spotty. Studies involving novice learners are more abundant than those focused on students enrolled in more advanced chemistry courses. Finally, dominant chemistry curricula at different educational levels are not designed to foster a gradual and meaningful development of the concept of chemical identity. The study of kinds of materials frequently undergoes dramatic shifts in framework with the introduction of the particulate model of matter, when the attention

moves from differentiating matter types based on comparison of measurable properties to first explaining generic behaviors (e.g. phase changes, compressibility, diffusion) using identity-less particles, and then making distinctions between substances based on symbolic features of their representations. These shifts often occur before learners have a chance to develop a solid understanding of ways of thinking about chemical substances within each framework.

Two possible ways of integrating concepts of substance and chemical identity into the chemistry curriculum were outlined above (Canac & Kermen, 2016; Vogelezang et al., 2015). Although significantly different in execution, these approaches both endorse instructors deliberately fostering students' conceptions of substance. As students construct these conceptions of substance, they will simultaneously develop ways to classify and differentiate substances, thus building their understanding of chemical identity. By presenting students with different substances, their interactions, and their representations, students will progress in their understanding of what cues are appropriate for classifying and differentiating substances.

CHAPTER 3

DEVELOPMENT OF THE CHEMICAL SUBSTANCE IDENTIFICATION (CSI) SURVEY

Introduction

As evidenced in the literature review, existing understanding of student thinking for some aspects of chemical identity is more robust than for others. The main contribution of this chapter is to present the rigorous development of an instrument that is informed by the hypothetical learning progression for chemical identity (CI) and captures students' ideas about characterizing and differentiating matter across a wide range of educational levels. This instrument is called the Chemical Substance Identification (CSI) Survey, and was developed over the course of two years. The CSI Survey is qualitative, i.e., it is intended to be used for collecting data that can be analyzed using qualitative research methods, and uses open-ended questions to elicit CI thinking in response to various contexts. The design specifications of the instrument included that it should be useful both in research for understanding and characterizing students' CI thinking and in the classroom practices of teachers that use formative assessment as a resource for making instructional decisions; thus, the

CSI Survey has also been designed so that it can be used by secondary and tertiary instructors of chemistry to assess their students' CI thinking.

The majority of the content in this chapter has already been published (Ngai & Sevian, 2016). This chapter contains additional information that was not included in the article due to space limitations of the journal. Some items that were placed in the supporting information in the article are included in this chapter, along with explanations as to how these were related to the process of developing the CSI Survey. In particular, information in this chapter not included in the published article includes additional details on how the survey questions were developed, a table of common terminology related to rigor in qualitative research, and examples of concepts covered in a typical chemistry curriculum that are related to chemical identity.

Guiding frameworks

Chemical Thinking

The Chemical Thinking framework informed the development of this survey. Authentic problems in chemistry involve multiple disciplinary crosscutting concepts, and in practice, CI thinking and structure-property relationship (SPR) thinking are often intertwined (Chemical identity: What is this substance? Structure-property relationships: What properties does the substance have?).

A main difference between them is found in the activity that drives the thinking. CI thinking is invoked in the characterization of substances, where unique features are selected in order to provide information about composition and structure. SPR

thinking is relevant for the explanation or prediction of properties of a substance, and relies on models for making predictions. SPR thinking is often used at the service of CI thinking when it is necessary to predict and explain the properties of substances for practical purpose. For example, in separation and purification, the unique properties of a substance must be predicted in order to use these properties to isolate the target substance from other substances in the mixture. Because authentic problems in chemistry involve several types of thinking, it was expected that the CSI Survey would elicit more than just CI thinking. Since the research objective of the CSI Survey is to capture student thinking that can be analyzed for CI thinking, a major concern during the development phases was how to maximize the CI thinking elicited by the questions in this survey.

While there are other approaches to defining central ideas in chemistry (Atkins, 2010; Gillespie, 1997; Holme, Luxford, & Murphy, 2015; Holme & Murphy, 2012), the Chemical Thinking framework offers a way of framing chemistry that expresses the authentic and practical nature of the discipline as both a science aimed at building knowledge and a technoscience aimed at utilizing chemistry to improve the human condition (Chamizo, 2013). Chemical scientists use chemical knowledge to synthesize, analyze, and transform matter for practical purpose. Regardless of whether students are prepared from a chemical thinking or other perspective, to reason with chemical knowledge in their daily lives or their careers, CI thinking is essential. Both authentic problems and traditional exercises can challenge students to use CI thinking.

Although chemical identity is not explicitly addressed in a traditional chemistry curriculum, there are many concepts common to most (if not all) chemistry curricula to which the relation of chemical identity can be made apparent. Table 3-1 outlines the relevance of chemical identity to some of these general chemistry concepts. This table is not exhaustive of the links that can be made between a traditional chemistry curriculum and chemical identity, but provides examples of how instructors and researchers can relate the two.

Table 3-1: Examples of concepts in a typical chemistry curriculum where chemical identity is relevant

Typical chemistry concept	Relevance to chemical identity
Acid-base reactions	When considering reactions, students must be able to classify substances as acids or bases in order to determine types of reactions and whether or not they will occur.
Intermolecular forces	To determine the types of intermolecular forces that might exist between substances on a molecular level, students must understand the chemical identity of a substance and be able to think in general terms about how the composition and structure (which are related to chemical identity) lead to the types of interactions that may exist between molecules.
Mixtures vs. pure substances	Most of the matter encountered in daily life is part of a mixture, and students in chemistry must first understand the differences between mixtures and pure substances in order to properly assign chemical identity. Mixtures are made of multiple substances with unique chemical identities, which can be used to separate and identify the components.
Nomenclature	In chemistry, nomenclature is used to reveal information about the identity of a substance. In order to properly assign nomenclature, students must first understand how to classify substances. For example, a substance must be first identified as ionic or molecular before it can be named.
Solubility	When asking questions of solubility, students need to classify substances (e.g. ionic vs. molecular) in order to determine whether a substance will dissolve in another substance, and to what extent.
Redox reactions	Chemical identity is involved when identifying oxidizing agents and reducing agents in order to decide what kinds of reactions might be possible with particular reagents.

Ensuring Quality during the Design of a Qualitative Instrument

A variety of researchers (Creswell & Miller, 2000; Lincoln & Guba, 1985; Morse, Barrett, & Mayan, 2002) have sought to establish criteria that can be consistently applied to qualitative work to ensure rigor. Some researchers have adapted criteria from quantitative work for use in qualitative studies (e.g. reliability and validity), while others have utilized criteria (e.g. credibility, transferability, dependability, and confirmability) that were developed specifically to evaluate qualitative work. These criteria have been interpreted and implemented in many ways, and are typically applied during data analysis. Table 3-2 outlines most of the accepted measures, and methods of achieving them, that have been used in qualitative research to establish quality of an instrument and the data it produces.

When possible, these established approaches for ensuring rigor in the research process informed the development of the CSI Survey. One of the most crucial influences on the development process was an argument made by many researchers, and articulated by Morse et al. (2002) that, “qualitative research is iterative rather than linear, so that a good qualitative researcher moves back and forth between design and implementation to ensure congruence among question formulation, literature, recruitment, data collection strategies, and analysis” (p. 17).

Where aspects of established criteria for rigor were incorporated into the development process, they are noted in the following development section. In some instances, these criteria were modified for use within the design of a qualitative instrument as opposed to the analysis of qualitative data. At other points during the

Table 3-2: Common terminology for establishing quality in qualitative research

Term	Methods of establishing criteria
Reliability – does the instrument measure the desired construct or produce the same results consistently?	<ul style="list-style-type: none"> • Test and re-test with same participants (Arjoon, Xu, & Lewis, 2013) • Verification strategies, including: <ul style="list-style-type: none"> ◦ Investigator responsiveness, methodological coherence, theoretical sampling, sampling adequacy, active analytic stance, saturation (Morse et al., 2002)
Validity – how accurately does the researcher’s account match the realities experienced by the participants? Does the instrument measure what is intended?	<ul style="list-style-type: none"> • Triangulation (Creswell & Miller, 2000) • Member checks (Creswell & Miller, 2000; Lincoln & Guba, 1985) • Disconfirming evidence (Creswell & Miller, 2000) • Researcher reflexivity (Creswell & Miller, 2000) • Prolonged engagement in the field (Creswell & Miller, 2000) • Collaboration (Creswell & Miller, 2000) • Audit trail (Creswell & Miller, 2000) • Thick description (Creswell & Miller, 2000; Lincoln & Guba, 1985) • Peer debriefing (Creswell & Miller, 2000) • Evaluation of instrument by expert panel (Adams & Wieman, 2011; Arjoon et al., 2013) • Analysis of participant responses (Arjoon et al., 2013; Shenton, 2004) • Participant interviews regarding their responses to probe their answers and determine their interpretations of the questions (Adams & Wieman, 2011; Arjoon et al., 2013; Shenton, 2004) • Pilot testing using participants with different levels of targeted knowledge (Creswell & Miller, 2000; Shenton, 2004) • Verification strategies (Morse et al., 2002) (see above) • Selection of a representative sample of population for pilot testing (Adams & Wieman, 2011) • Scrutiny of research from outside researchers (Creswell & Miller, 2000)
Credibility – can internal validity be established? Are the researcher’s recordings and knowledge claims about the multiple realities credible or accurate to original participants?	<ul style="list-style-type: none"> • Using well-established research methods (Shenton, 2004) • Familiarity with culture of targeted population or prolonged engagement (Lincoln & Guba, 1985; Shenton, 2004) • Member checks (Lincoln & Guba, 1985; Shenton, 2004) • Triangulation through different data collection methods (Lincoln & Guba, 1985; Shenton, 2004) • Random sampling to eliminate bias (Shenton, 2004) • Peer scrutiny of research (Lincoln & Guba, 1985; Shenton, 2004) • Negative case analysis (Lincoln & Guba, 1985)
Transferability – are the findings transferable to other contexts?	<ul style="list-style-type: none"> • Thick description of context (Lincoln & Guba, 1985; Shenton, 2004)
Dependability – what is the quality of this research process?	<ul style="list-style-type: none"> • Audit trail (Lincoln & Guba, 1985; Shenton, 2004)
Confirmability – what is the quality of the product of this research process? Are the findings objective?	<ul style="list-style-type: none"> • Audit trail (Lincoln & Guba, 1985; Shenton, 2004) • Outline of researcher’s own beliefs and assumptions (Lincoln & Guba, 1985; Shenton, 2004) • Acknowledge limitations in study and discuss their potential impact (Lincoln & Guba, 1985; Shenton, 2004)

development phases, there were no set criteria for evaluating rigor; thus, the steps taken to establish quality and subsequent modifications to the instrument have been outlined so that readers may evaluate the rigor of this process for themselves and also have sufficient information to replicate this process in their own work if they wish. The process of collecting evidence to establish the quality of the instrument and to influence instrumental design decisions resulted in a more constructive approach for rigor than an evaluative one, as recommended by Morse and collaborators (Morse et al., 2002). These steps are further elaborated in the development section of the paper.

Stakeholders

A primary constraint on the development process was that the product should be useful both as a research instrument to investigate learners' CI thinking and as a classroom formative assessment tool for teachers to use in informing instructional decisions. Design-based research (Cobb, Confrey, Lehrer, & Schauble, 2003; Sandoval & Bell, 2004) approaches also combine both basic and applied research positions in cyclical development of educational products, which has been illustrated previously as well (Szteinberg et al., 2014). Therefore, before the design of the instrument itself began, the stakeholders relevant for this instrument were determined. Involvement of stakeholders in the research process ensures that the vision of the benefits held by the researchers is actually realized in the field, which can be achieved by including those who are directly and indirectly linked to the research product during the research process (Penuel, Confrey, Maloney, & Rupp, 2014). As

shown in Figure 3-1, four groups of stakeholders were identified: students, teachers, educational researchers, and disciplinary experts.

Figure 3-1. Stakeholders input-output model

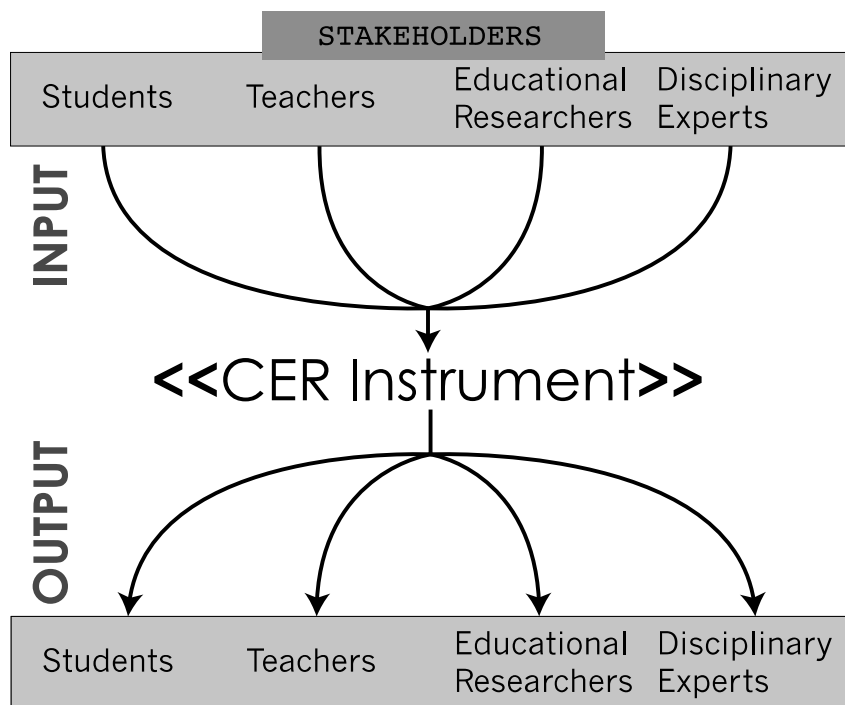


Figure 3-1. Stakeholders input-output model, illustrating how the chemistry education research (CER) instrument results from the input of stakeholders and also is intended to advance the goals of the same stakeholders.

In this approach, the potential contributions and expected gains of each stakeholder inform the development process to create an instrument that delivers benefits to its intended recipients. Each stakeholder group contributes expertise and knowledge, represented by the input portion of the figure. Students reveal their challenges learning chemistry, and teachers offer insight on the implementation of educational resources such as the instrument under design. Educational researchers

provide the theories of learning used to guide the instrument design, and disciplinary experts identify the skills and knowledge necessary to become more expert in chemistry. Design decisions are influenced by consideration of what these stakeholders offer, and the product holds promise to deliver specified outputs or gains to each stakeholder. These outputs serve as the driving force for the instrument's development. For students, the instrument provides the opportunity to express chemical thinking. For teachers, it can uncover students' ideas, which enables teachers to make instructional decisions based on data. The instrument can be used to effect change in chemistry education through its use by education researchers to inform curriculum design and teaching resources. Finally, disciplinary expertise is advanced by clarifying how CI thinking is enacted by experts. Data collected using this instrument, along with other measures, will ultimately serve to characterize CI thinking and potentially refine elements of the CI learning progression. The combined outputs have the potential to advance chemistry education by preparing students who are better trained to use chemistry knowledge for practical purpose.

Development of the Chemical Substance Identification Survey

Ultimately, the purpose of the CSI Survey is to capture how students think about and utilize CI thinking in chemistry contexts so that it might be studied and better understood. Seminal texts on collecting and analyzing qualitative data (Charmaz, 2014; Patton, 1990; Silverman, 1994) informed the development of the CSI Survey. Content analysis will be used to analyze the data collected with the CSI Survey. Determining the type of analysis to be performed on the data collected with the CSI Survey allowed for methodological coherence to be established by matching the type

of data needed to explore and refine understanding of students' chemical identity thinking with the methods used to produce and analyze the data (Morse et al., 2002). Since the succeeding analytical work uses content analysis (see Chapter 3), a qualitative instrument that utilizes open-ended questions was developed. For reference, Boxes 3-6 contain an abbreviated view of the finalized questions for the CSI Survey, organized by set (A-D). For questions asking for a dichotomous answer, a follow-up question or statement was included in the complete version that asked students to explain or justify their responses. The complete sets as seen by students (questions, follow-up questions, and pictures if included) are in the Appendix.

In the Boxes, following each question in the CSI Survey, the targeted CI thinking is outlined, with anticipated reasoning pattern(s) in bold and associated assumptions, where expected, in italics (see Figure 2-1). The statements that follow are examples of predicted manifestations of the reasoning patterns and/or assumptions in student responses. Predicting how students might respond based on existing knowledge of chemical identity was useful because it helped to determine whether the questions had the potential to elicit CI thinking. In all questions, other CI thinking could be used (for example, more advanced thinking tended to occur when using this survey with experts and some upper level students). Only a selection of the different types of CI thinking has been outlined in the boxes, for the sake of brevity. The Appendix contains examples from the collected pilot data that were included in the article published in the *Journal of Chemical Education* (Ngai & Sevian, 2016); these are presented in a format intended to serve as a resource for teachers who may wish to use the CSI Survey.

Box 3. CSI question set A

A1. Your friend's favorite earring is made of a light gray metal. How would you determine if this is silver?

- **Objectivization, Principlism, Compositionism, Interactionism:** Students may utilize explicit or implicit properties when trying to identify a metal. They also might consider the composition and/or molecular structure of the substance for identification purposes.

A2. Your friend's mother tells you this earring is made of pure silver. Your friend accidentally lost her earring and you found it a few months later. You noticed that it was no longer shiny and that it was now a dark gray/black color. Is the earring still made out of silver, or is it a different substance?

- **Compositionism - elementalism:** Some students might focus on the color change and use that to infer that a chemical reaction (and thus a change in chemical composition) has occurred, changing the identity of the metal from silver to something else.

A3. You decide to create a poster that has the title: "What is chlorophyll?" What would you put on this poster, and how would it help you explain what chlorophyll is to the other students?

- **Objectivization - functional usage:** Students might define chlorophyll based on its function or purpose in plants.

A4. Chlorophyll can be isolated from the leaves of a tree growing in the forest and from algae growing in a pond. Is the chlorophyll from the leaves of the tree the same or different as the chlorophyll from the algae in the pond?

- **Objectivization - historicality:** Some students may reason that the source of a substance has an impact on its chemical identity, and may think that these chlorophylls are different.

Box 4. CSI question set B

B1. You have a cup of an unidentified liquid in front of you. How would you determine whether or not this is water? (photo of cup with clear liquid is provided)

- **Objectivization, Principlism, Compositionism, Interactionism:** When trying to identify a liquid, students may utilize explicit or implicit properties. Other students might suggest determining the composition and/or molecular structure of the substance in order to identify it.

B2. You heat a pot of water over a stove and it begins to boil. What is in the bubbles that are rising to the surface?

- **Objectivization - surface similarity:** Since the gaseous substance in the bubbles has a different appearance than the liquid substance, some students might reason this means the chemical identity of the substances is different. Others may compare the substance in the bubbles to other, more familiar gases.

B3. In its natural state, oxygen is a gas. If you had an unlabeled cylinder filled with gas, how would you determine if it is oxygen?

- **Objectivization, Principlism, Compositionism, Interactionism -** When trying to identify a gas, students might utilize implicit over explicit properties. More advanced students might suggest determining the composition and/or molecular structure of the substance in order to identify it.

B4. Carbon dioxide also occurs naturally as a gas. How would you tell the difference between carbon dioxide and oxygen? Please explain your response.

- **Principlism - additivity:** It is likely that some students will reason that the addition of carbon to O₂ adds new properties to CO₂ that can be used to differentiate the gases.

Box 5. CSI question set C

C1. You meet someone who has never heard of caffeine. What would you say or do so that this person could recognize caffeine in the future?

- **Objectivization** - *functional usage*: Some students might only define caffeine by its stimulating effect on humans.

C2. Caffeine is present in many plant seedlings and acts as a pesticide to discourage insects from eating the unprotected plants. Is the caffeine found in seedlings the same as the caffeine found in energy drinks, such as Red Bull, or is the caffeine different?

- **Objectivization** - *historicality*: Students might reason that the source or process of synthesis impacts the chemical identity, and thus reason that caffeine in seedlings is chemically different than the caffeine in Red Bull.

C3. What could the object below be made out of? How would you know this? (photo of a roughly cut chunk of metal shown that is metallic gray in appearance)

- **Objectivization, Principlism, Compositionism**: Since the object is not identified, students may tend to rely on the appearance of the substance in the photo and might use these features to infer properties for classification.

C4. Could the object below be made of the same substance as the object in the picture you saw previously? (photo of an unlabeled metal can shown)

- **Objectivization, Principlism, Compositionism**: Since this is a more familiar object, students might focus on salient features that they can use to classify the object, and then use explicit or implicit properties to compare the two objects.

Box 6. CSI question set D

D1. There are white, crystalline granules on the table in front of you. How would you be able to determine if this is sucrose (also known as table sugar)?

- **Objectivization** - *surface similarity*: Students might focus on the described appearance of the granules in order to determine chemical identity.

D2. Let's assume the white granules are sucrose (table sugar). You take the sucrose and heat it over a flame until it turns from a solid into a liquid. The liquid now has a brown, caramel color. Is the liquid still sucrose, or is it a different substance?

- **Principlism** - *substantialization*: Since the granules are no longer white, students might think that the granules have lost the component that gives them the white color but that overall the chemical identity is maintained.

D3. You have a cup of an unidentified liquid in front of you. How would you determine whether or not this is ethanol? (photo of cup with clear liquid is provided)

- **Objectivization, Principlism, Compositionism, Interactionism**: When identifying a liquid, students might use explicit or implicit properties. Some might suggest determining the composition and/or molecular structure of the substance in order to identify it.

D4. You heat a pot of ethanol and it begins to boil. What is in the bubbles that are rising to the surface?

- **Interactionism**: Some students might reason that the heat provides energy to the molecules, and that the bubbles are ethanol in the gaseous phase. They might use this to infer that the chemical identity is maintained in the bubbles.

Through four phases, stakeholders contributed to the development of this instrument. These phases are outlined below, with particular emphasis on ways in which stakeholders influenced decisions made during the process.

Phase 1: Targeting Chemical Identity Thinking

The first step in the development process was to design questions that could elicit CI thinking. A variety of substances were explored via pilot testing and interviewing with students, to identify potential topics for questions concerning the identification and differentiation of substances. The questions were framed in contexts designed to target CI ideas found in existing literature, as highlighted in the hypothetical learning progression (see Figure 2-1).

Some questions were built from empirical studies that formed the basis for the hypothetical learning progression, so that analysis of data from later implementation of the instrument could be compared to prior results. For example, many studies have explored how students conceptualize phase changes in water (Bar & Travis, 1991; Bodner, 1991; R. Osborne & Cosgrove, 1983) and prototyping of all liquids to water (Krnel, Watson, & Glažar, 1998). Thus, a range of substances was selected that exist as solids, liquids, and gases under ordinary conditions. Prior research also points to familiarity as a powerful heuristic (Gilovich, Griffin, & Kahneman, 2002; Goldstein & Gigerenzer, 2002), and three assumptions (functional usage, surface similarity, and historicity) are closely linked to familiarity. Therefore, some substances were included that would be more familiar (water, oxygen) and others that would be less so (ethanol, chlorophyll). In order to target CI thinking that involves differentiation (the second question of CI), processes in which substances may or may not change their CI (i.e. separations, phase changes, combustion) were incorporated in the contexts for the questions.

Using the hypothetical learning progression to guide question development ensured that hypothesized CI thinking could be elicited, but the questions were left open-ended to allow for other CI thinking to emerge. To determine whether the initial questions elicited CI thinking, they were tested in an interview format with a small population of students representative of the target population (grade 8 through final year of undergraduate training in chemistry) to see if students responded with the expected CI ideas. The students for all pilot testing were chosen based on availability during or after class time from schools local to University of Massachusetts Boston. The pilot testing began with interviews (N=15) as this is a method frequently used for assessing whether participants interpret the questions in the way the researchers intended, evaluating researchers' understanding of participants' responses, and determining if the questions elicit the desired responses from participants (Arjoon et al., 2013; Lederman, Abd-El-Khalick, Bell, & Schwartz, 2002). Five students enrolled in university general chemistry were then given the same questions and asked to write their responses, and these written responses were followed up with interviews to probe student thinking in more depth. The author conducted all interviews and survey implementation.

Data analysis during this phase helped establish validity of the questions by evaluating whether the questions prompted participants to use CI thinking. The data collected from Phase 1 testing were first coded by the author for the presence of CI thinking as defined by the hypothetical learning progression. The original student response and the author's coding and interpretations were then presented to three other researchers and examined for agreement and disagreement. For example, the

student response below was coded by the first researcher to hold ideas about source because the student focused on where the chlorophyll came from (rose bush vs. oak tree) to make a claim about the chemical identities of the chlorophyll. The author also assigned a code about function, since the student made the argument that the chlorophylls have different jobs, which makes them different from each other. The other researchers also noted these CI ideas in their review of the data, and the following discussion led to a consideration of the types of physical and chemical properties that students with different extents of training in chemistry may use in CI thinking.

Question: Chlorophyll is a compound used in plants to convert sunlight into energy. Scientists extracted chlorophyll from the leaves of a rose bush and from the leaves of an oak tree. Is the chlorophyll from the rose bush the same as the chlorophyll from the oak tree?

Student: They are, it also depends, cause they're not the same type of trees, just like how our DNA is different from one another, so the chlorophyll may have the same job to convert the sunlight into energy but the structure might be different and it's just how there are green leaves there are yellow leaves so the amount of chlorophyll and the type of the chlorophyll and the job it does is totally different from one another so they're different.

Through this process of group coding student responses from Phase 1, it was found that students pay attention to easily observable characteristics such as shape, function, and color, and often generalize when referring to CI ideas. The group

coding process served as a member check by determining whether multiple researchers would independently identify CI thinking in the responses to the CSI Survey, and was one step for validating that the CSI Survey elicits the constructs it was designed to uncover.

The coding also uncovered student thinking about structure-property relationships. Because SPR thinking is often used at the service of CI thinking, this was expected. Analysis of the student responses that exhibited this revealed that some of the questions themselves directed students to this thinking, such as the following example, in which the student reasoned about why sugar and wood are flammable:

Question: Both sugar and wood are flammable. Why can both of these substances be burned?

Student: Well I know wood can be burned...I mean I know sugar can be lit because you can caramelize sugar, and then as for wood I know you always use that for firewood, and um well I know it's a substance, an organic substance, so I guess when it reacts with oxygen then it would make CO₂ and water...it's probably not the same, but they have specific properties that allow them to be burned.

Since the primary intent of the CSI Survey was to obtain data on CI thinking for the research purposes of the CSI Survey, it was necessary to clarify why some questions elicited SPR rather than CI thinking. Comparison of the questions that elicited more SPR thinking to those that elicited more CI thinking revealed that questions that direct a participant toward considering why or how the properties enable

differentiation elicit SPR thinking, while questions that ask for the use of properties to differentiate elicit more CI thinking.

In order to focus the questions on CI thinking, the questions were restructured. As it was already established that CI consists of two core questions, the questions in this survey were revised so that, for each substance, there was a question that targeted the identification of that substance (core question 1) and the differentiation of that substance (core question 2). Designing paired questions that each focused on a core CI question for the same substance generated a new concern to test in later phases: whether the instrument would capture a variety of CI thinking by separating the two CI questions. It was also decided that in all cases the question corresponding to core question 2 should follow the question corresponding to core question 1 because in order to differentiate one substance from another, the former may first be identified. Conversely, if the question concerning differentiation were asked first, students might not outline their thinking about how to identify the substance in the first place. Phase 1 thus resulted in the design of paired questions that would be revised based on the extent to which they elicited CI or SPR thinking.

Phase 2: Expert Validation

The second phase of the instrument development used an expert panel to evaluate the instrument and its goals by seeking validation and feedback from experts in the field of chemistry and experts in chemistry education research. In this phase of peer scrutiny, experts were asked to respond to the version of the survey questions that emerged from Phase 1 and provide feedback about the survey through a

questionnaire. The expert input collected during Phase 2 was then used in various ways to evaluate the data that would be produced by this instrument.

Content Validation. As experts in chemistry and chemistry education outside of the Sevian research group, these individuals were uniquely qualified to provide insight into the development of this instrument. First, by answering the questions from their own points of view, these experts provided data that could be analyzed for CI thinking. As in Phase 1, the author and other researchers in the group read the expert responses and looked specifically for CI concepts, per the hypothetical learning progression. The CI thinking revealed in the expert responses was typically more advanced than the CI thinking demonstrated by participants in Phase 1, which was expected. For example, in the following excerpt, an expert's response to one of the questions includes multiple strategies for identifying the unknown white substance, and utilizes unique structure (through polarimetry) and the interactivity (burning, solubility) of the substance to identify it.

Question: How would you determine if the white powder is sucrose, also known as table sugar?

Expert: So, polarimetry is a good way to analyze sugars. May use it. It's fast...but you need the instrument. If I'm at home and feeling playful, maybe char a little sample and see how it burns. Table sugar crystals are very distinctive from other granules one may find at home, so I'd use visual inspection too. Throw a few crystals in water and see if they dissolve...

Although this is an example of a more advanced reasoning pattern, this expert also displays an appropriately used reliance on an assumption of appearance. Because advanced CI concepts were observed in the expert responses, it was inferred that the questions had the potential to elicit a variety of CI thinking, the primary goal of this instrument.

The feedback questionnaire asked the experts to characterize the types of chemistry knowledge they used to respond to the survey. They indicated a range from high school chemistry concepts to organic and physical chemistry. The variety of chemistry concepts they identified as relevant indicated that the questions did not limit students to using specific chemistry concepts or ideas, and that the questions should be approachable by students with different levels of chemistry training. The expert responses also demonstrated that chemistry-specific knowledge was used when responding to these questions.

Refinement of Survey Structure: Although in most cases, the questions provoked thoughtful and detailed responses from the experts, the experts had many suggestions on improving the question structure and wording. These comments were captured in a feedback questionnaire (see Appendix), which asked specifically about the difficulty level and wording of the questions. Experts noted that in order to obtain detailed responses from students, the questions would have to prompt for these details. Thus, the questions were revised so that there was an initial question and a follow-up question that asked participants to explain or justify an initial response. One expert remarked that some of the word choices were confusing and she proposed alternatives. To address this concern, the questions were deconstructed into parts

(substance utilized, context or setup of question, instruction or question posed). An example of the deconstructed questions at this stage in the development is shown below in Table 3-3. The parts of each question were compared and standardized so that the questions were clearer and more consistent in their format. This step was of particular importance in the design of the CSI Survey, as the different versions were intended to elicit a similar range of CI thinking, and standardization of the questions makes it more likely that this can be achieved.

Table 3-3. Example of deconstructed questions

Q?	Substance	Composition	Phase	Familiarity	Context	Stimuli	Targeted CI idea
1a	Water	Pure	Liquid	Yes	Real-world	How would you determine whether or not this is water?	Identification of a liquid
1b	Water Bubbles (vapor)	Pure	Gas	Yes	Real-world	What is in the bubbles that are rising to the surface?	Does a substance maintain its ID when going through a phase change?
2a	Oxygen	Pure	Gas	Yes	Chemistry	If you had an unlabeled cylinder filled with gas, how would you determine if it is oxygen?	Identification of a gas
2b	Carbon dioxide and Oxygen	Pure	Gas	Yes	Chemistry	How would you tell the difference between carbon dioxide and oxygen?	How do you tell the difference between two gases?

Another concern raised by an expert was the lack of instruction regarding what hypothetical tools were at the disposal of the participant. In response to this, the initial written directions preceding the survey were modified to inform participants that they “may use knowledge from your own experience, knowledge from the classroom, and guesses to answer these questions.” These instructions also stated that there were many acceptable answers, participants were not being graded, and their teachers would not see their responses. It was noted that prior to implementation of the survey, the researcher should explicitly indicate in oral instructions that students may hypothetically use any equipment or knowledge available to them in their answers, and that each participant’s individual thinking is valuable for this study.

Lastly, experts identified which questions they perceived would be more difficult for students. As student responses were examined, it was observed that the questions on which students had the least to say were the ones that experts predicted would be more challenging. Questions were classified into two groups: easier and more difficult. In order to encourage participants to provide lengthier written responses, it was important that they not be discouraged by a difficult question and fail to respond to the next one (Weinstein & Roediger, 2010). Thus, questions were paired based on perceived difficulty, so that in each set the easier question always preceded the more difficult one.

Phase 3: Pilot Testing with a Representative Population

Phase 3 focused on determining whether the improved survey was feasible to implement in a classroom, how the changes to the questions impacted participant

responses, and whether participants at all of the targeted educational levels would understand the questions.

General Evaluation of Revised Survey Questions. To obtain a general sense of how long it took students to complete this survey and whether the questions were clear, five students from a first-semester university general chemistry course were asked to complete the survey and were then interviewed about their responses. At this point in Phase 3, there were two versions of the survey, each containing 10 questions. Versions were randomly assigned to the participants. A brief analysis of the written responses and interviews of students indicated that the questions were clear and interpreted as intended, indicating that the questions were valid in the sense that participants and researchers understood them in the same manner. A range of CI thinking was observed when coded, and demonstrated that separating the questions into the two core questions of CI would capture a variety of CI thinking. For example, the following student response to the two core questions about oxygen produced unique CI thinking; in the first, reactivity (as the student understands it) is considered, and in the second question the student considers odor as a differentiating factor.

Question: In its natural state, oxygen is a gas. If you had an unlabeled cylinder filled with gas, how would you determine if it is oxygen?
Please explain your response.

Student: Add some hydrogen to it and see if water molecules will form, because H_2O is water and if there really is oxygen in the cylinder adding hydrogen will help you figure out for sure what's in there (in terms of if it's oxygen or not).

Question: Methane also occurs naturally as a gas. How would you tell the difference between methane and oxygen? Please explain your response.

Student: Methane, I think, has a stronger or different odor than oxygen.

On average, each participant took 30 minutes to respond to the survey, regardless of the version. This was deemed to be too much class time to allocate if the survey were to be valuable to instructors, so each version was split in half. This resulted in four versions of the survey, each containing four to six questions.

Classroom Implementation. To be able to collect data on a large scale using this instrument, it should be feasible to implement the survey during class time. Large-scale implementation strengthens the probability that the broadest range of participants is included in a study. Implementation during class time provides efficiency in data collection for the researcher, as well as efficiency for the instructor.

When interviewed, five teachers (2 middle school, 3 high school) indicated that the written survey should take students no longer than 15 minutes to complete. To test this, students in an 8th grade class (N=13) were randomly assigned one of the four versions of the survey. The researcher told students that they had 15 minutes to complete the questions. The time students took to complete the survey ranged from 5-25 minutes, at which point they were asked to hand in their responses regardless of whether they were complete. Although some students were stopped early, only one student out of thirteen left any questions blank (however, some student responses consisted only of “yes,” “no,” and “I don’t know”). Most students provided complete

answers to all of the questions, thus it was concluded that the students who were stopped at the end of the time limit were primarily providing further details.

The four versions of the survey were next implemented in a second-semester university general chemistry course (N=121). The entire process, including verbal instruction and collection of the surveys, took approximately 20 minutes. Similar to the 8th grade class, some students finished in 5 minutes, while other students took the entire allotted time. Since a majority of students completed the survey within 15 minutes, it was judged that the versions with fewer questions were more feasible to implement during class than the longer versions with more questions.

Establishment of Validity through Data Analysis. The pilot data collected from the general chemistry course were analyzed for CI thinking using NVivo, a qualitative analysis software package, to keep track of the codes and the author's memos regarding coding decisions and patterns observed in the data. In qualitative analysis, memos can serve as part of an audit trail that can be used by the researchers to maintain consistency during future analyses and for others to evaluate the coding process. The analysis consisted of coding for the reasoning patterns observed in each response and counting the instances of observed CI thinking, seen in Table 3-4. This analysis of student responses revealed that students utilized a variety of CI thinking in their responses across all versions of the CSI Survey, providing verification that the CSI Survey sets elicited the desired constructs. Although it is clear that ways of thinking coded as objectivization and principlism were more prevalent than compositionism and interactionism, this is not unexpected for students in a general chemistry course, and the distribution is expected to shift toward more advanced

thinking with further training in chemistry. Additionally, since there are coded instances of compositionism and interactionism within this pilot dataset and observed in expert responses collected during Phase 2, it can be expected that the four versions of the CSI Survey have the potential to elicit all four major reasoning patterns.

In many cases, students responded with thinking patterns that were considered to be related to CI, but that did not fit under the major reasoning patterns defined in the hypothesized learning progression. Based on this, it was inferred that the CSI Survey elicited a wide range of CI thinking, as intended, and also that the full implementation of the CSI Survey is likely to allow for CI thinking to be explored and characterized more deeply than the comprehensive literature review that led to the hypothesized learning progression. During analysis of these pilot data, it was observed that the content of students' answers made sense in relation to the questions asked, implying that participants were able to interpret the questions as designed by the researchers and were able to do so consistently.

Table 3-4. Counts of reasoning patterns coded in phase 3 general chemistry pilot data

<i>Set and Question</i>	<i>Objectivization</i>	<i>Principlism</i>	<i>Compositionism</i>	<i>Interactionism</i>	<i>other CI</i>
A1. Silver	13	7	0	3	2
A2. Oxidized silver	10	2	4	2	12
A3. Chlorophyll	23	0	2	0	2
A4. Chlorophyll source	22	2	2	0	4
B1. Water	12	18	0	0	1
B2. Water bubbles	3	0	8	1	19
B3. Oxygen	16	9	0	0	4
B4. Oxygen vs. methane	16	7	0	0	7
C1. Caffeine	26	0	2	1	0
C2. Caffeine source	22	0	2	2	0
C3. Metal chunk	20	3	1	0	6
C4. Chunk vs. can	26	1	0	0	3
D1. Sucrose	14	11	1	0	1
D2. Caramel	10	1	5	1	10
D3. Ethanol	9	13	0	0	5
D4. Ethanol bubbles	4	1	8	0	15

Total participants: N=121

^aPlease refer to the Appendix for a rubric that contains details about the different reasoning patterns and how to identify them in student responses.

The student responses were coded for the major reasoning patterns and assumptions in the hypothetical learning progression. For example, the use of appearance or another sense to identify or differentiate a substance was coded as objectivization. The following two student responses utilize sensory information in their CI thinking, and were counted as instances of objectivization. In response to the question concerning water (Set B, Q1) one student used both appearance and odor as indicators for chemical identity.

Student: I would not taste it because it might not be water but I will smell it and look at the color. Because water is colorless and odorless then I will know whether or not it is water.

Another student used sensory information in a similar manner, but in response to a different question on a different set (caramel question, Set D, Q2).

Student: Different substance. It has a different color, this is most likely a sign that it is not sucrose anymore.

When students considered the components of a substance or its composition in their response, it was coded as compositionism. In the following example from Set A (Q4), a student stated that the chlorophylls from the two sources are different, and reasoned that it is because they have different compositions.

Student: Different. Because there is probably a different charge, and composition depending on the pH of the water it's been exposed to, or the temperature variation it has been exposed to.

In response to the question about the unidentified chunk of metal, in Set C (Q3), a student was unwilling to make a claim about the identity of the metal and stated that he/she would need information about the composition in order to do so.

Student: I would need to know the chemical comp.

This response was also coded as an instance of compositionism. From this analysis, it was observed that different assumptions and ways of reasoning appeared to be elicited across questions in all sets.

Qualitative analysis of the data also showed that the follow-up questions, which were added during Phase 2, helped by enhancing the responses of students so that more justifications were provided in their answers. Although it was not possible to quantitatively determine how much more detailed the student responses were, the

follow-up questions did not detract from student answers, and were thus kept for the final version of the survey.

Phase 4: Teacher Validation

The final stage in the development of the survey sought the feedback of experienced science and chemistry teachers who could potentially be the end-users of this survey in their classrooms.

Evaluation of Implementation Plan. Five teachers (two 8th grade science teachers and three high school chemistry teachers) were initially provided electronic copies of the four versions of the survey, and asked to complete an online questionnaire before meeting for an open discussion with the researchers about implementing the CSI Survey in classrooms. The teachers were familiar with CI concepts and the purpose and design of the survey, and were asked for their input on how data collection using this survey could occur within a class period.

To ensure that students completed the surveys with detailed answers and within a 15-minute period, the teachers suggested that the survey be converted to a computer-based format. They reasoned that their students already complete many activities and standardized testing on the computer, so it could be expected that students would feel comfortable completing a survey on the computer and would potentially provide lengthier answers when not limited by handwriting each response. Recent studies indicate that paper-and-pencil tests that have been converted to a computerized format do not significantly impact student responses unless the test incorporates significant reading passages (e.g. must scroll through the text) (Wang, 2010). Since the CSI Survey was identical in wording and format to the paper-based version, it was

assumed that students' answers would not be impacted by its conversion to a computer-based format.

For the full implementation, GoogleDrive was used as the computer-based platform to collect data during classroom administration of the CSI Survey. The CSI Survey was built as a GoogleForm, which provided a similar format as a standard online survey. GoogleForms allowed for redirection based on question responses, and so the first question of the survey asked students to select the multiple choice option that contained their month of birth. The GoogleForm redirected students to a specific set of the CSI Survey based on their choice to this question. As students completed the CSI Survey, their responses were automatically compiled into a GoogleDrive spreadsheet. This automatic compilation allowed for the student responses to be used in interviews immediately after survey completion. A GoogleForm was created that replicated the CSI Survey, and a GoogleDrive add-in (Autocrat) was used to automatically populate the response fields of the replicated CSI Survey with the student's answers. The form with the student's responses in the field was then downloaded as a pdf and pulled up on an iPad to use during the interview with the student. This allowed the interviewer to go over the student's responses in real-time with the student during the interview.

Informed consent process

Consent was obtained from all students who participated in the development phases of the CSI Survey and its final implementation. This study obtained IRB approval from the University of Massachusetts Boston, and followed standard IRB procedures for obtaining consent from students. For students in 8th grade through 12th

grade, written parent consent was obtained unless the student was old enough to provide consent for himself/herself (18 years of age). For students at the university level, consent was obtained through written consent forms during the development phases and then through a virtual consent form that preceded the CSI Survey. For all data analysis during both the development phases and final implementation, student responses were de-identified and assigned a code number.

Implications

Development Process of a Qualitative Instrument

This chapter has outlined a rigorous procedure for the development of an instrument for collecting qualitative data using a constructive approach that incorporated measures to ensure quality in the process. Integral in this iterative development process was the involvement of stakeholders. The needs of the stakeholders drove instrument development, and the stakeholders contributed valuable expertise through many of the methods of the qualitative instrument development process. The input of the stakeholders influenced many design decisions, from determining the structure and format of the instrument to establishing whether the instrument elicited the types of data useful to stakeholders. A cyclical development process allowed for verification steps to be built in and for researchers to respond to the outcomes of these steps. Checking that the process included methodological coherence, an appropriate sample population, concurrent data collection and analysis, confirmation of ideas in the data, and recurring theory development are methods that were used to ensure a quality instrument was produced. A large body of research exists on the development of valid and reliable quantitative

instruments (Arjoon et al., 2013; Sanger, 2008) and informed the development of this instrument. This chapter contributes an example of a rigorous development process, based on this body of research, for a qualitative instrument in chemistry education research.

Concluding remarks

CI thinking is important both for scientifically literate citizens and for those who intend to become chemists. Because of this, it is essential to characterize how CI thinking progresses with training in chemistry. This chapter has outlined the rigorous process used to develop an instrument that can be used to collect data for characterizing students' CI thinking. The development process addressed the inputs and gains of relevant stakeholders, and the steps to incorporate stakeholders' expertise, concerns, and goals while also ensuring an instrument of high quality was developed that can serve as a model for other researchers developing qualitative instruments.

CHAPTER 4

RESULTS OF THE CSI SURVEY – THEMES IN CHEMICAL IDENTITY THINKING

Introduction

Motivation

Solving modern day societal challenges requires scientifically literate citizens who are able to apply scientific reasoning, models, and skills learned in the classroom. Producing scientifically literate citizens requires the transformation of instructional practices to match the needs of these future citizens. It is no longer enough to communicate the knowledge of science to students; they must engage in the practices of science while in the classroom.

The Chemical Thinking framework outlines crosscutting concepts that comprise the practices of chemists. Chemical identity is foundational to the other five disciplinary crosscutting concepts, and is essential for solving many societal challenges using chemistry. Since chemical identity thinking is important for the general population in addition to students training to become chemists, instruction that develops chemical identity thinking is important. In order to accomplish this, a

better understanding of chemical identity thinking and how it evolves with training in chemistry is needed.

Research questions

The following research questions are the focus of this chapter:

R1: In what ways do students think about and apply chemical identity?

R2: In what ways do the patterns of students' chemical identity thinking correspond to training in chemistry?

Characterization of chemical identity thinking requires evidence of how students solve problems involving chemical identity. The CSI Survey presents students with a variety of substances and asks questions that probe how they classify and differentiate substances. In order to explore the relationship between chemical identity thinking and training in chemistry, the CSI Survey was administered with students across a wide range of education levels.

Data collection

Implementation of the CSI Survey

The CSI Survey was implemented in classrooms at multiple public middle schools and high schools in the Boston area, as well as in courses at the University of Massachusetts Boston. The instrument was administered via computer interface in order to control the quality of the graphics shown, to capture data in a format that

allowed for immediate follow-up interviews, and to encourage students to provide lengthier responses. At the beginning of the survey students were asked to select the month of their birth. This randomly assigned them the set (A, B, C, or D) of questions. On average, students spent 10 minutes completing the survey; some students took as little as 5 minutes, while others took closer to 20 minutes. The CSI Survey was implemented during class time at the middle school and high school levels. Students completed the CSI Survey all at once or took turns throughout the class period depending on the schedule of the class for that day. Prior to starting the CSI Survey, the author read aloud the instructions that were provided to the students on the first page of the CSI Survey. She also stressed that the responses students provided would not be graded, their teacher would not see their answers, and that it was important to complete the CSI Survey individually as every student's thought process was valuable for the study. In most cases, students were observed taking time to thoughtfully complete the survey and asked the author questions when necessary. Such questions were typically concerned with the "correctness" of the answer (to which the author replied many answers existed), or with the range of experiences students were allowed to talk about (e.g. students asked if they could mention previous experiments or experiences from their daily lives, which the author encouraged they include in their responses).

At the middle and high school levels, students were randomly selected by the teacher to be interviewed (some teachers used cards, others dice, etc.) and these students received a \$5 Dunkin Donuts gift card for their participation in the interview. The interview took place immediately after students completed the CSI Survey, with

the author and student relocating to the hallway or another room to conduct the interview. Interviews involved going over the student's answers to the CSI Survey, with the author asking the student to explain what he or she was thinking when responding to the questions. The author also asked follow-up questions, which typically concerned the student's meaning of certain words such as "natural" or "processed" to ensure later interpretation of these words were not misconstrued by the author and other researchers during data analysis. The general interview protocol can be found in the Appendix. Interviews ranged from 5-15 minutes in length.

At the university level, students completed the CSI Survey during designated times outside of their classes. For the general chemistry and organic courses, this occurred in conjunction with their lab classes. Laptops were provided by the university and once students were finished with their lab work, they were given the opportunity to take the survey for extra credit towards their lab grade. The author issued the same verbal instructions as given to the middle and high school students and monitored students while they completed the survey. The physical chemistry students signed up for pre-determined times outside of class to take the survey while monitored by the author, as there was not a lab time when the CSI Survey could be administered.

After completion of the CSI Survey, the undergraduate students were asked if they would like to participate in an interview about their responses. The author arranged the interview times to take place no more than 3 days after completion of the CSI Survey, and in most cases the interviews were the same or following day.

Students received a \$10 gift card to the university's cafeteria as a token of appreciation for their time.

Table 4-1. Participant numbers

Class level	No. of schools	No. of participants	No. interviewed
8 th grade science class	3	78	9
Regular/Honors chemistry (10 th grade)	2	70	10
Advanced placement chemistry (11 th /12 th grade)	4	78	10
General chemistry (1 st -2 nd year university)	1	150	10
Organic chemistry (2 nd -3 rd year university)	1	48	10
Physical chemistry (3 rd -4 th year university)	1	36	8
Total	8 unique schools	460 students	57 students

Analytical framework

Much like quantitative data, qualitative data can be analyzed in a variety of ways. There are many guides to qualitative data analysis (e.g. Patton, 1990; Saldaña, 2015; Silverman, 1994), and methods range from loose guidelines to strict step-by-step instructions. Selecting the appropriate methods of data collection and analysis are dependent on the goals of the research. For this study, developing a richly detailed understanding of students' chemical identity thinking was the primary purpose of this research. The data collected using the CSI Survey comprised 460 student responses. Each student responded to one of the four sets of the CSI Survey, and each set involved four main questions (two sets of paired questions, each set involving a different substance). Since the questions were open-ended, this resulted in student responses that varied in length. Some students responded in as few as three or four words, while others constructed paragraphs of multiple sentences. These responses

contained information on the ways in which students think about chemical identity, as students were asked to identify and differentiate substances. Despite the prompts, students did not always explicitly state how they would identify and differentiate the substances presented to them. Thus, interpretation of students' chemical identity thinking based on the information provided in their responses was a necessary part of the analytical process.

Both grounded theory and content analysis offer guidelines on qualitative analysis methods that are appropriate for this study. At their core, both seek to infer meaning in raw textual data and use the products of these methods to describe the reality of the phenomenon under analysis (Lindkvist, 1981). In order to determine which option was the best fit for the aims of this study, both grounded theory and content analysis were explored in great detail. An overview of grounded theory and content analysis is presented in the following paragraphs in an effort to provide a context for the methodological decisions in the analysis of the CSI data.

Grounded theory

Grounded theory is a methodology that can be used to guide the rigorous construction of a theory that has been grounded in data from participants' experiences. This theory can be used to explain, infer, and predict the phenomenon under study. Although grounded theory is not limited to qualitative data analysis, this is its most popular application (Cho & Lee, 2014). The earliest form of grounded theory was developed by Glaser and Strauss (Glaser & Strauss, 1967), and they have more recently presented an updated version of grounded theory (Glaser & Strauss, 2009).

Grounded theory as a methodology presents guidelines that begin at the onset of the research process. Generally, researchers using grounded theory are discouraged from reading too heavily into literature about the phenomenon they wish to explore in order to prevent bias or other perspectives from influencing how they interpret participants' experiences (Glaser & Strauss, 2009). More recent champions of grounded theory, however, acknowledge that reading the available literature is a necessary component of good research; without knowing what already exists in the field, it is impossible to determine what gaps exist and what phenomena are worth exploring (Charmaz, 2014; Suddaby, 2006; Thornberg, 2012). Grounded theory experts agree that although understanding the literature is necessary, when conducting analysis using grounded theory, researchers must set aside what they already know, or be prepared to critically examine or critique what others have put forth, in an effort to keep an open mind to the themes that are present in the data.

Grounded theory data analysis is driven by the process of constant comparison, which serves to guide researchers in making sense of the data. A sample of qualitative data is collected, typically through interviews. The data are then examined for meaning through the procedure of open coding. During the process of open coding, the researcher assigns first-level codes (sometimes referred to as child codes or meaning units) to every episode of meaning within the text, which are the researcher's first interpretation of the data. Codes are intended to capture the meaning in the data (Charmaz, 2014). The researcher has a few options when determining the size or length of text to code in this initial stage; s/he can choose to delineate ideas or experiences within a participant's response to code, use the natural breaks caused by

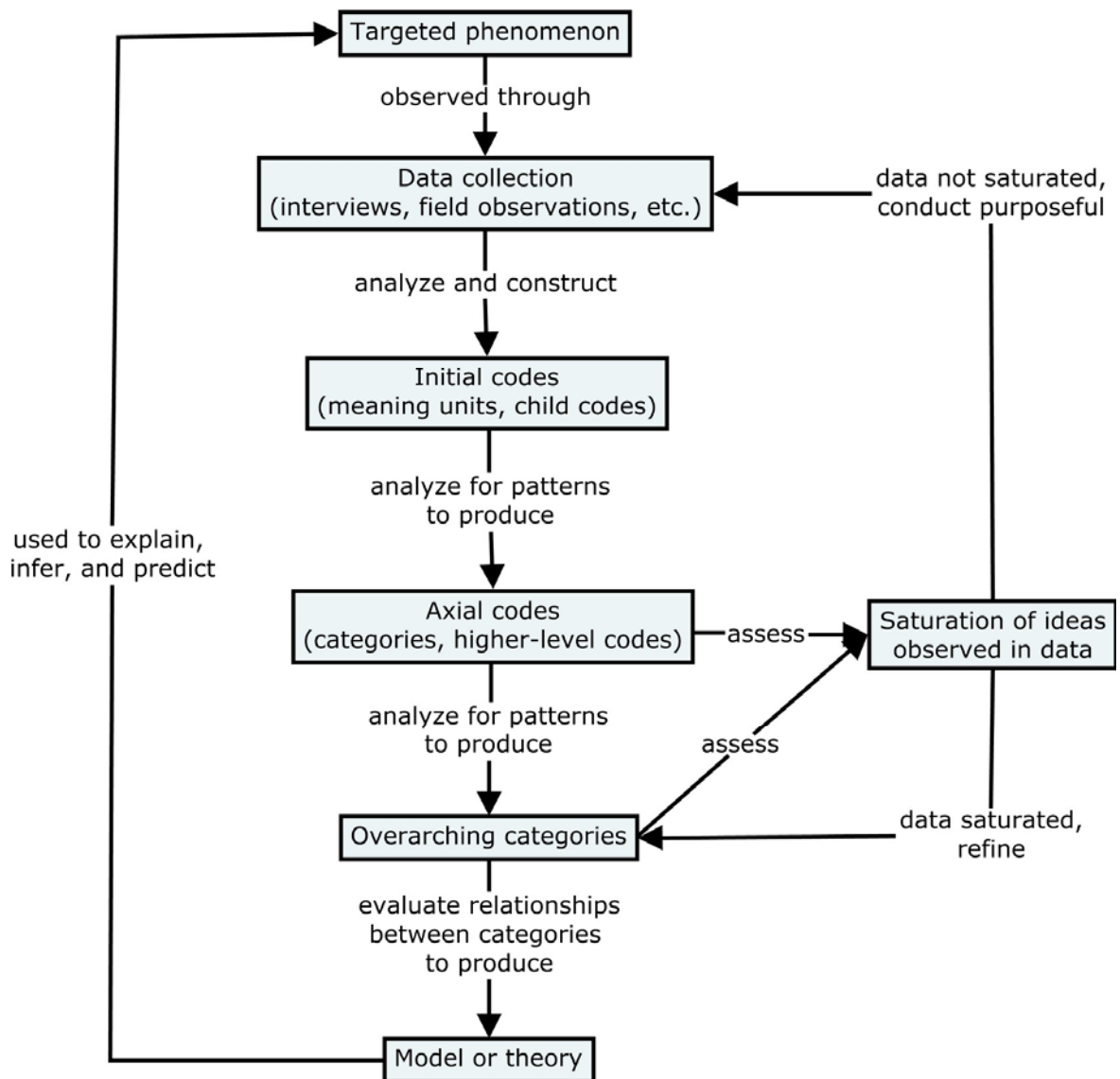
interviewer questions to segment chunks of data to code, or even assign codes on a literal line-by-line basis in the text. At this stage, the codes typically incorporate exact words or phrasing used by the participants in an effort to reflect the original intentions of the participants. Codes can be re-used, and the codes are constantly compared to assess redundancy and to look for patterns. Once the researcher has constructed the initial codes, she/he can begin to investigate patterns within the codes. This process of comparing the codes to each other, to the raw data, and across participants in order to investigate similarities and differences is referred to as constant comparison. During this discovery stage, the observed patterns are captured via the creation of the next level of codes, which are often referred to interchangeably as categories or axial codes. Constant comparison occurs again at this level, producing yet another level of codes. Through this process of coding, a hierarchy of codes or categories is produced, with each level becoming more abstract in its representation of the participants' experience (Charmaz, 2014; Corbin & Strauss, 2008; Glaser & Strauss, 2009).

During the data analysis, additional data are collected to further explore meanings found in the data through constant comparison. The additional data can be collected to confirm the existence of certain codes, to explore the experiences of participants not yet captured in the participant population, or in an attempt to disconfirm what is being observed in the data (which is referred to as negative case analysis) (Charmaz, 2014; Cho & Lee, 2014; Corbin & Strauss, 2008). The new data are coded using the highest level of the existing codes in order to verify and refine the existing codes; alternatively, if the data do not fit within an existing code, new codes must be created to capture the new information. Data collection and analysis thus

alternate until saturation has been achieved. Saturation implies that no new knowledge or understanding is obtained from collecting more data, and that the concepts developed from the grounded theory analysis are well defined. A representation of the general process that occurs when grounded theory is used as a methodology is shown in Figure 4-1. This is not a static process; these steps may change or be modified in accordance with the goals of the research, and Figure 4-1 only represents a generalized procedure outlined by other researchers.

In order to produce the final theory or model, the researcher must explore the relationships between the final categories that have been produced through coding. Examination of these categories and their influence on the participants, the context, and the overall experience of the participants is important to generate a comprehensive theory that explains the targeted phenomenon and can be used to make inferences or predictions. Many researchers talk about the creativity required to make the interpretive leap from the final codes or categories to overall theory. The codes must be tied together in a cohesive manner, and ultimately must represent the participants' experiences as a whole (Charmaz, 2014; Corbin & Strauss, 2008; Glaser & Strauss, 2009).

Figure 4-1. Grounded theory process



Content analysis

Content analysis is a qualitative analytical method used to produce a description of a phenomenon through the construction of concepts or categories (Elo & Kyngäs, 2008; Hsieh & Shannon, 2005; Lindkvist, 1981). Initially, content analysis was used as a quantitative method to systematically compare the content of different texts, such as hymns, newspaper articles, and speeches (Cho & Lee, 2014; Elo &

Kyngäs, 2008). More recently, it has been used to derive meaning from qualitative data, particularly by researchers in sociology, nursing, and psychology.

Content analysis provides general guidelines on analysis of qualitative data. There are different types of content analysis, from the more conventional approach where pre-existing literature and knowledge informs the study but is simultaneously questioned through the inductive methodology, to a directed and deductive approach that can be guided more explicitly by theory and can provide evidence to support or refute theory (Hsieh & Shannon, 2005). Both employ a systematic coding process similar to that of grounded theory, where codes are constructed from the raw data and categories of codes are created based on observed or inferred patterns. The process of creating categories delineates the patterns noticed in the data, and researchers are forced to determine how to best categorize the meanings found in the data, as it is likely the data have multiple meanings or interpretations (Cavanagh, 1997). Content analysis ultimately provides structure to the data, in that the final categories or themes can be used to describe the original experience in a more explicit manner.

Grounded theory vs. content analysis

Although the general intention of both grounded theory and content analysis is to capture the meaning of a participant's experience, they differ in a few key aspects. Grounded theory is accepted as a methodology, meaning that it provides guidelines for rigorous research procedures from the beginning to the end of a project (Cho & Lee, 2014). Although grounded theory does provide guidance on methods of data analysis, it can also be used to drive the research design as a whole. Content analysis, on the other hand, serves only as a method for data analysis.

In terms of data analysis, content analysis differs from grounded theory methods in that it does not require re-sampling the participant pool (theoretical sampling). In this manner, content analysis employs data reduction, where extraneous information not relevant to answering the research question is not explored via additional data collection (Cho & Lee, 2014). Grounded theory seeks to capture the entire experience, whereas content analysis might be more focused on capturing specific variables or components of an experience.

The final products of studies employing grounded theory vs. content analysis are also different. Studies following the tenets of grounded theory seek out the relationships between the identified categories and transform the overall conception of the data to a more abstract level than content analysis. In many cases, studies using content analysis are satisfied with the construction of the final categories or themes that describe the experience of the participants. These categories do not need to be tied together in a uniform theory like that of grounded theory (Cho & Lee, 2014).

Table 4-2. Comparison of grounded theory and content analysis

Research component	Grounded theory	Content analysis
Typical form of raw data	Interviews	Responses to open-ended questions
Experimental hypothesis	No hypothesis tested, existing literature ignored or mentally “set aside”	Hypothesis or theory can be explicitly tested
Core methods	Constant comparison AND theoretical sampling	Inductive coding OR deductive coding
Final product	Theory	Categories or themes

Grounded theory and content analysis in chemistry education research

Many studies in chemistry education research refer to core components of grounded theory and content analysis, such as open coding or constant comparison,

but do not make explicit commitments to either analytical approach. These methodological theories have been utilized in many other disciplines, and studies from these other disciplines were used as exemplars for this work. One study used grounded theory to study the process of interpreting change in management (Isabella, 1990), and another investigated social practices in private dentistry offices (Sbaraini, Carter, Evans, & Blinkhorn, 2011). These studies provided concrete examples of how to implement the steps outlined by grounded theory. Another article compared a study guided by grounded theory to a study that implemented content analysis in order to contrast the two (Cho & Lee, 2014). This article provided an explanation of how content analysis was used to answer research questions about the environment of Korean American nursing homes. Another article published in the *Nurse Researcher* outlined the specific steps needed to conduct content analysis (Hickey & Kipping, 1996), which were helpful when making methodological decisions in this study.

Data analysis methods

Although patterns of chemical identity thinking had previously been suggested based on the literature, the author sought to reveal CI thinking in the data without the influence of the hypothesized learning progression for CI. While many of the steps taken in the design of the CSI Survey and the analysis correspond to methods proposed by both grounded theory and content analysis, it was ultimately decided that the constraints and affordances corresponding to content analysis better fit the goals of this project. There are two main reasons behind this choice; the first is based on the study's weaker defense for theoretical sampling. Although it can be

argued that the many pilot phases in which data were collected and then analyzed to inform the CSI Survey development were a form of theoretical sampling, the results from these analyses were only used for the pilot study and contributed in a substantial manner to developing an initial understanding of CI thinking. Inductive coding and constant comparison were both utilized in this study, which allowed patterns of chemical identity thinking to emerge that were rooted in the data collected using the CSI Survey. Second, at the time of publication, the relationships between the emergent categories had not been explored. Thus, the categories or themes fully described the strategies taken by students for determining chemical identity, but a generalized theory was not produced by the conclusion of this study. The development of a theory for CI thinking is a future research goal, and can be built on the foundation of the categories presented in this doctoral work.

The data were analyzed in a cyclical process that involved analysis by the author followed by analysis by other researchers. The data from the CSI Survey were split into two sets, shown in Table 4-3. The questions in the CSI Survey were matched based on their contexts when possible (see Table 3-3: Example of deconstructed questions for how the questions were broken down), and one set of questions was randomly chosen for the first half of the analysis. Deliberately splitting the dataset in half ensured that the analysis took place on a wide variety of student answers, while leaving half of the data to test the emergent categories on to refine the categories. Although the dataset that was used in the complete analysis did not include the interviews from students, the researchers used these interviews in the early stages of the analytical process to ensure that the typed responses to the CSI

Survey were reflective of what students were thinking. In most cases, the researchers found that the additional details students provided in their interviews did not contribute significantly to the content of the typed responses students provided for the CSI Survey.

Table 4-3. Splitting the CSI Survey dataset

Set 1	Set 2
Water and water bubbles	Ethanol and ethanol bubbles
Caffeine and caffeine source	Chlorophyll and chlorophyll source
Silver and oxidized silver	Sucrose and burnt sucrose
Oxygen and oxygen vs. carbon dioxide	Chunk of metal and metal can

The student responses to the questions in Set 1 of the CSI Survey dataset were used in a ground-up approach for analysis, where child codes were constructed from the raw data and patterns were sought in the child codes and used to construct categories. Three levels of categories were ultimately created, rooted in the patterns observed in the previously established set of categories. Figure 4-2 represents the coding process followed for this inductive approach. Bidirectional arrows indicate that both the author and group worked to analyze the patterns in the codes and categories, and the products of each level were subject to change as the next level was constructed. Table 4-4 notes the number of child codes and subsequent categories developed at each level of the analytical process. A list of the categories created for each level is located in the Appendix.

Six final categories were established after coding the first half of the dataset, and they were used to code the second half of the dataset in a top-down approach. The six categories (change, composition and structure, experimental values, history, object that it's in, purpose and effect upon use) were applied to the raw data in a

cyclical process by the author and other researchers similar to the analytical method for the first half of the dataset. This allowed the author to determine if the same patterns of chemical identity thinking were present in the responses from students to different questions with different substances and to see if new ways of thinking about chemical identity were uncovered. Although no entirely new categories emerged from coding the second half of the dataset, the original categories were split into eight categories to more accurately capture the unique themes within the data. This process further refined how the categories were defined, and examples of how these categories were applied were collected.

Figure 4-2. Category development process

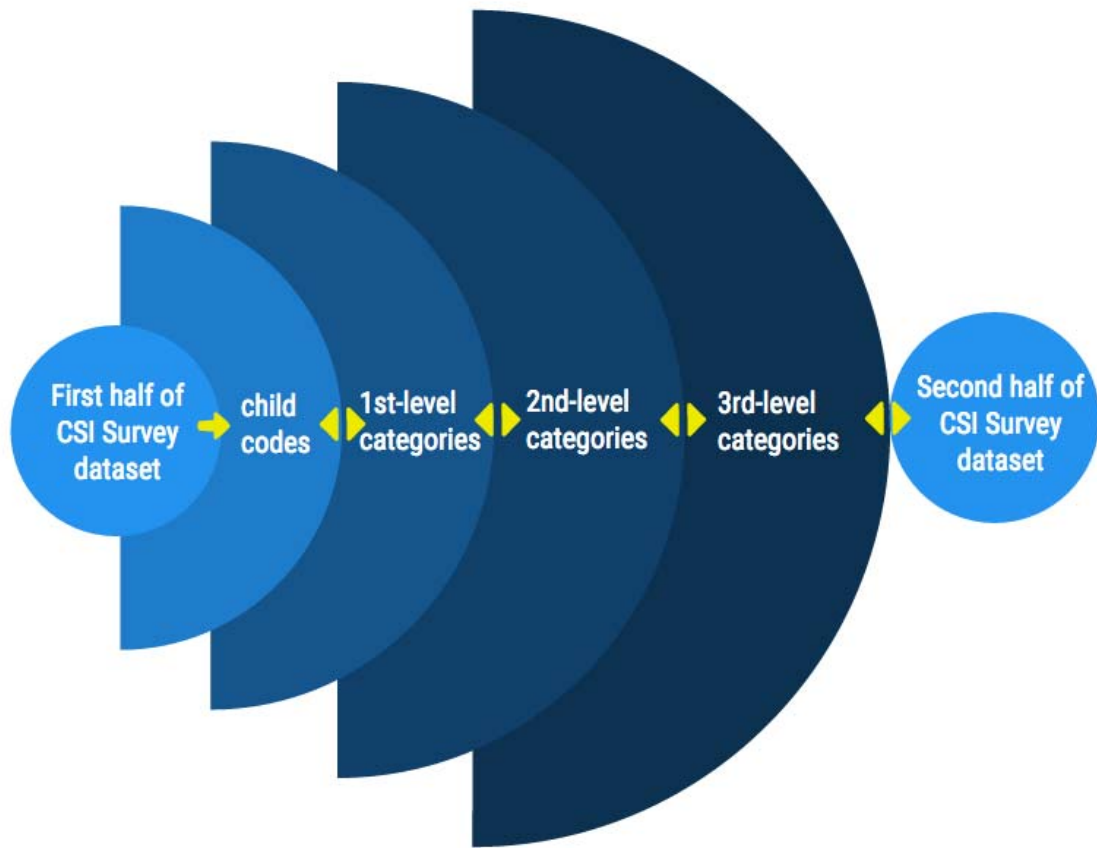


Figure 4-2: The category development process is represented as a series of levels, where the researchers grounded the next highest level of categories in the lower level of categories (represented by arrows), the circles represent the data while the half circles represent the categories that are grounded in the data but increasing in abstraction

Table 4-4. Steps and products from coding analysis process

Step	Players	Product	No. unique codes or categories
Code first half of dataset	Author	Child codes	908
Analyze child codes for patterns	Author, group	First-level categories	73
Analyze first-level categories for patterns	Author, group	Second-level categories	18
Analyze second-level categories for patterns	Author, group	Third-level categories	6
Apply third-level categories to second half of dataset and refine third-level categories	Author, group	Refined third-level categories	8
Apply final third-level categories to entire dataset	Author, group	Dataset coded with highest (third) level categories	NA

Eight consistent themes (corresponding to the eight third-level categories) involving chemical identity thinking emerged from the data collected using the CSI Survey. Brief descriptions of these themes are presented in Table 4-5 below. These final eight categories developed from coding the second half of the data were then applied to the first half of the dataset to ensure that the refined categories were valid for the entire dataset. Throughout this process, other researchers checked the author's application of the categories and also participated in group coding using the final categories.

Table 4-5. Themes of chemical identity thinking

Theme	Defining characteristics
Change	Students may focus on the changes to a substance occurring through a process, event, or transformation, and reason about the chemical identity of the substance based on the type of change that is happening or has already happened or the external agents that may be invoking the change on the substance
Class	Students may place the substance into a more general class of substances in order to make inferences about the substance's chemical identity
Composition and structure	Students may use the components of the substance and their arrangement at either a macroscopic or microscopic level to reason about the chemical identity of the substance
Function	Students may consider the function or purpose of a substance on its own or when in a mixture or object form to determine the chemical identity of the substance
Organism effect	Students may consider the effect a substance has on a living organism to determine the chemical identity of a substance
Sensory information	Students may rely on information provided to them by their senses in order to make judgments about the chemical identity of a substance
Source	Students may reference where a substance came from to establish its chemical identity or to differentiate it from other substances, they may think that an essential component or quality is imparted by the source
Tests and experimental values	Students may suggest performing tests or experiments on substances to aid in claims about chemical identity, and may wish to compare experimentally obtained values or observations to those defined in the literature

Results

Although the intention of this research is to characterize students' chemical identity thinking, obtaining analyzable data towards this goal is not straightforward. Chemical identity is comprised of two main practices: classifying and differentiating substances. While it is possible to directly ask students to differentiate substances, it is more difficult to get students to talk about how they classify substances, which is often implicit in how they identify substances. Thus, the questions in the CSI Survey were structured around two questions related to chemical identity: 1. What is this substance? And 2. How is this substance different from other substances? The first question targets how students identify substances, from which their classification strategies can be inferred. The second question targets how students differentiate

substances. Questions of chemical identity often involve both classification and differentiation, so students' responses contained a mix of chemical identity thinking.

The following section presents the themes of chemical identity thinking uncovered in the data, and grounds these themes in original student responses. When statements made by students are included, a code name is used to identify the student. The prefix (see Table 4-6) denotes the grade level of the student, and the second half of the code is the number in which the participant responded to the CSI Survey. For example, 1049 represents a student number 49 in 10th grade, while F117 is the 117th freshman student to take the survey.

Table 4-6. Student code prefixes

Prefix	Grade level
8	8 th grade (general science)
10	10 th grade (honors or regular chemistry)
AP	11 th /12 th grade (AP chemistry)
F	General chemistry (1 st /2 nd year university)
O	Organic chemistry (2 nd /3 rd year university)
P	Physical chemistry (3 rd /4 th year university)

In total, 2199 unique references were assigned codes. Only one CI theme code was assigned to any given student statement; no text was double coded with the CI themes. In some cases, students responded that they did not know how to respond to the question. There were 89 instances that were coded as “I don’t know,” representing 4% of the entire dataset. Some student responses were coded as “not relevant” because either the students did not respond to the question that was asked or the meaning of the student’s response was unclear or uninterpretable. There were 124 statements coded as “not relevant,” which were checked with other researchers during

the group coding process for agreement. These instances represented 5.6% of the total dataset.

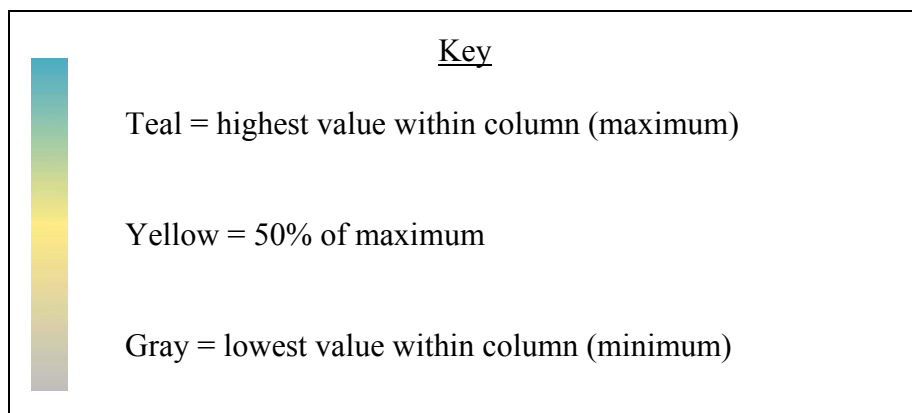
Once the entire dataset was coded with the themes of chemical identity thinking, the intersection of themes and CSI Survey questions was explored. The number of coded references was totaled for each CSI Survey question. Then, the references were split into counts of coded themes for each question. These counts were used to calculate the frequency or prevalence of each theme within the responses to a specific CSI Survey question. The frequencies are presented as percentages in Table 4-7.

Table 4-7 makes it possible to visualize in which question(s) a theme appeared most frequently. The table has been color coded to reflect the frequencies of student responses coded for a specific theme. Within each theme (column) the cells have been colored based on their values and how they compare to each other within a theme. The coloring is a three-color gradient based on percent, with green corresponding to the maximum value within that theme, yellow to 50% of the maximum value, and red to the minimum value. The assignment of the colors is theme-dependent; that is, each theme will have a unique maximum value, 50% value, and minimum value. Comparing the prevalence of student responses within a theme helped to illustrate major differences in how often that theme appeared in the CSI Survey questions. Each theme had at least one question where its prevalence was $< 1\%$; since most themes had multiple questions with a prevalence $< 1\%$, this influenced the coloring so that there were not an even number of questions above and below the 50% mark. This allowed for questions where a theme was highly prevalent to stand out from the other

questions. Table 4-7 provides a detailed picture of coded theme frequencies, and specific theme frequencies will be discussed in the following section outlining each of the CI thinking themes.

Table 4-7. Percentage of references within a question coded as a theme of CI thinking

		Chemical identity theme							
		Change	Class	Composition and structure	Function	Organism effect	Sensory info	Source	Tests and experimental values
Question labeled by substance	caffeine	0.0	8.5	0.5	21.6	32.2	4.0	29.1	0.5
	caffeine source	8.2	13.4	9.7	20.1	20.9	0.0	15.7	0.0
	chlorophyll	0.0	5.0	6.1	40.6	2.8	15.0	18.9	0.6
	chlorophyll source	1.6	6.5	8.9	29.8	0.8	7.3	26.6	0.8
	ethanol	0.0	4.3	2.5	0.0	0.6	28.6	0.0	57.8
	ethanol bubbles	46.3	9.7	14.9	3.0	0.0	1.5	3.0	6.7
	metal chunk	0.0	50.8	3.2	1.6	0.0	30.6	0.8	3.2
	metal can	5.2	13.0	3.9	7.8	0.0	33.8	4.5	23.4
	oxygen	0.0	1.8	0.9	0.0	8.2	13.6	0.0	57.3
	oxygen vs. carbon dioxide	0.0	0.0	7.5	6.6	8.5	6.6	0.0	50.0
	silver earring	0.0	2.3	3.1	0.0	4.6	15.4	0.0	62.3
	oxidized silver	28.4	12.1	10.3	0.0	0.0	6.0	6.0	32.8
	sucrose	0.6	1.2	10.3	0.0	0.0	32.7	0.6	50.9
	burnt sucrose	48.9	8.5	18.4	0.7	0.0	5.0	8.5	5.7
	water	0.0	2.5	0.0	0.0	0.0	43.3	0.0	50.8
	water bubbles	60.4	10.9	11.9	2.0	1.0	0.0	0.0	0.0



Themes of chemical identity thinking

1. Tests and experimental values

Tests and experimental values was the most commonly observed chemical identity theme in students' responses. A total of 533 instances in the data were coded with this theme, which represented 24.2% of the entire dataset. Student responses that were coded with this theme suggested tests and values associated with the substances that could be used to identify and/or differentiate them. This line of thinking was most commonly observed in students' responses to the question about whether the earring was made of silver or not, and 62.3% of students' responses to the silver question were coded with this theme *tests and experimental values*. Five other questions (ethanol, oxygen, oxygen vs. carbon dioxide, sucrose, and water) also had a high frequency of the theme *tests and experimental values* within the student responses. In the metal can and oxidized silver questions, *tests and experimental values* was present in moderate levels. The remaining eight questions contained little to no thinking within the *tests and experimental values* theme. In a few cases, the pair of questions was split between frequently and rarely observed (ethanol and ethanol bubbles, sucrose and burnt sucrose, water and water bubbles).

Table 4-8. Prevalence of *tests and experimental values* theme

Total coded references	Question(s) where theme was frequently observed	Question(s) where theme was sometimes observed	Question(s) where theme was rarely observed
533	Ethanol Oxygen Oxygen vs. carbon dioxide	Metal can Oxidized silver	Burnt sucrose Caffeine Caffeine source Chlorophyll Chlorophyll source Ethanol bubbles Metal chunk Water bubbles
% of total dataset	Silver earring Sucrose Water		
24.2			

When responding to the CSI Survey questions, students incorporated thinking within the *tests and experimental values* theme in many different ways. Sometimes, students stated the specific values that they expected a substance to have, such as student F71, who responded to the unknown liquid question and said, “Theoretically, you could test the liquid for its pH level. If it is about 7, the liquid is probably water.” Boiling point, freezing point, pH, and density were common values that students referred to in their responses. In many cases students talked about the actual values associated with a substance (e.g. water boils at 100°C), but in other cases they stated that comparing the observed value to the literature or expected value would be useful for classifying and/or differentiating the substance.

Other types of student thinking within the *tests and experimental values* theme involved the expected behavior of substances. For example, when responding to the sucrose question, student P17 said, “I would first test to see if the white crystals dissolved in water. If they did not, then I would immediately be able to tell that they were not sucrose.” Student P17 apparently drew on knowledge that sucrose is water soluble, and suggested a test that can be performed to determine if the unknown white

crystals exhibit this behavior. Other students suggested tests based on chemical reactivity of substances, such as student 1029 who proposed:

“I would conduct a chemical reaction that involves oxygen. For example, I could conduct a synthesis reaction with aluminum and oxygen to form aluminum oxide. If aluminum oxide has formed, then it would confirm that the unlabeled cylinder filled with gas is oxygen.”

Student 1029 appeared to rely on the expected behavior of oxygen when it interacts with aluminum in order to identify the unknown gas in the cylinder. This student and others may have assumed that the behavior and properties of substances do not change and could be reliably used to classify and differentiate substances. Thus, if water has a boiling point of 100 degrees Celsius, this value can reliably be used in boiling tests to differentiate water from other substances. A variety of tests and experimental values associated with substances were proposed by students to determine the chemical identity of a substance.

2. Sensory information

Thinking along the lines of *sensory information* was the second most prevalent theme; there were 344 references coded with this theme, which represented 15.6% of the total dataset. This type of thinking was most common in responses to the question that asked students to determine if an unknown liquid was water. Four other questions (ethanol, metal chunk, metal can, sucrose) had high frequencies of the *sensory information* theme. Responses to three questions (chlorophyll, oxygen, and

silver earring) contained moderate frequencies of *sensory information* thinking. The remaining eight questions contained little to no *sensory information* thinking.

Table 4-9. Prevalence of *sensory information* theme

Total coded references	Question(s) where theme was frequently observed	Question(s) where theme was sometimes observed	Question(s) where theme was rarely observed
344	Ethanol Metal chunk Metal can Sucrose Water	Chlorophyll Oxygen Silver earring	Burnt sucrose Caffeine Caffeine source Chlorophyll source Ethanol bubbles Oxidized silver Oxygen vs. carbon dioxide Water bubbles
% of total dataset			
15.6			

Students incorporated many types of sensory information into their responses, but the substance’s appearance was most frequently cited. Many students responded in a similar vein to student 823, who said, “I would look at the color, because I know silver is usually a shiny gray metal” in response to determining whether the earring is made out of silver. Student F29 also used appearance, and reasoned, “but I think the can is the same because it is shiny and patterned” when asked if the chunk of metal could be the same substance as the metal can.

Students also used other features that could be examined via the senses, such as texture and smell. Student F82 said, “color of the gas and smell of the gas would help me determine what gas it is” when answering how s/he would figure out if the gas inside the cylinder is oxygen. Some students combined multiple pieces of sensory information, such as student 1029 who said:

“I would examine it physically and identify its properties. Is it clear? Is the liquid thick? Thin? Is there anything within it? What color is it? What does it

smell like? From the information I have obtained, if it matches the criteria of being clear and odorless, I would assume that it is water. If it doesn't, it is not water.”

In these cases, students appeared to compare sensory information about the substance at hand to prior knowledge of sensory information associated with that substance.

Other students used sensory information derived from hypothetical tests of the substance.

3. Change

The theme *change* was the third most prevalent form of chemical identity thinking observed in the data. There were 247 references coded with the *change* theme, representing 11.2% of the dataset. This type of thinking was exhibited most frequently in the water bubbles question, as 60.4% of all coded references for this question were related to *change*. The burnt sucrose and ethanol bubbles question also exhibited high levels of *change* thinking in student responses. The responses to the oxidized silver question contained moderate levels of *change* thinking. Despite moderate to high levels of *change* thinking in these four questions, there were twelve questions in which *change* thinking was rarely observed or not present at all.

Table 4-10. Prevalence of *change* theme

Total coded references	Question(s) where theme was frequently observed	Question(s) where theme was sometimes observed	Question(s) where theme was rarely observed
247	Burnt sucrose Ethanol bubbles Water bubbles	Oxidized silver	Caffeine Caffeine source Chlorophyll Chlorophyll source Ethanol Metal chunk Metal can Oxygen Oxygen vs. carbon dioxide Silver earring Sucrose Water
% of total dataset			
11.2			

Thinking that fell within the *change* theme considered the state of the substance. Substances can be encountered in what appears to be a static state or they can appear to be in a state of transition. Students made inferences about the type of transformation that was occurring or could occur in the context to make judgments about the chemical identity of the substance. They reasoned about the ways the substance did or did not change in cases where there was perceived to be a state of transition, or ways that substances could or could not change in cases where it was perceived to be static in order to determine the chemical identity of the substance and to compare it to other substances. For example, student F122 argued that the silver earring did not change identity after being “left out” and said, “the silver earring is pure silver and the substance does not change unless it goes through a chemical process.” Student F122 apparently perceives that the identity of the silver remained stable, and then argues why no transition occurred. To make this argument, student F122 outlines what IS necessary for a transition of the silver to occur (chemical process).

In order to justify the stability or transformation of a substance, some students went beyond classifying the change that did or did not occur to a substance and explained the mechanism of the change. Student 1046 described the state of the water molecules before heat was applied to explain why s/he thought there were H₂O particles inside the bubbles and said, “Because when water is together the Hs and Os link but when they are boiled the heat separates compounds from one another.” Student 1046 talks about the change that is occurring in order to reason about the identity of the substance in the bubbles. Including the mechanism of the change (separation of Hs and Os due to heat) supports this student’s reasoning that the water molecules are preserved but separated. Some students chose to include the mechanism behind change or mechanism behind substance stability, while others did not and only described the change or stability of the substance.

Other students focused on the presence and/or types of external agents that could have caused the substance to change. For example, in response to the oxidized silver question, student 835 reasoned that it was still silver because, “a substance cannot change unless you add multiple sources of heat or other factors.” This student argued that without any obvious “factors” to stimulate change, it was impossible for the substance to undergo changes in chemical identity on its own. This tendency to seek out the agents that play a role in influencing the substance is another example of a pattern of student thinking that fell within the *change* theme.

The student responses about change occurred the most frequently when the context brought up a possible change (e.g. boiling, oxidation, melting/decomposition), which is evidenced by the high prevalence of *change* thinking observed in response to

the burnt sucrose, ethanol bubbles, and water bubbles questions. However, reasoning involving change also appeared outside of these questions. For instance, when asked to compare the metal chunk to the metal can, student F141 said, “I believe that previous substance (metal chunk) could be the same because it could be shaped into a can through welding and use of technology in order to use that substance for an applicable use.” Student F141 considered the type of change that could occur to the metal chunk to shape it into a metal can, and reasoned that the welding and other processes used to shape the metal will not affect its chemical identity. It was common for students to describe what may have happened to a substance in the past when thinking within the *change* theme to explain the chemical identity of a substance.

4. Function

Thinking within the *function* theme was observed in 208 instances, which corresponds to 9.5% of the entire dataset. *Function* thinking was most prevalent in responses to the chlorophyll question, where students were asked what they would put on a poster with the intent to teach others about chlorophyll, and the chlorophyll source question, where students were asked whether chlorophyll from two different sources was the same or not the same. Four questions (caffeine, caffeine source, metal can, oxygen vs. carbon dioxide) prompted responses that contained moderate amounts of *function* thinking. There were ten questions where *function* thinking was not observed or was barely present.

Table 4-11. Prevalence of *function* theme

Total coded references	Question(s) where theme was frequently observed	Question(s) where theme was sometimes observed	Question(s) where theme was rarely observed
208	Chlorophyll Chlorophyll source	Caffeine Caffeine source Metal can Oxygen vs. carbon dioxide	Ethanol Ethanol bubbles Metal chunk Oxygen Sucrose Burnt sucrose Silver earring Oxidized silver Water Water bubbles
% of total dataset			
9.5			

When students exhibited reasoning within the *function* theme of chemical identity thinking, they defined or described the substance(s) in terms of purpose or function. Within responses to the chlorophyll question, students frequently mentioned that the function or purpose of chlorophyll is to provide food to the plant through the process of photosynthesis. For example, student F16 said, “I would put a picture of plant(s) photosynthesizing. It would be a picture that dissects the process of photosynthesis and would provide information on how chlorophyll plays its role in all of it.” This student, like many others, emphasized the role of chlorophyll in the process of photosynthesis: the purpose of the chlorophyll is to be used by plants.

The purpose or function was also associated with the ways in which the substance is encountered in everyday experiences. This way of thinking within the *function* theme was observed in response to the caffeine questions. For example, student AP75 said, “I would tell them about all of the items which caffeine can be found in, such as coffee and certain soft drinks. I would tell them about the uses and purpose of caffeine, and the effects it can have on humans.” In the case of caffeine, students often related the purpose or function of to its effects on humans. When

students spoke about the purpose of ingesting caffeine for its stimulating effect it was coded as *function*, whereas when students described the effects of ingesting caffeine as a way to define or describe caffeine, it was coded as the *organism effect*.

Function was observed in the responses from students to other questions besides caffeine, as in the chlorophyll source question. When responding to whether the chlorophyll that is extracted from algae is the same or different as the chlorophyll from an oak tree, student 1058 said, “The chlorophyll would be the same in both situations as the purpose is still the same. It is still being used in photosynthesis to convert light into energy.” Again, the focus is on the purpose of the substance – in this case the function of chlorophyll in the process of photosynthesis is the sole component for student 1058’s claim that the chlorophylls are the same. *Function* thinking was used to determine if two substances are the same or different.

5. Class

The *class* theme was observed in 202 instances of students’ responses, which comprised 9.2% of the dataset. *Class* thinking appeared most frequently in responses to the metal chunk question. Within the nine questions where *class* thinking was sometimes observed, the *class* theme represented 5-13% of the student responses to these questions. The *class* theme had the highest number of questions where class was moderately observed. There were six questions where *class* thinking was rarely observed in student responses.

Table 4-12. Prevalence of *class* theme

Total coded references	Question(s) where theme was frequently observed	Question(s) where theme was sometimes observed	Question(s) where theme was rarely observed
202	Metal chunk	Burnt sucrose Caffeine Caffeine source Chlorophyll Chlorophyll source Ethanol bubbles Metal can Oxidized silver Water bubbles	Ethanol Oxygen Oxygen vs. carbon dioxide Silver earring Sucrose Water
% of total dataset			
9.2			

Explicitly or implicitly using classes of substances was a popular way for students to infer or deduce the chemical identity of a substance. *Class* thinking was most commonly observed in responses to the metal chunk question. Students often began their responses with a statement similar to AP38, who stated, “It is probably some type of metal.” Some students concluded their responses with this classification, while others provided a justification of what features placed the unknown substance into the category of “metals.” When substance features are used at the service of placing a substance into a class, these other ideas about substance were secondary to the main purpose of determining class. These secondary ideas about substance were also captured, and this is discussed in a later section of this chapter regarding cues.

By placing substances into a more general class or category, students were observed using the behaviors or properties typical of substances in that class to determine chemical identity. For example, student 1041 stated that although the earring had changed colors, it was still silver because, “metals rust being exposed to factors like rain, wind and other stuff which it could have come in contact with while it was lost.” It was inferred that this student classified silver as a metal, and then

reasoned that metals exhibit a characteristic rusting behavior. It appears that the student thought the chemical identity is maintained because rusting is typical of metals and silver falls within this category. In this case, the student placed the substance into a class and then used the class to justify or explain the observed phenomenon.

Students were also observed following the reverse reasoning sequence, where they focused on the class of the unknown substance to then determine its identity. When reasoning about the substance inside the bubbles in the boiling water, student F82 argued that oxygen is inside the bubbles, “because oxygen is a gas and bubbles are gas bubbles.” This student classified the bubbles as being made of a gaseous substance (i.e. there is a class of substances that are “gaseous substances”) and then might have considered the possible range of substances relevant to the context. Within these relevant substances, student F82 chose the one substance that fit within the “gaseous substance” class (oxygen).

Class thinking was also used to make arguments about the chemical identity of substances involved in mixtures. Students explained observed behavior by classifying a substance or material as pure or a mixture. For instance, regarding the oxidized silver question, student P20 stated:

“Most earrings are not made of 100% pure materials; they are often a mixture of two or more to make the work of the jeweler easier giving a desired shape. So, it is normal that the earrings get a little oxidized, but they can get cleaned and shine again.”

Student P20 made two references to *class* in this argument. The first separated pure materials from mixtures, and student P20 classified the earring as a mixture. Next, student P20 explained that because the earrings are a mix of substances, it is normal for them to get oxidized. Student P20 appears to implicitly assign one or more of the substances within the earring as belonging to a class of substances that can be oxidized and also implied that the other substance (likely silver) does not belong to that class.

6. Source

The *source* theme was coded for in 178 references, which made up 8.1% of the dataset. *Source* thinking was most prevalent in student responses to the caffeine question, and 29.2% of student responses to this question were coded with this theme. *Source* thinking was also frequently observed in student responses to the chlorophyll and chlorophyll source question. In five questions, *source* thinking was moderately observed. In the remaining eight questions, *source* thinking was rarely observed or not present.

Table 4-13. Prevalence of *source* theme

Total coded references	Question(s) where theme was frequently observed	Question(s) where theme was sometimes observed	Question(s) where theme was rarely observed
178	Caffeine Chlorophyll Chlorophyll source	Burnt sucrose Caffeine source Ethanol bubbles Metal can Oxidized silver	Ethanol Metal chunk Oxygen Oxygen vs. carbon dioxide Silver Sucrose Water water bubbles
% of total dataset			
8.1			

Student responses that were categorized as part of the *source* theme incorporated the source of the substance(s), the history of the substance(s), or both. *Source* thinking appeared frequently in response to the second question for both caffeine and chlorophyll, where students were directed to consider the source of the substance. In many cases, students argued that caffeine and chlorophyll that come from two different sources (e.g. two different types of plants) are different. When talking about the source of a substance to make claims about chemical identity, students sometimes described the conditions that the substance came from. For instance, student O2 stated that the chlorophyll extracted from the algae is different from the chlorophyll extracted from the oak leaves. Student O2 continued on to say,

Conditions in which the chlorophyll is observed are very different. The algae is grown in a pond with direct contact to water, while the trees take water from the ground, so the chlorophyll in the algae must have a different affinity to water.

Student O2 differentiated the chlorophylls by their affinity to water, which, s/he reasoned, can be attributed to the different environmental conditions these chlorophylls came from. Thus, student O2 appeared to think that the source of the chlorophyll contributed a characteristic feature to the chlorophyll that could be used to classify and differentiate it.

Students were also observed using the history of a substance to classify or differentiate it. For example, in response to the melting sucrose question, student 847 stated, “It is still sucrose because even though it change forms and colors, it is still from the sucrose.” This student apparently disregarded cues about appearance and

shape in favor of the history of the substance: this substance that is different in form and color came from sucrose, so therefore it must still be sucrose. This type of thinking appeared in student responses to many different questions and was linked to the original source of the substance. This implied that students might think part of a substance's chemical identity is contributed by the source. This implicit way of considering chemical identity is evident in student AP74's response to the caffeine source question:

It is the same type of caffeine but the use is different because insects react differently to the caffeine. One substance can have many uses. The caffeine is the same because coffee has caffeine and coffee is a plant seedling.

At first, it appears that AP64 focused on the function of the caffeine. It becomes evident, however, that the student argued that the function does not correspond to chemical identity, because s/he says, "one substance can have many uses." The student moved on to talk about the relationship between coffee, caffeine, and plant seedlings, and concluded that based on her/his knowledge of the source of the caffeine present in coffee, the caffeine in the context of the question are the same. This implies that student AP64 thought there is something *beyond* the use of the caffeine and linked to the source that gives the caffeine its identity. Without further probing, it is impossible to know exactly what feature or attribute student AP64 believed is imparted by the source. For example, the student could be thinking about a generalized essence associated with the caffeine, or perhaps specific atoms that comprise the caffeine molecule.

7. Composition and structure

The *composition and structure* theme was present in 150 student references, which represented 6.8% of the total dataset. *Composition and structure* thinking was most prevalent in three questions: burnt sucrose, ethanol bubbles, and water bubbles. This theme was moderately observed in six questions, and rarely observed in seven questions. In most cases, the pairs of questions were split in terms of how frequently *composition and structure* thinking appeared. For example, although *composition and structure* thinking was frequently observed in the ethanol bubbles question, it was rarely present in responses to the ethanol question. The ethanol question preceded the ethanol bubbles question in the CSI Survey.

Table 4-14. Prevalence of *composition and structure* theme

Total coded references	Question(s) where theme was frequently observed	Question(s) where theme was sometimes observed	Question(s) where theme was rarely observed
150	Burnt sucrose Ethanol bubbles Water bubbles	Caffeine source Chlorophyll Chlorophyll source Oxidized silver Sucrose Oxygen vs. carbon dioxide	Caffeine Ethanol Metal chunk Metal can Oxygen Silver earring Water
% of total dataset			
6.8			

References to the composition and/or structure of a substance as part of its chemical identity were observed in student responses to the CSI Survey. Thinking within the *composition and structure* theme included when students explicitly or implicitly used the components or composition of a substance to guide their reasoning about a substance's chemical identity. This theme also included when students spoke about arrangement of the components within a substance. These ideas about

composition and structure frequently occurred simultaneously, so they were merged into one theme of chemical identity thinking.

Composition and structure thinking was observed in relation to both the macroscopic and submicroscopic level, although it was more common for students to tie *composition and structure* thinking to the submicroscopic level. For example, in response to the burnt sucrose question, student 820 states, “Its still the same thing. The elements that make up the sucrose have not changed. Its sucrose but in a different form. The heat from the flame changed the form of the solid sucrose into liquid sucrose.” Student 820 is basing her/his conclusion that the sucrose has maintained its chemical identity on the notion that the elements that make up the sucrose have not changed. Student 820 appears to account for the noticeable changes with a change in form, which might relate to structure or possibly the proximity of the elements of sucrose to each other.

In some cases, students referenced composition and structure ideas very generally. For example, student AP61 said, “Caffeine has a specific chemical structure. Its presence in different solvents does not change its chemical identity.” From this it can be inferred that the student was referring to chemical structure on a molecular level. Other students were more specific, like student F57 who said, “Since it is pure silver the metal is composed of only the element silver, therefore it is still silver.” Student F57 made claims about the chemical identity of the earring based on components that s/he identified as elements. Thus, chemical identity was tied to the identity of the element making up the substance.

Other students used *composition and structure* thinking to explain phenomena, such as the differing effects of caffeine on insects vs. humans. Student AP74 explained:

I think the caffeine would be the same. However, to different organisms they would have different effects, but the elements involved would be the same.

They could be arranged in different ways and thus serve different purposes.

And at distinct ratios there could be differences in the concentration and lethal dose.

Student AP74 based the chemical identity of caffeine on the specific elements in caffeine, and attributed its different effects to a different arrangement of the elements.

For student AP74, composition at a submicroscopic level determines chemical identity, but structure still plays a role in the macroscopic behavior of the substance.

Although *composition and structure* thinking did not dominate students' responses for any question in particular, it appeared to be evenly distributed amongst the questions in comparison to other themes of chemical identity thinking.

8. Organism effect

Thinking within the *organism effect* theme was found in 124 references, which comprised 5.6% of the dataset. This theme was the least prevalent out of the eight themes of chemical identity thinking. *Organism effect* thinking was most frequently observed in the paired questions caffeine and caffeine source. Following this, *organism effect* thinking was next most commonly observed in the paired

oxygen and oxygen vs. carbon dioxide questions. *Organism effect* thinking was rarely observed in the remaining 12 questions.

Table 4-15. Prevalence of *organism effect* theme

Total coded references	Question(s) where theme was frequently observed	Question(s) where theme was sometimes observed	Question(s) where theme was rarely observed
124	Caffeine Caffeine source	Oxygen Oxygen vs. carbon dioxide	Chlorophyll Chlorophyll source Ethanol Ethanol bubbles Metal chunk Metal can Silver earring Oxidized silver Sucrose Burnt sucrose Water Water bubbles
% of total dataset			
5.6			

The theme *organism effect* dominated students' responses to the questions about caffeine, and involved using the effect of a substance on a living organism to reason about its chemical identity. For example, students frequently described how caffeine made them feel in order to identify caffeine. Student 871 said, "when caffeine is entered into the human system, it causes an increase of energy," while student AP74 stated, "Drinking it would make you more thirsty but awake at the same time." How caffeine affected organisms was also used to reason that the caffeine from the plant seedlings was the same as the caffeine from Red Bull, as student F43 argued, "because caffeine has a diuretic effect, it probably doesn't affect us as strongly as it affects tiny insects. A diuretic might be perceived as toxic for them so they innately stay away." Other students, however, used the effect on organisms to reason that the caffeine from the two different sources is different, as student 1056 justified, "if it was the same caffeine acting as a pesticide, we would not be able to consume it." In

these cases, the action of caffeine on humans and insects was used as a defining characteristic that could be used for the purposes of identification and differentiation.

Although the organism effect was most commonly observed in students' responses to the caffeine questions, students brought up the organism effect in other CSI Survey questions as well. For example, in response to the water bubble question, student F65 stated that the substance in the bubbles was oxygen changing from a liquid form to a gas form. Student F65 knew it was oxygen because "there are no harmful effects of breathing the bubbles. If it was Hydrogen gas I would assume it would be harmful. O₂ obviously is not." There are several possible steps embedded within this student's thinking. Implicit in this statement is the student's assumption that the substance in the bubbles could only be oxygen gas or hydrogen gas. Based on this knowledge, student F65 might have next recalled previous experiences with boiling water and recognized that the bubbles are filled with a gas that is nontoxic to humans. Thus, s/he reasoned that it must be oxygen gas and not hydrogen gas in the bubbles, based on implicit knowledge that oxygen is not harmful to humans.

In response to the silver earring question, some students spoke about the interaction of silver with the skin of the person wearing the jewelry. This was perceived as a way to determine if the jewelry truly is silver or another metal. As observed in the other themes, personal experience can play a role when applying the organism effect to reason about the chemical identity of a substance.

Distinguishing primary reasoning from supporting information

Some students incorporated multiple chemical identity themes into their responses, and the desire to capture this complexity lead to the separation of the

theme that was driving the argument from themes used to support the main argument. In most cases, a single chemical identity concept was driving the student's reasoning, with other chemical identity themes contributing to the main argument. In order to distinguish the primary chemical identity theme used by the student from the minor chemical identity themes, the chemical identity themes were assigned to two different tiers during coding. The first tier corresponds to the main factor driving the student's reasoning about the chemical identity of a substance and was labeled as "primary". The second tier denotes that the chemical identity themes were used as a minor contributing factor to the overall argument, and were labeled as "props". In each tier, the chemical identity themes are the same (the eight final themes), but when they were assigned to a student's response they were labeled as either primary or a prop. In all cases previously presented in the description of the themes, the theme in which the example statement was presented was coded as a primary theme for that statement. For all student responses, the chemical identity theme corresponding to the main reasoning was identified. When chemical identity themes that played a secondary role in the reasoning were also found, they were coded and classified as props. Props cannot stand alone, and were only coded for after the primary chemical identity theme driving the reasoning had been identified.

An example of a student's response where multiple props contributed to the primary argument is presented below in Table 4-16. The codes applied for the props and primary argument observed in this student's response are indicated in the column on the right, with the corresponding text from the student's response on the left. Student AP51 selected "different substance" in response to the question about

whether the earring was the same substance or different substance after turning dark gray/black. Student AP51 explained this choice and said:

Table 4-16. Student AP51's coded response

Student AP51's response	Codes and explanation
<p>“Certain metals have the potential to be oxidized,</p> <p>in which their chemical formula is changed,</p> <p>thus their physical appearance changes as well. For example, iron and copper experience rust, in which their color changes from grey to orange-brown, or brown to green, respectively.</p> <p>This occurs once the metal is oxidized, or oxygen molecules interact with the metal atoms, forming FeO or CuO₂.</p> <p>Therefore, because there is evidence that the silver changed in physical appearance, and the fact that silver is a metallic substance, it is reasonable to say that the silver is now a different substance, after it has been oxidized.”</p>	<p>prop: Class – classification of silver as a metal that could be oxidized</p> <p>primary: Composition – chemical composition changes as result of oxidation</p> <p>prop: Sensory info – the color change is indicative of the composition changing</p> <p>prop: Change – explaining the type of change, oxidation, going on and how it impacts the composition</p> <p>Summary sentence combining the previously mentioned props and primary argument.</p>

There are many themes of chemical identity thinking in student AP51's response to the question about whether the earring is still silver or a different substance. The basis of this student's response is that the chemical formula changed, which drives all other chemical identity themes presented in the student's response. She/he started with the observation that silver is a metal that can be oxidized, which would lead to a change in chemical formula. This change in chemical formula is what prompts the change in physical appearance, thus explaining the change in color from silver to dark gray/black. Finally, AP51 explained the mechanism of the oxidation, which is the type of change occurring to the silver. Student AP51 based her/his argument that the chemical identity of the silver changed (a new substance is produced) on the point that the chemical formula (composition) has changed, and

used chemical identity thinking related to class, sensory info, and change in order to support this argument.

There were some instances where students presented a multi-component argument regarding the chemical identity of a substance. In the example in Table 4-17, student P17 made two separate claims about chemical identity of the white crystal granules in the sucrose question.

Table 4-17. Student P17's coded response

Student P17's response	Codes and explanation
<p>“I would first test to see if the white crystals dissolved in water. If they did not, then I would immediately be able to tell that they were not sucrose.</p> <p>If they did dissolve, I would perform a flame test, as I know that sucrose is an organic compound and should not produce a colored flame.</p> <p>If a colored flame was produced, I would be able to say that the compound was not sucrose. If The flame was not colored then I would take an IR spectrum of the compound (dissolved in some inert solvent) and compare it to the structure of sucrose (which I'd have to look up).”</p>	<p>primary: Tests & experimental values – a solubility test can be used to rule out the substance's identity as sucrose</p> <p>prop: Tests & experimental values – uses a flame test to determine whether the substance belongs to a certain class</p> <p>primary: Class – classifying it as an organic or inorganic compound will help determine chemical identity</p> <p>prop: Tests & experimental values – use an instrument to get the IR spectrum</p> <p>primary: Composition & structure – the IR test provides information about the structure of the crystals, which can be compared to the known structure of sucrose in order to determine chemical identity</p>

Not all students incorporated multiple chemical identity themes into a single response, like student P17. However, when students did use multiple arguments corresponding to separate chemical identity themes as in student P17, the primary chemical identity theme behind each separate argument was identified. Thus, in those cases, there were multiple chemical identity themes identified as primary – one for each argument made in the overall response.

Incorporating multiple chemical identity themes into a response was not limited to the more advanced students. In Table 4-18, an 8th grader used more than

one chemical identity idea to justify her/his conclusion that the burnt sucrose is still sugar.

Table 4-18. Student 874's coded response

Student 874's response	Codes and explanation
<p>“It's still sugar because it didn't get mixed with another substance</p> <p>for a chemical reaction to happen so it still is sugar</p> <p>plus if u taste it, it still taste like sugar”</p>	<p>prop: Class – this substance is pure and not a mixture</p> <p>primary: Change – this is NOT a chemical reaction – a chemical reaction needs to happen to change identity, and you need another substance in order to have a chemical reaction</p> <p>primary: Sensory info – taste remains the same, which indicates the chemical identity is maintained</p>

Overall, props were identified in 417 student references along with their primary reasoning counterparts. The most common CI theme used as a prop was *sensory info*, which was used as a prop 137 times. In many of these cases, appearance was used as a prop in conjunction with the theme *tests and experimental values*. *Change* and *class* have the next highest counts for props, with 93 and 89 coded references respectively. The props corresponding to these three themes comprised more than 75% of the observed props. Props were most often observed in the oxidized silver question, which was mostly divided between *sensory info* and *change* themes. A high frequency of props was also found in responses to the metal chunk question (primarily based on *sensory info*) and the burnt sucrose question (split between *change* and *sensory info*). The high prevalence of props in student responses to these three questions indicates multiple chemical identity themes were considered relevant by students when answering the CSI Survey questions. Additionally, the low frequency of props in responses to the questions chlorophyll, oxygen, oxygen vs.

carbon dioxide, and water suggests that only one chemical identity theme may have been needed for students to feel that they had completely answered the question.

Table 4-19. Counts of chemical identity themes used as cues

		Props								
		Change	Class	Composition and structure	Function	Organism effect	Sensory info	Source	Tests and experimental values	Total props
Questions	caffeine	0	5	0	2	2	0	7	0	16
	caffeine source	3	10	1	2	5	1	5	0	27
	chlorophyll	0	0	0	0	0	0	0	0	0
	chlorophyll source	0	7	2	1	3	3	3	0	19
	ethanol	0	0	0	0	0	2	0	8	10
	ethanol bubbles	12	8	6	0	0	0	1	2	29
	metal chunk	0	0	6	1	0	54	0	5	66
	metal can	3	3	0	3	0	8	0	6	23
	oxygen	0	3	1	0	0	2	0	1	7
	oxygen vs. carbon dioxide	0	0	1	0	0	0	0	0	1
	silver earring	0	1	0	0	0	9	0	3	13
	oxidized silver	32	13	0	0	0	31	1	0	77
	sucrose	1	4	1	0	0	3	0	8	17
	burnt sucrose	33	7	1	0	0	21	0	1	63
	water	0	0	0	0	0	3	0	2	5
water bubbles	9	28	4	0	1	0	1	1	44	
	Total props	93	89	23	9	11	137	18	37	417

Although there are many examples of students using multiple props as part of their responses, not all students utilized chemical identity themes as props. Table 4-20 below presents the percentages of students who used props organized by grade level. Although a greater percentage (74%) of students in the AP chemistry classes used props than students in other levels, students in the physical chemistry classes tended

to use more props per student (1.7 props made per student in physical chemistry vs. 1.4 props per student in AP chemistry).

Table 4-20. Usage of props by grade level

	8 th grade	10 th grade	AP Chem	Freshmen	Organic	Physical
# students using props	34	46	58	88	27	26
Total # students	78	70	78	150	48	36
% students using props	44%	66%	74%	59%	56%	72%
Total props used	44	65	83	138	43	44
Average props used per student	1.3	1.4	1.4	1.6	1.6	1.7

Additional examples of thinking that fell within each theme for primary reasoning and props as well as examples of coding more complicated instances of student thinking were compiled in the complete CSI codebook, which can be found in the Appendix. This codebook was developed through the coding process and was subsequently used as a reference for the final round of coding.

Discussion

Implications for research

While students' conceptions of matter as a whole or their conceptions of specific substances (e.g. water) have been explored (Johnson, 2000; Krnel, Watson, & Glažar, 1998; Solomonidou & Stavridou, 2000; Stavy, 1988, 1991), students' chemical identity thinking has not been explicitly investigated until now. Since questions of chemical identity are inherent to many problems that can be addressed by chemistry (Ngai, Sevian, & Talanquer, 2014), eliciting CI thinking using the CSI Survey and characterizing their responses using the eight themes of CI thinking could be useful for understanding how students are solving problems in chemistry. If students cannot appropriately apply chemical identity thinking, it is unlikely they will

be successful in solving more complex problems in chemistry that involve multiple disciplinary crosscutting concepts.

Evaluating students' chemical identity thinking can lead to a better understanding of how students define substances. Conceptions of substance are implicit in chemical identity thinking, and future work could design questions to separate the two. It is possible that students hold multiple conceptions of substances, and when faced with challenges of chemical identity, choose the conception they find to be most relevant to the problem at hand. For example, when responding to the chlorophyll source question, student AP71 claimed that "it [the chlorophylls from two different sources] is probably the same as they provide the same function in each of the organisms." This response was characterized as the *function* theme of CI thinking and potentially rests on a concept of substance that conflates materials and objects, which is a more intuitive way of thinking about substances and chemical identity. When responding to the oxidized silver question, however, student AP71 said that the earring is a different substance because "It is very possible that silver reacted with air and oxidized or there were other chemical reactions that slightly changed the composition." This response was coded as *composition and structure* thinking, and within this response it is possible to infer that student AP71 perceives substances as having a specific chemical composition. This corresponds to a transitional level of thinking. Although the conceptions of substance students have were not investigated in the research presented in this thesis, student AP71's responses are one example of how conceptions of substance might be inferred from these data about students' chemical identity thinking.

It was observed that students did not consistently reason with the same CI thinking across questions, indicating that it is possible the question and/or substance prompted specific themes of CI thinking. For example, it was observed that students did not consistently consider chemical identity at a microscopic or macroscopic level across questions or themes. This was observed in the responses to the burnt sucrose question, where students were more likely to respond with ideas about composition and structure of the sucrose on a submicroscopic level. For instance, in response to the burnt sucrose question, student 1045 stated that, “It’s a different substance because of the change in color. It signifies that the bonds of the sucrose have been broken and cannot be placed back together, so it’s a new substance.” Student 1045 is thinking on a submicroscopic level about the chemical identity of the substance by reasoning about the bonds of the sucrose and the role they play in the chemical identity of the sucrose. Yet this same student based her/his response to the ethanol bubbles question on *change* thinking and stated that there was water vapor in the bubbles because, “the water in the ethanol would change its phase from a liquid to a gas.” If student 1045 is thinking about water and ethanol on a submicroscopic level, it is not clear from this response. This could mean that in some instances, students think about substances on the macroscopic level, while in other cases something (e.g. substance, context of problem) prompts them to shift to the molecular level. Research that explores the relationship between context, substance conception, and chemical identity thinking could be useful for obtaining a better understanding of substance + chemical identity as a whole.

Chemical identity thinking learning progression

Although it is clear that the context of the question (including the way the question was phrased, whether it pertained to core question 1 or 2, and the substance involved in the question) influences the type of chemical identity thinking observed in students' responses, it is also apparent that a wide range of chemical identity thinking exists and is applicable in many contexts. The eight themes of CI thinking were observed in responses at each educational level, which means it is likely that a range of sophistication within each theme exists. Exploring the different levels of sophistication and the ways in which students applied chemical identity thinking can contribute to a learning progression for chemical identity thinking. Although such analysis goes beyond this thesis, some evidence already indicates that it would be fruitful to carry out such an analysis to illuminate a first idea of a learning progression. The following inferences stemming from the initial analysis of the data include:

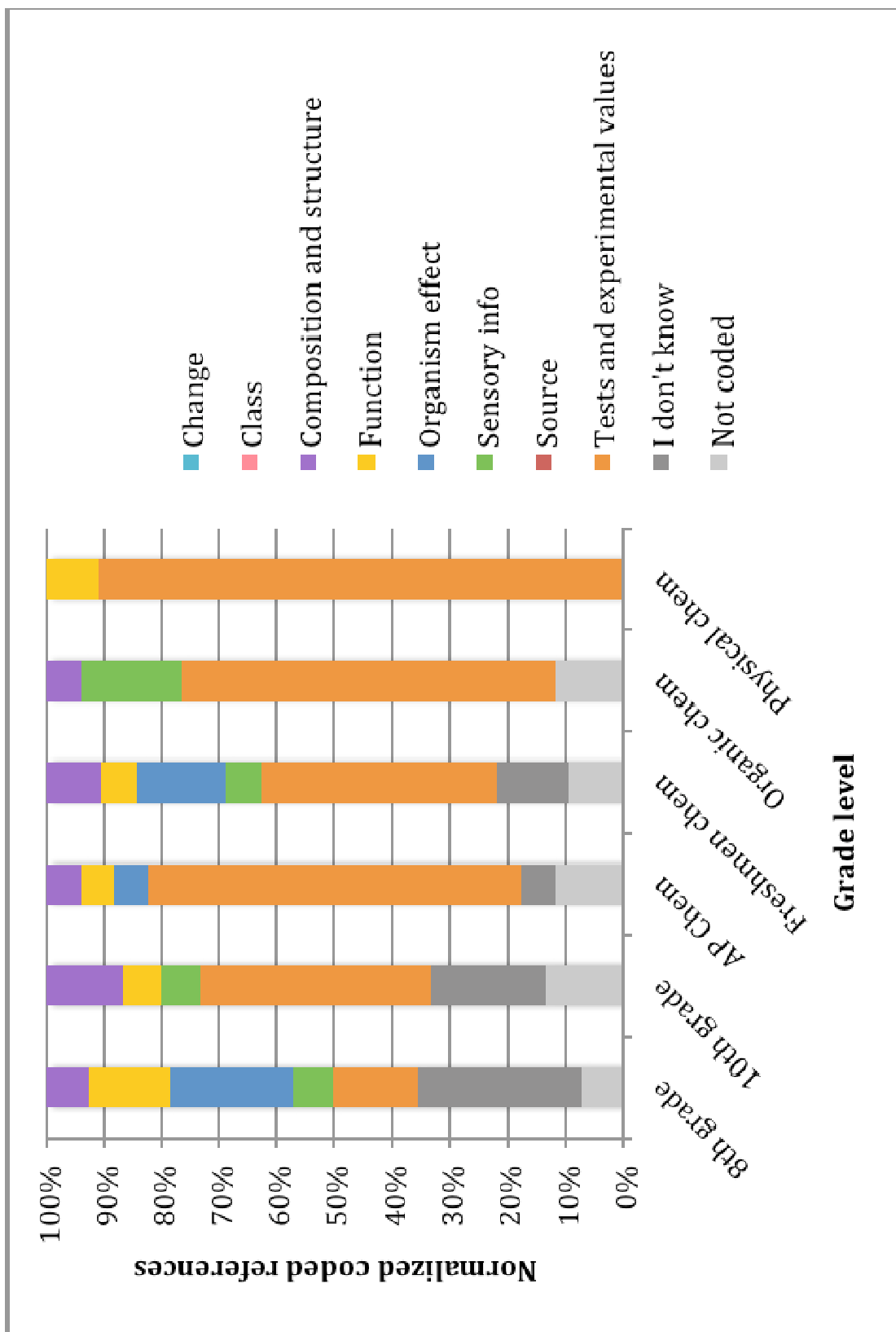
- As observed in the responses from students that were coded as *change*, in many cases, a focus on the type of transformation that is occurring can help students reason about conservation of chemical identity of a substance. When students classified the type of transformation occurring (e.g. chemical vs. physical) they were more likely to supply evidence on a microscopic level in support of that classification.
- The frequent application of *tests and experimental values* thinking included a broad range of sophistication. Students at more novice levels in their chemistry training were more frequently observed using extensive values such as mass or volume to classify and differentiate substances. Sorting through the

range of tests and experimental values students deemed appropriate for substance characterization would be useful for understanding how students' application of *tests and experimental values* shifts with training in chemistry. For example, Figure 4-3 below presents the distribution of codes for the question oxygen vs. carbon dioxide. The frequency of *tests and experimental values* thinking generally increases with grade level. Examining the distributions of CI thinking within each question and across grade levels can provide insight on the ways in which CI thinking progresses.

- Students' reliance on certain CI themes as props to support their primary reasoning might also contribute to a learning progression for chemical identity thinking. Students at the upper levels tended to use more props per response than students at the novice level (see Table 4-20), suggesting that with training in chemistry, students are able to incorporate more chemical identity themes into their arguments. It has also been observed that students at advanced levels prioritized using *composition and structure* and *experimental values and tests* as props over other CI themes. Investigating how students used these props in their reasoning can help characterize how sophistication of CI thinking and argumentation progresses.
- As mentioned previously, it is likely that context played a role in the chemical identity theme students relied on when answering the CSI Survey questions. Out of the sixteen questions in the CSI Survey, the responses to twelve of these questions were dominated by one CI theme. For these twelve questions, the one CI theme accounted for more than one third of the CI thinking in

student responses to that question. Not a single CSI Survey question showed evidence of all eight CI themes in the responses, and on average, five CI themes were observed in response to each question. This suggests that the contexts themselves limit the types of CI thinking that can be elicited. In turn, it is likely that the CI theme used for the primary argument prompted specific CI themes to be used as props. For example, students' responses to the water bubbles question primarily incorporated the *change* theme of CI thinking. *Class* was observed most frequently as a prop for this question, indicating that students might be prompted to think about *class* along with *change*. This relationship between CI themes and whether they were relied on for the primary reasoning or as props could further characterize a learning progression for chemical identity thinking.

Figure 4-3. Coding distribution for oxygen vs. carbon dioxide question



CHAPTER 5

PROBING THE RELEVANCE OF CHEMICAL IDENTITY THINKING IN BIOCHEMICAL CONTEXTS

Introduction

Biochemistry as an interdisciplinary field

Over the past decade, learning in biochemistry has been investigated by educational researchers through many different methods. Assessments have been developed for measuring the content knowledge of students before they enter upper level biochemistry and biology courses (Shi, Wood, & Martin, 2010; Villafaña, Bailey, Loertscher, Minderhout, & Lewis, 2011). Researchers have also investigated students' understanding of specific concepts, such as enzyme-substrate interactions, within biochemistry (Linenberger & Bretz, 2015). Other studies have characterized overall conceptual difficulties for biochemistry and biology students (Loertscher, Green, & Lewis, 2014).

Biochemistry has long been recognized as a discipline that integrates concepts from both biology and chemistry (AAAS, 2011; NRC, 2009; Wright, Provost, Roecklein-Canfield, & Bell, 2013). To perform well in biochemistry, students must

have a fundamental understanding of the concepts and practices comprising biology and chemistry. Many chemical concepts drive the phenomena and patterns observed in biochemistry; for example, the concept of inter- and intramolecular forces is presented in many general chemistry textbooks and is responsible for the behavior of protein folding, an essential phenomenon studied in biochemistry.

Despite an obvious link between chemistry and biochemistry, however, how students apply chemistry-specific concepts in biochemical contexts has only been investigated by a handful of researchers. Recently, Wolfson et al. (2014) have collected data on how well students transferred their understanding of energy from chemistry contexts (e.g. Gibbs free energy changes) to biochemistry contexts (e.g. energy flow in dynamic systems). Warfa and Odowa (2015) used creative exercises to investigate the links students made between a range of general chemistry concepts and biochemical contexts. Villafañe et al. (2011) designed a multiple-choice assessment to evaluate students' understanding of foundational concepts for biochemistry that come from the disciplines of chemistry and biology. Chemistry concepts included bond energy, free energy, dispersion forces, pH/pK_a, and hydrogen bonding. Haudek et al. (2012) focused on how students applied concepts of acid-base chemistry in biological contexts, and used computer software to analyze students' explanations about the behavior of biological functional groups.

Other instruments have been developed to assess student understanding of biochemical concepts, which can include concepts students previously learned in chemistry. For example, the Molecular Life Sciences Concept Inventory (MLS-CI) is one such instrument that was designed to measure students' understanding of ten "big

ideas” in biochemistry (Wright & Hamilton, 2008). These included some concepts that students are likely to learn in chemistry prior to biochemistry, such as energy and molecular structure. A diagnostic assessment was developed by Shi et al. (2010) for students entering molecular and cell biology classes, which contained concepts specific to the field of biology and biochemistry. These instruments, along with others not mentioned here, primarily target concepts that are unlikely to be encountered in chemistry contexts.

Evaluation of the chemical concepts students bring to their biochemistry courses and the ways in which students apply them could provide valuable insight to biochemistry instructors about their students’ chemistry knowledge. It may be beneficial for instructors to deliberately foster connections between previously learned chemistry concepts and new biochemical contexts; this support might encourage students to independently apply their chemical knowledge to biochemical contexts.

Studying chemical identity in biochemistry

The interdisciplinary nature of biochemistry implies that many chemical concepts are relevant to the contexts and phenomena explored by biochemists. Problems in chemistry and biochemistry share many of the same concerns, and the concepts and thinking applied in each discipline may overlap. Since chemical identity (CI) thinking is foundational for many concepts within chemistry (see chapters 2-4), the hypothesis driving this study proposes that CI thinking has major relevance in biochemistry. CI thinking encompasses the knowledge, reasoning, and practices that are relevant to classifying and differentiating substances. The study presented in this

chapter is an extension of the research on CI thinking presented earlier in this thesis, and does not propose to investigate all the facets of CI thinking within the context of biochemistry. The nature of the instruments presented in this chapter elicit CI knowledge only, and thus this chapter explores the ways and extent to which CI knowledge is consequential in biochemistry.

Guiding framework – Model of Educational Research

When considering challenges in science education, it is essential to consider both the science content itself and the educational practices for teaching the targeted science content. The model of educational research (MER) guides researchers in considering both educational research and practice, and proposes a model to investigate and transform science content so it can be taught most effectively (Duit, Gropengießer, Kattmann, Komorek, & Parchmann, 2012). The MER is divided into three components:

1. Clarification and analysis of science content
2. Research on teaching and learning
3. Design and evaluation of learning environments

The MER offers guidance on conducting research within each component to create a product that integrates science content and practice. Research within the first component analyzes and clarifies the targeted science content. This entails characterizing expert understanding of the science content in the context of its educational significance. The perspectives of many disciplines (e.g. philosophy of science, history of science, pedagogy) are often considered during research within the first component in order to identify the core concepts and guiding principles relevant

to the science content. As a result of this research, the expert perspective of the science content is established, which is generally more nuanced than the version of the science content understood by novices.

Research within the frame of the second component identifies the views of students and teachers regarding the science content. This can include difficulties students have learning the science content, their affective views regarding the content, and teachers' perspectives on how to evaluate students learning the science content. The learning processes and modes of instruction necessary for students to grasp the science content are also explored. Ultimately, learning sequences and activities for the targeted science content may be developed and evaluated based on the student and teacher perspectives.

The third component of the MER uses the results from components one and two to form the foundation for the design of learning environments for the targeted science content. Research carried out in this component identifies the key features necessary to learn the targeted science content based on the understanding of the science content developed in component one. These key features of the science content are then transformed for teaching, so that the research and teaching are seamlessly integrated to create a supportive learning environment.

The MER guides the design of the research presented in this chapter, and the study is divided into two parts corresponding to the first two components of the MER. Although learning environments for chemical identity in biochemical contexts were not explored as part of this study, this type of research corresponding to the third component of the MER can be carried out based on the results presented in this thesis.

It was necessary to establish the presence of a link between CI and biochemical contexts before designing and evaluating learning environments for the classroom.

The two parts of this study were completed sequentially. First, expert perspectives of CI within biochemistry were characterized, following the guidelines of the MER's first component. By determining the ways and contexts in which expert biochemists utilize CI knowledge, the relevance for students training to be biochemists can be identified. The second part of this research identifies how students view and utilize CI knowledge within biochemical contexts, and in doing so addresses the goals of the second component in the MER. This work is guided by the following research questions:

Overarching research question: In what ways is CI knowledge relevant in biochemistry problems?

- R1: In what ways do practicing biochemists deem chemical identity relevant in biochemistry problems?
- R2: How do students who are training to be biochemists use CI knowledge in biochemistry problems?

Research design and results

Research question 1 – use of chemical identity by expert biochemists

Data collection

Whether experts in biochemistry considered CI in their own work was investigated to determine if and how CI is relevant when solving biochemical

problems. To accomplish this, an online survey was designed and distributed to people who self-identified as practicing biochemists. Participants were encouraged to send the survey to other known biochemists, and in this manner the survey was distributed nationwide and internationally. The survey was kept anonymous, although basic demographic information was collected to ensure diversity within the participant pool.

The survey began by asking participants to give a brief description of their own research. This served to establish that the participants are experts in a wide range of biochemical areas, and not just focused on one area of biochemical research. Next, the survey provided participants with a brief definition of CI (see the Appendix for the complete survey) and asked whether they considered CI thinking to be relevant or useful for their own work. Following this question, participants were asked to provide an example of a problem in biochemistry they felt required CI thinking. This provided a perspective on CI through the lens of expert biochemists; how did they interpret CI thinking, and in what biochemical contexts did they perceive CI thinking as useful?

Results from expert biochemist survey

Thirty-four biochemists participated in this survey, and almost all participants (n=33) provided a summary of their own research. At the time of survey completion, the participants were pursuing a range of research interests: protein identification and purification, enzyme characterization, examination of biochemical pathways, and gene regulation, to name a few broad topics mentioned by participants. Although some research interests overlapped, for the most part, the participants were unique in

their research focus. Table 5-1 provides the general demographic information of the participant pool, showing that the participants come from different backgrounds.

Table 5-1. Expert biochemist participant demographics (N=34)

In the U.S.	In Academia
26	32
Outside of the U.S.	In Industry
8	2
Terminal degree(s): PhD Biochemistry, PhD Chemistry, PhD Molecular Biophysics, PhD Molecular Cell Biology	
Professional societies in which currently a member: ASBMB, ACS, AAAS, RNA society, ASM	
Journals frequently read for research purposes: Science, Nature, Journal of Biological Chemistry, Nature Chemical Biology, Nature Cell Biology	

A majority of the participants (n=27) provided examples of biochemical problems in which they considered CI to be relevant. In many cases, the examples involved the separation of components in a mixture and then identification of the molecule or protein of interest. Another common response was the classification of substances, either for the purpose of finding similar substances or for determining the properties of a specific substance of interest. In most cases, multiple ways of CI thinking were considered, such as using the composition and structure of substances in a mixture in order to separate them via a biochemical test. Some participants identified their research as clinical, and they stressed the importance of knowing the precise CI of the substances they work with when preparing drugs or medicines. For example, participant 4 commented:

Impurity identification is crucial in my job. It's important because to put a drug into people you need to know what's exactly in the vial. The way we do this is by making large amounts of our target molecule and then through

chromatography separate all the impurities and try to identify them through mass spec, sequencing, and bio-assay.

This type of problem seeks to answer the first core question of chemical identity: what is this substance? In this case, a major practice belonging to CI underlies the goal of this research: creating a pure product. Participant 21 provided another example of a biochemical problem that seeks to answer the first core question of CI, and said:

In discovering and elucidating new biochemical pathways we have on numerous occasions been faced with the task of identifying intermediates in the pathway. Knowing the identity of these intermediates is crucial to understanding the pathway as a whole and how it fits in to the overall metabolic network.

The participants also mentioned biochemical problems addressing the second core question of CI: how is this substance different from other substances? Participant 34 described a method for distinguishing proteins, and said:

In protein chemistry, in which you are expressing a recombinant protein in an expression system such as *Escherichia coli*, we must consider the chemical identity of the protein being produced, so that it can be distinguished from the background proteins of the expression system. To do this, we standardly utilize PAGE [polyacrylamide gel electrophoresis] analysis to assess by size, however it is important to also confirm this with enzyme assays (if an enzyme), mass spec analysis, or western [blot] analysis to be completely sure

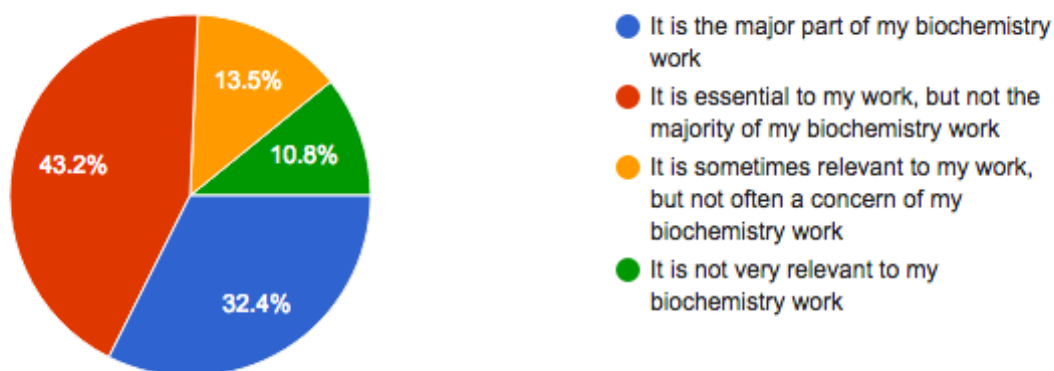
as different proteins could have the same mass, and therefore be indistinguishable on a PAGE gel.

Other examples given by the expert biochemists included determining the structure of proteins, the development of new biochemical analogs, and using enzymes to transform substances. The participants almost always included one or more experimental strategies for determining the CI of a substance, including mass spectrometry, gel electrophoresis, NMR, cell cultures, and other laboratory techniques. Based on the survey responses, it is clear there are many biochemical contexts where CI knowledge is relevant, and biochemists have a plethora of available methods to establish CI.

These and other examples provided by the expert biochemists gave an overview of CI in biochemical contexts. In most cases, the interpretations of CI made by expert biochemists coincided with the previously established understanding of CI thinking, which included both general CI knowledge and themes of CI practices (see Chapters 2 & 4). Out of the 30 examples provided by the participants, 21 examples (70%) contained at least one or more types of CI knowledge as defined by previous research. These responses supported the hypothesis that CI thinking is used by experts in biochemistry, and participant responses to the final, closed-ended question about the relevance of CI in their work (*To what extent do you consider answering questions of chemical identity to be significant in your biochemistry work?*) corroborated this conclusion. These responses are represented in the figure below.

The majority (26 participants, 76%) of the expert biochemists responded that questions of CI are either the major part or essential to their work as biochemists.

Figure 5-1. Responses of expert biochemists to question: "To what extent do you consider answering questions of chemical identity to be significant in your work?"



Research question 2 – chemical identity use by students studying biochemistry

Choice of creative exercises as an instrument for revealing use of chemical identity

To answer the second research question, an instrument was needed that could reveal whether students naturally use CI knowledge when thinking within a biochemical context. In the past several decades, many instruments have been developed to evaluate student thinking, but creative exercises best fit the requirements of this study. Creative exercises (CEs) were originally developed by

Trigwell and Sleet (1990) as an alternative assessment of the knowledge of students that could also benefit students' learning processes. Creative exercises present a context to students, who are instructed to provide a specific number of statements relevant to the context. Students are graded on the correctness and uniqueness of the statements. Trigwell and Sleet compared the effects of their creative exercises on student knowledge of acid/base equilibria to both traditional closed-ended problems and concept mapping. They discovered that students demonstrated they had the necessary content knowledge to successfully solve the closed-ended exam question and to relate specific, pre-identified concepts for the concept mapping task, but these same students did not successfully apply these concepts to the creative exercise. Trigwell and Sleet concluded that students are more easily able to apply previously learned content knowledge when the goals of the task are explicitly defined, and that creative exercises could be used to help foster students to make the connections between new contexts and previously learned content knowledge on their own. This, they hypothesized, would result in deeper learning.

Creative exercises have been recently used in chemistry (Lewis, Shaw, & Freeman, 2010; Ye & Lewis, 2014) and biochemistry courses (Warfa & Odowa, 2015) to assess what previously learned chemistry concepts students deem relevant to the "new" context of the creative exercise. Using creative exercises allowed these researchers to characterize the types of previously learned concepts students applied to new contexts. This use of creative exercises to capture the variety of linkages students make between content knowledge and new contexts inspired their use in this study. Previous studies have used gas laws, molecular shapes (Ye & Lewis, 2014),

thermodynamics, and enzyme kinetics (Warfa & Odowa, 2015) as contexts for the creative exercises to name a few examples.

Design of creative exercises

The first creative exercise (CE1) for this study mimicked a creative exercise designed by Warfa and Odowa (2015), where they presented the structure of an amino acid (glutamic acid) as the context. The study presented in this chapter used a dipeptide (glutamyl cysteine) as the context for CE1. The instructions provided for this first creative exercise were the same as those provided for the following creative exercises. CE1 and the other creative exercises designed in this study are included in the Appendix.

The contexts for the other three creative exercises designed in this study were derived from the problems or scenarios identified by the biochemistry experts as instances where they believed CI to be relevant. Using the expert responses to inspire the contexts ensured the creative exercises elicited CI relevant to biochemistry. Additionally, the contexts were designed to be broad enough so there were many acceptable responses; thus, any CI knowledge in students' responses was present because the students thought it relevant to the problem. Furthermore, basing the contexts on problems expert biochemists encounter in their own research provided authenticity to the creative exercises (Eilks & Hofstein, 2015).

The second creative exercise (CE2) presented the structures of two molecules: Molecule A is arachidonic acid and Molecule B is prostaglandin E1. Neither molecule was labeled, other than "molecule A" and "molecule B". This context was inspired by participant 8, who spoke about classification tasks in biochemistry:

We try to categorize enzymes into different reactive classes using a library of enzyme substrates where we vary the chemical reactive group on the substrates and then screen them against different enzymes to classify them into different chemical groupings.

It was anticipated that students would classify molecules A and B in addition to pointing out compositional features in the provided chemical structures. At the point when CE2 was implemented, students had already learned about fatty acid synthesis, metabolism, and hormones.

The third creative exercise (CE3) was derived from participant 28 describing the challenge of differentiating proteins and RNA molecules. This participant stated:

If a protein or RNA is the product of the reaction I'm studying then I need to prove that it was indeed synthesised. I routinely differentiate between protein and RNA molecules based on their chemical composition or physical properties, i.e. length, charge etc. Modern molecular biology techniques allow us to specifically label proteins and RNA with fluorescent markers so many times we prove chemical identity by following fluorescent signals.

DNA and RNA are commonly studied in introductory biochemistry, and thus students were expected to be familiar with these substances. The context for CE3 thus presented two solutions of DNA: one healthy and one damaged from UV radiation. No pictures or structures were provided.

The context for the fourth creative exercise (CE4) was inspired by the biochemistry expert responses about application of CI thinking for clinical research questions. Participant 21's comments about biochemical pathways and intermediates

(refer to page 136) along with other participants' responses about the transformation of biochemical substances prompted the use of acetaminophen excretion pathways as the context for the final creative exercise. Metabolism is a central topic in biochemistry, and students typically encounter examples of metabolic pathways early in the curriculum. CE4 presents three different excretion pathways for acetaminophen, each adding a different substituent to the original structure.

Implementation of the CEs

The creative exercises were implemented in a second-semester undergraduate biochemistry course. There were 27 students who completed at least 3 out of the 4 CEs, and these students were primarily biochemistry and chemistry majors. Although the creative exercises were timed so that they generally followed the presentation of biochemical topics relevant to the creative exercise (e.g. CE2 followed unit on fatty acids), it was expected that students would also respond with other previously learned chemistry knowledge. This study was designed for secondary data analysis (e.g. data were blinded by an external researcher before data were analyzed), and upon review of the study design, IRB determined that approval was not needed for data collection.

CE1 served to familiarize students with the format and expectations of creative exercises. It was implemented as an online homework assignment, and students received feedback on the quality of their statements in addition to their grades. Since this was the first encounter students had with creative exercises and because it was given as a homework assignment and not in class, the responses to CE1 were not used for data analysis. Furthermore, Ye and Lewis (2014) have established that CEs administered outside of class are not as valid because the

environment is less controlled. The other three CEs were implemented during class time as announced quizzes. The topic of the CE was not released prior to implementation, and students were given five minutes to respond to the CE. This format corresponds to other published research using creative exercises (Warfa & Odowa, 2015; Ye & Lewis, 2014).

For each CE, the author brainstormed a list of correct and relevant statements for which the students might receive credit. This list was checked by the professor of the biochemistry course, and immediately after the CEs were due this initial rubric was made available to students. The rubric was revised as the student responses were graded, and expanded to accommodate statements made by students that were not initially part of the rubric but fit the grading criteria. The final rubric was made available to students with their grades for each CE. The average scores for each CE are listed in Table 5-2. These averages are based only on the scores of those students who completed the CEs.

Table 5-2. Average scores for creative exercises

Average	CE1 – dipeptide	CE2 – fatty acids	CE3 – DNA	CE4 – acetaminophen
Score	4.4	4.5	4.3	4.3
Percentage	88%	89%	87%	86%

Analysis of creative exercise data

When the student responses to the creative exercises were graded, each statement made by the student was categorized by the generic statement it fell under on the rubric (regardless of whether the statement was correct or incorrect) or as irrelevant (not related to the context, no credit received for these statements). The

rubrics were thus a comprehensive collection of the knowledge students brought to the CEs. The rubrics for CE2, CE3, and CE4 were then coded by two researchers for the presence of CI knowledge. Each researcher coded the rubrics independently before discussing the codes, and agreement on the coding for each statement was reached. The statements not coded as belonging to CI were identified as structure-property relationships (another disciplinary crosscutting concept, see Chapter 1) or not relevant to either CI or structure-property relationships. When the CI knowledge included in statements made by students was examined, the CI knowledge was disregarded if only one student provided a statement relevant to that specific theme of CI knowledge. Thus, a minimum of two students was needed to contribute statements to a specific theme of CI knowledge for it to be considered relevant for that creative exercise.

For students to complete the creative exercises successfully, they were required to provide correct, relevant, and unique statements in response to the prompt. The creative exercises did not specifically ask students about the chemical identities of the substances presented in the prompts, as this would have violated the open-ended nature of the creative exercises. Because students were only asked to provide statements, it was unlikely that students would provide full arguments related to chemical identity in response to the creative exercises. Thus, in lieu of chemical identity thinking, the general CI knowledge was identified that could form the basis of an argument about chemical identity (e.g. be used in the practice of classifying and differentiating substances) when coding for the presence of CI. This was largely guided by the themes uncovered by previous work on CI (see Chapter 4). Although

this does not capture students' chemical identity thinking intact, the creative exercises do reveal the CI knowledge students have at their disposal for arguments about CI.

Results from creative exercise data

Although CI knowledge was found in each of the rubrics accompanying the creative exercises, the range of CI knowledge was limited. The CI theme corresponding to each statement that contained CI knowledge was identified. The CI themes observed in each creative exercise are outlined in Table 5-3.

Table 5-3. Chemical identity themes identified in creative exercise rubrics

Creative Exercise context	Chemical identity themes identified in rubric
CE2 – fatty acids	<ul style="list-style-type: none">• Composition and structure• Class• Function
CE3 – normal and damaged DNA solutions	<ul style="list-style-type: none">• Change• Composition and structure• Class• Function• Tests
CE4 – acetaminophen metabolism	<ul style="list-style-type: none">• Source• Composition and structure• Function

For every creative exercise, more than half of the statements on the corresponding rubric were coded with one of the chemical identity themes. The prevalence of each CI theme in the creative exercise rubric can be found in the first column under each creative exercise heading in Table 5-4. Each statement provided by students in their responses to the creative exercises was categorized by each unique statement on the rubric; this was used to determine how frequently students responded with statements related to CI and represented as counts, which was then used to calculate the percentage of the total count of statements made by students in

response to that creative exercise. These are located in the second column under each creative exercise heading in Table 5-4. For all creative exercises, more than half of the total statements provided by students were related to CI themes. These values are not indicative of the grades the students received for the creative exercise, as the researchers were more interested in what types of CI knowledge was elicited in the creative exercises rather than the scientific accuracy of the statements.

Table 5-4. Prevalence of CI themes in creative exercise rubrics

Chemical identity themes	CE2		CE3		CE4	
	Rubric statements (total = 28)	Student counts (total = 179)	Rubric statements (total = 42)	Student counts (total = 134)	Rubric statements (total = 42)	Student counts (total = 137)
Source					1 (2%)	5 (4%)
Change			3 (7%)	5 (4%)		
Composition & structure	8 (29%)	78 (44%)	12 (29%)	47 (35%)	11 (26%)	60 (44%)
Class	2 (7%)	25 (14%)	2 (5%)	8 (6%)		
Function	5 (18%)	15 (8%)	1 (2%)	2 (1%)	2 (5%)	5 (4%)
Experimental values & tests			6 (14%)	12 (9%)		
Structure-property relationships	7 (25%)	51 (28%)	3 (7%)	15 (11%)	15 (36%)	29 (21%)

Discussion

Observed CI themes in CE responses

Although six unique CI patterns of thinking were identified in the student responses (*source, change, composition & structure, class, function, experimental tests and values*), *composition and structure* represents the majority of the statements coded as related to CI. Out of the total number of unique statements (N = 112) that were included in the rubrics for the CEs, 31 statements were coded as related to the *composition and structure* theme for CI thinking. This represents close to 25% of the

total possible statements. In response to all three creative exercises, students provided 450 statements. Out of the students' responses, 185 of the students' statements belonged to the 31 rubric statements coded as *composition and structure*. This represents approximately 41% of the students' responses.

The prevalence of statements related to *composition and structure* indicates that students regarded *composition and structure* as relevant for the biochemical contexts provided in the creative exercises. In CE2 and CE4, molecular structures were provided as part of the context. This might contribute to the greater prevalence of student responses related to this theme; although each CE had a similar percentage of possible *composition and structure* related statements that could receive credit (29%, 29%, and 26% respectively), the percentage of statements provided by students corresponding to the *composition and structure* statements were higher for CE2 and CE4 (44% and 44% vs. 35%). The statements coded as *composition and structure* included general observations about the substances or molecules presented in the CE context, such as mentioning the degree of unsaturation and location of the double bonds for the fatty acids in CE2 or identification of the types of functional groups attached to the benzene ring in CE4.

The presence of the chemical structure in the context was not necessary to elicit *composition and structure* statements, however, as evidenced by the responses to CE3. Statements involving *composition and structure* for CE3 included those noting the different units that make up DNA (base + pentose sugar + phosphate group) and descriptions of the types of bonds that form between base pairs as a result of DNA damage. Students were not provided with any images or structures related to

DNA, nor did the context indicate that the UV radiation impacted the composition or structure of the DNA. Thus, the overwhelming presence of *composition and structure* ideas in students' responses to the creative exercises appears to indicate that students have little trouble linking *composition and structure* to biochemical contexts. The composition and structure of molecules and macromolecules is discussed frequently throughout a typical biochemistry curriculum, with some textbooks (e.g. Lehninger) bringing up these concepts as early as the introductory chapter. This is in contrast with the results from the CSI Survey, where *composition and structure* concepts were observed in only 6.8% of the dataset, indicating one potential difference between CI thinking in the discipline of chemistry vs. biochemistry.

Function was the only other chemical identity theme observed in all three of the creative exercises. It appeared most frequently in CE2, representing 18% of the rubric statements and 8% of student responses. In CE3 and CE4, its representation was low, with 5% or fewer of both the rubric and student statements coded as related to *function*. In responses to the CSI Survey, the function of a substance was generally linked with the purpose of an object or material that the substance is a component of; thus, it is typically associated with the macroscopic level of substances. The majority of the substances in the CSI Survey were presented on the macroscopic level, and students were observed to reason about features observed at both the macro and micro level. The substances in the creative exercises (fatty acids, DNA, acetaminophen), however, are generally described at the microscopic or molecular level, and were more frequently represented at this level in the contexts. The meaning of function for a substance might vary when considered at the molecular level, and the idea of

function in biochemistry is likely to be tied to microscopic processes. For example, one of the rubric statements for CE2 coded as function was “Molecule A is used in phospholipids and in cell membranes, molecule B is a type of hormone used in signaling pathways.” This statement directly links the molecules in the context to their purpose in biological systems.

The other statements coded as *function* in CE3 and CE4 related to the function of DNA as the genetic code for living organisms and the use of acetaminophen as a pain reliever. These are generally accepted definitions or uses of these two substances, but few students included these statements about function in their responses. There are a number of reasons that might explain why students did not include these statements. First, at this level in their undergraduate education, the biochemistry students might be trained to look beyond the more obvious usage or function of substances. *Function* thinking was more commonly observed in the CSI Survey in response to questions where the substance might be encountered in daily life (e.g. caffeine and chlorophyll). Secondly, as mentioned previously, certain patterns of CI thinking might be tied to features of the context. The CE contexts could be construed as related to biochemistry content discussed in the course, especially since the CEs were implemented as part of the course assignments, but the contexts in the CSI Survey were not obviously tied to science courses or school knowledge. The class during which students participated in the CSI Survey was often a science course, but the contexts themselves did not indicate science or chemistry knowledge was needed to answer the questions. Thus, ideas related to *function* might be perceived as more

relevant for non-science contexts, and when encountering contexts perceived as related to science students might draw on CI knowledge other than function.

Ideas related to the CI theme of *class* appeared in CE2 and CE3. Students frequently placed each of the molecules presented in CE2 into a class (fatty acid, eicosanoid). This statement, coupled with noting that Molecule A is the precursor for Molecule B, encompassed 14% of the statements students provided in response to CE2. In CE3, statements related to *class* only accounted for 5% of the rubric statements and 6% of the student statements. These statements involved classifying the type of linkages formed in the DNA and the class of enzymes responsible for repair. Classifying molecules and proteins and understanding the precursors needed to build biomolecules is an important task in biochemistry, as evidenced by expert responses. Experts commented on identifying the class of an unknown molecule and differentiating classes of molecules as a type of task in biochemistry they encounter in the field.

The themes *change* and *tests and experimental values* appeared in student responses to CE3. For *change*, students commented on what happened when the UV radiation interacted with the DNA. Their focus on characterizing the process (e.g. the DNA is chemically altered) prompted these statements to be coded as the *change* theme of chemical identity thinking, and represented 7% of the rubric statements and 4% of statements made by students. The statements coded as *tests and experimental values* were the second most frequent CI theme present in CE3, at 14% of the rubric statements and 9% of the students' statements, and all involved using different laboratory techniques to separate and identify the normal vs. damaged DNA. The

ways in which students utilized these different tests is similar to the ways in which more sophisticated students suggested using laboratory instruments (e.g. mass spectrometry) to identify the substances in the CSI Survey. Students who spoke about laboratory instruments were primarily in the organic chemistry and physical chemistry courses, which means they were at a similar level of education (e.g. 2nd, 3rd, and 4th year university) as the students in the biochemistry course. The relatively low presence of *tests and experimental values* in responses to the CEs suggests that when students are not specifically asked to identify and differentiate substances (as they are in the CSI Survey) they are unlikely to talk about these types of methods.

The *source* theme was only observed in student responses to CE4, and its frequency was low in comparison to the other observed themes (2% of the rubric statements and 4% of students' statements). The one rubric statement corresponding to *source* noted that acetaminophen is a component of or can be found in drugs. This was likened to statements made by students in the CSI Survey who talked about chlorophyll being located in plants and caffeine found in coffee. Relating a substance to the mixture and/or object it is typically encountered in *without* referring to its purpose or function within that mixture/object is a way of thinking about source. Although there was only one statement on the rubric that referred to *source*, five separate students provided statements that fell within this category. Something about the context of CE4 triggered students to consider *source* in this creative exercise and not the others; possible triggers include familiarity with this compound outside of biochemistry and the fact that this was the only substance presented in the creative exercises that is exogenous to the body. Students are less likely to encounter

arachidonic acid or DNA in commercial products, which may have prompted them to draw on their biochemistry knowledge instead.

Although six unique CI themes were observed in students' responses to the creative exercises, *composition and structure* ideas were more prevalent than the other themes. No theme dominated the responses in the CSI Survey to the same extent; the theme *tests and experimental values* was observed most frequently in the data (25% of student responses). These trends may be linked to the context of the problem, the targeted discipline (chemistry or biochemistry), the emphasis of the biochemistry curriculum, or a combination of these variables. Further studies would be necessary to determine if *composition and structure* is a more dominant CI theme in biochemistry as compared to chemistry, and whether the specific substance under question influences the type of CI thinking elicited. The emphasis of certain CI themes in the biochemistry textbook and in biochemistry courses can be investigated to see if they have an effect on what students perceive as relevant when solving problems in biochemistry.

Explaining the presence of CI knowledge

Although there were eight themes of CI thinking revealed from the responses to the CSI Survey, the creative exercise responses did not elicit the same range of CI knowledge. A variety of reasons might have contributed to this outcome. The first is that even for the CSI Survey, not every set (four sets, A, B, C and D were designed and implemented) elicited all eight themes of CI thinking (only sets A and C did). Thus from previous work and from these creative exercises, it can be inferred that the types of CI knowledge observed is in part linked to the nature of the context. This is

not surprising, as CI thinking encompasses a wide range of practices, and it is unlikely they will all be applicable to every problem in chemistry or other interdisciplinary problems. If a response based on one way of using CI is satisfactory for the problem at hand, there is no need to provide additional CI thinking. Additionally, every context will have certain features that are likely to be more salient than others, and students and experts are more likely to respond to those obvious cues. These cues are dependent on the nature of the problem.

Secondly, it is likely that certain types of CI thinking are more relevant for problems in biochemistry than others. The majority of the examples provided by the expert biochemists utilized *composition and structure*, *tests and experimental values*, or both. The prevalence of *composition and structure* in expert responses reinforces the claim that this theme of CI thinking might be more relevant in biochemical contexts than the general contexts in the CSI Survey.

The presence of *tests and experimental values* in expert biochemists' responses might be attributed to the design of the survey. Participants were explicitly asked how they would identify and/or differentiate substances in their example biochemical problem. The creative exercises, on the other hand, did not explicitly direct students to consider identification and differentiation of substances, which might explain the lower presence of this theme in students' creative exercise responses.

Finally, the creative exercises were not designed to elicit the broadest possible range of CI knowledge and thinking. However, this was a goal of the research using the CSI Survey, so the questions in the CSI Survey were specifically designed to

uncover as many types of CI thinking as possible. The creative exercises, in contrast, served to determine if students would naturally respond with CI knowledge to the given biochemical contexts, thus establishing a link between CI and biochemistry.

Additional insights gained from coding creative exercise data

Coding the creative exercise data also served to further refine the definition of chemical identity. It became clear that there is a similar concept of chemical identity that is unique to the discipline of biology or biochemistry (perhaps both). This way of characterizing substances might be called “biochemical identity” in future research, and was exhibited when students classified substances based on biological classes (e.g. types of cells) or identified molecules by the specific role they exhibit in a biological or biochemical pathway (e.g. repair enzyme). These statements were coded as not relevant for chemical identity, but do indicate the possibility of discipline specific interpretations of substance identity.

Structure-property relationships (SPR) were also observed in students’ responses to the creative exercises (>10% of students’ statements for each CE, see Table yyy). Both CI and SPR involve noticing a feature of a substance or molecule, but this way of thinking transitions to SPR when a property of the substance is attributed to the noticed feature. For example, one of the statements students received credit for in response to CE4 about acetaminophen metabolism was: “The added substituents all increase the polarity of the acetaminophen.” Noticing that substituents have been added to the acetaminophen and commenting on the types of substituents that were added relates to CI, whereas noting that these substituents increase the acetaminophen’s polarity relates to SPR. SPR was also noticed in expert responses

about examples of chemical identity (e.g. enzyme activity in relation to its active site), and clearly plays a large role when solving problems in biochemistry. The SPR identified in the creative exercises was not differentiated in the same manner as the CI themes, as the goal of this study was to understand and characterize the application of CI knowledge.

Limitations and future work

Due to the nature of the creative exercises, it is impossible to know why students thought their statements were relevant to the context of the exercise, or in what ways students would use the knowledge they presented in these creative exercises. Students were rewarded for providing relevant and correct statements, and were not required to justify them. Open-ended questions that ask for justification or cognitive interviews could be used to probe student reasoning for linking specific chemical identity concepts to the provided biochemical contexts.

Although expert biochemists were surveyed to collect biochemical scenarios in which chemical identity concepts would be used, the creative exercise rubrics were developed based on student responses alone. This resulted in a lack of variety of expert biochemical ideas with regard to the types of CI knowledge that might be applied to the creative exercise contexts. The observation of *composition and structure* ideas used in conjunction with *tests and experimental values* in expert biochemists' survey responses indicates there are other relationships between CI themes that were not captured in either the CSI Survey data or CE data. To gain a better understanding of the range of responses possible for these creative exercises, they should be administered with expert biochemists as well as students.

The model of educational reconstruction is not meant to be followed in a linear sequence of steps. Future studies can build from the research in this study and might repeat the first (clarification of science content) and second (research on teaching and learning) components to further refine the concept and use of CI in biochemistry and the characterization of student and teacher perspectives on CI thinking. During this process, learning activities and environments promoting learning about CI within the space of biochemistry can be constructed and tested, and can in turn inform future studies falling within the first and second components.

Conclusion

The survey of expert biochemists and analysis of student responses to the creative exercises illustrate the ways in which CI knowledge is relevant to biochemical contexts. Certain CI themes, such as *composition and structure* and *class*, occur more frequently than others. Based on these observations, students may need more assistance linking some themes of CI knowledge to biochemical contexts than others. Instructors can use the creative exercises to determine what themes of CI knowledge their students do not link to biochemical contexts and then facilitate students' linkages of previously learned concepts to new problems in biochemistry. Creative exercises can also be used to reward students for linking previously learned content knowledge to new contexts.

Examining the themes of CI thinking in the context of biochemistry has added depth to the existing understanding of the themes. It is useful to consider them from another discipline, as this study demonstrates that CI knowledge is relevant outside of the field of chemistry. This helps provide a more comprehensive understanding of

chemical identity thinking, and suggests that there might be other unique ways of characterizing substances in other disciplines. Future work can explore these other discipline-specific ways of investigating the identity of substances, and determine what themes of CI knowledge are more relevant for the discipline of biochemistry than others.

CHAPTER 6

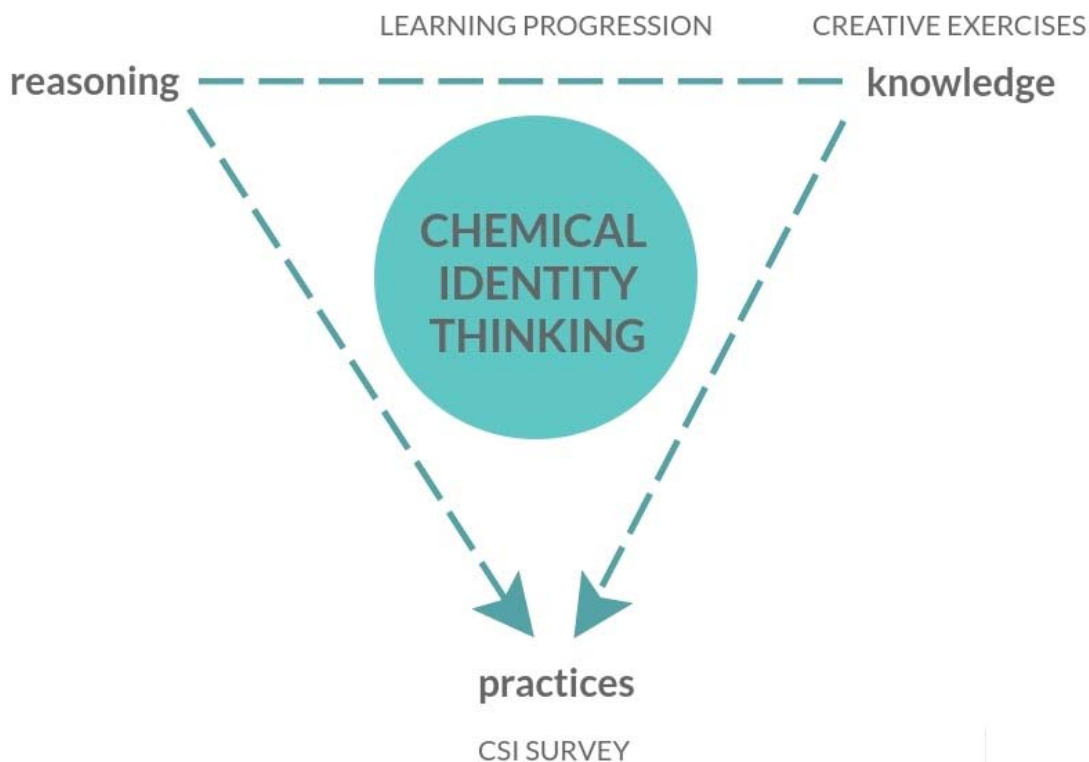
IMPLICATIONS AND CONCLUDING REMARKS

Summary of findings from chemical identity research

Chemical identity thinking is comprised of the knowledge, reasoning, and practices necessary for classifying and differentiating substances. The practice of CI generally incorporates both CI knowledge and reasoning. These facets of chemical identity thinking and their relationships are illustrated in Figure 6-1.

Chemical identity is a crosscutting concept in chemistry, and CI thinking was investigated via multiple perspectives. The literature review characterized CI thinking as a whole, along with assumptions that may be guiding and constraining CI thinking. A hypothetical learning progression regarding students' conceptions of substance and CI thinking was proposed based on the existing research explored in the literature review. The CSI Survey data analysis revealed eight common themes in how students classified and differentiated substances, or the practice of CI. Lastly, the relevance of CI knowledge was explored through a survey of expert biochemists and the use of creative exercises with biochemistry students.

Figure 6-1. Components of chemical identity



Chemical identity from the literature

The review of the literature revealed and generated a deeper understanding of several potential assumptions guiding chemical identity thinking and patterns in ways of thinking about substances. These are captured in Figure 2-1, the hypothetical learning progression for CI, presented in chapter 2. The different conceptions of substance, listed in row (a), range from substances as classes of stuff to substances as discrete units with composition and structure. These conceptions of substance influence the properties students choose to classify and differentiate substances, as outlined in row (b). The patterns in these ways of thinking about substances and CI have been loosely grouped into four major ways of thinking (*objectivization*,

principlism, compositionism, and interactionism) for the hypothetical learning progression. The different assumptions that guide chemical identity thinking have also been organized based on the ways of thinking they are likely to be associated with. These assumptions provide insight both into students' conceptions of substance and their CI thinking.

Chemical identity from the CSI Survey

Students' responses to the CSI Survey were analyzed for how they identified and differentiated substances and eight themes related to the practice of CI were uncovered. These eight themes (*change, class, composition & structure, function, organism effect, sensory information, source, and tests & experimental values*) represent the common patterns in how students classified and differentiated substances in response to the CSI Survey. Some themes were observed more frequently than others (e.g. *tests & experimental values*), and it is likely that the context of the question influences the CI themes observed in student responses. All themes were present in all educational levels, however, indicating that there likely are varying degrees of sophistication of thinking about CI within each theme.

Chemical identity in other disciplines

As a foundational disciplinary crosscutting concept in chemistry, CI thinking is necessary for solving many chemical problems. CI thinking is also relevant for the general public, and is important for the many types of daily decisions that involve substances. Because of its foundational nature, it was hypothesized that CI is relevant for solving problems in biochemistry, which is an interdisciplinary field. Research tested this hypothesis from the perspectives of both expert biochemists and

biochemistry students, and found that there is a range of ways that these participants considered CI to be relevant. The CI themes *composition & structure* and *tests & experimental values* were observed most frequently in the data. For this study as well, it is likely that the contexts played a role in prompting the specific CI themes to emerge; however, the overwhelming presence of these two particular themes suggests that they might be more relevant than the others for biochemical problems.

A construct map for concepts of substance and chemical identity

Components from the literature review and the recent work investigating CI thinking have been used to create the construct map presented in Table 6-1. This construct map proposes revised types of student thinking (intuitive, transitional, normative), conceptions of substance, and CI thinking from the hypothetical learning progression for CI proposed in chapter 2. These revisions are based on additional literature and the analyzed CSI data that followed the initial literature review for chemical identity.

Student thinking that involves intuitive reasoning is more likely to correspond to the hypothesized *objectivization* way of thinking. The intuitive conceptualization of substance, classes of stuff, has similarities to the early perspective of the four natural kinds that constitute substances (Ball, 2004). Thinking about substances only at the macroscopic level can lead to conflation between object and material. This macroscopic perspective lends itself to differentiation based primarily on explicit properties, and student thinking about chemical identity is guided by *historicality*, *surface similarity*, and *functional usage* assumptions.

Maturing from the intuitive to transitional level may involve students recognizing the difference between material and object and the limits of explicit properties for determining chemical identity. At the transitional level, substances are conceived as made of constituents that provide specific properties (*principlism*) or as constituents with specific chemical composition (*compositionism*). This type of thinking is similar to Ellis' argument of essentialism (Ellis, 2002), where elements or other components contribute the essential properties of the substance. The components and their essential properties are the features students use to differentiate substances, and thus they are more likely to rely on intensive explicit properties and/or the composition of a substance when considering the chemical identity of a substance. Several assumptions might be most likely to guide and constrain student thinking about substances and chemical identity, including *additivity*, *substantialism*, and *elementalism*.

Progressing from a transitional level to a normative level may require students to start thinking about the organization of substance components and the interactions among different types of particles at various scales of distance and time. Students no longer just view substances as made of parts, but rather think of substances as made of components with specific structures. This relates to the microstructure argument of substance, where the composition and structure of individual components within a substance dictates identity (Bursten, 2014; Ellis, 2002). Once the value of structure has been recognized, students can also move to thinking about the interactions between substances and their emergent behavior (Luisi, 2002; van Brakel, 2000; VandeWall, 2007). At the normative level, students can fluently shift between the

submicroscopic level (e.g. molecules, ions) and other levels of organization (e.g. structure of molecules, collection of molecules in a system). Students differentiate substances based on their composition and structure in addition to their emergent behavior. Assumptions that are likely to guide thinking within this level include *emergence* and *structuralism*.

Table 6-1. Chemical identity construct map

(What is this stuff? How can I tell it apart from other stuff?)

<p>Normative Thinking <i>Interactionism:</i> Substances are dynamic entities within a system that can interact with each other to produce specific behavior of substances</p>	<p>Concept of substance Substances are comprised of particulate units (molecules, ions), with specific composition and structure, within which there may be other levels of organization (e.g., atoms connected in specific ways within molecules, tertiary structure in proteins).</p> <p>Differentiating properties Differentiation is based on molecular composition and structure.</p>	<p>Assumptions <i>Emergence:</i> Stable properties emerge from dynamic interactions among components that occur at submicroscopic scales.</p> <p><i>Structuralism:</i> Interactions occur at submicroscopic scale between structural components, giving rise to properties at larger scales.</p>
<p>Threshold concepts:</p> <ul style="list-style-type: none"> • Fluid consideration of individual units (molecules, ions, unit cells) with deterministic behavior and dynamic interactions with probabilistic behavior • Recognition of affordances and limitations of different models, and predictions based on simultaneous consideration of different models 		

<p>Transitional Thinking <i>Principlism:</i> Properties of matter are due to the presence or absence of principles, which can be removed or added without altering the identity of a substance. These principles are responsible for behavior or properties.</p>	<p>Concept of substance Materials are considered to be constituents of objects. These constituents contribute specific properties.</p> <p>Differentiating properties Differentiation is based on explicit properties considered to be intensive.</p>	<p>Assumptions <i>Additivity:</i> Perceivable properties are the result of weighted average of properties of individual components.</p> <p><i>Substantialism:</i> Components of the substance are responsible for some properties, homogeneous substances are considered mixtures of components when convenient and considered single substances under other circumstances.</p>	<p>Transitional Thinking <i>Compositionism:</i> Tendency to cue on explicit differences of composition of a substance or material to the exclusion of structure, strong association between representational features and characteristic properties or types of materials.</p>	<p>Concept of substance Substances are considered as constituents of materials, and they have specific chemical composition. Substances can have different arrangements of particles.</p> <p>Differentiating properties Symbolic (e.g., chemical formulas) and iconic (e.g., drawings of particles) representations of substances allow for differentiation. Names and chemical formulas provide information about components of substances that helps to identify classes of substances.</p>	<p>Assumptions <i>Elementalism:</i> Substances are static objects made of small parts with fixed properties and structures.</p>
<p>Threshold concepts:</p> <ul style="list-style-type: none"> • Material kinds are the constituents of objects • Differentiation between properties of a material and properties of an object <ul style="list-style-type: none"> ○ Recognition of intensive properties for categorization • Perception has limits, experimental testing is useful 					

<p>Intuitive Thinking <i>Objectivization</i> of substances: use of object-relevant properties to classify substances</p>	<p>Concept of substance Materials are considered as distinct classes of stuff. Materials and objects may be indistinguishable.</p>	<p>Assumptions <i>Historicality</i>: Origin and past history determine identity. The identity of a substance is conserved through changes.</p>
	<p>Differentiating properties Differentiation is based on explicit properties without distinguishing intensive vs. extensive. Classes of substances are formed according to what something does or can do (e.g., its use or appearance)</p>	<p><i>Surface similarity</i>: Appearance determines identity, especially tactile features such as shape, color, texture, and smell.</p> <p><i>Functional usage</i>: Actions and uses determine identity of a substance or material. Substances with similar functions are assumed to have similar characteristics.</p>

Future research will incorporate the CI thinking within the eight identified themes of CI practice presented in chapter 3 of this thesis into the construct map. Every CI theme was observed to some extent in every education level surveyed, which indicates there may be varying degrees of sophistication within each theme corresponding to educational level. This means that the CI thinking driving the themes of CI practice could be present at every level within the current construct map, but might be guided by different assumptions at each level. Investigating the progression of student thinking within each theme will reveal possible levels and assumptions associated with that theme of CI practice.

It is likely that the assumptions that will be revealed that guide thinking within each CI theme will intersect with students' conceptions of substance. Students' conceptions of substance (what they think substances are) influence their CI thinking (the classes of substances that can exist and the cues that can be used to differentiate these classes). The interactions between concept of substance and CI have already been observed in students' responses to the CSI Survey. For example, some students answered that the silver earring is a different substance after being left out for a period of time because the appearance of the earring is different (transformed to a dark, black substance). The cue these students focused on to differentiate the earrings was appearance, which was guided by a *surface similarity* assumption. This manifestation of CI thinking is influenced by the conceptions of substance held by these students. Students who answered this way likely conceptualized substances as objects that have properties (*objectivization*) and thus considered appearance to be a property of the silver earring that can be used to determine chemical identity.

Further exploration of the intersections between conceptions of substance and CI will refine the existing construct map. Additional examples of these intersections can provide a better understanding of how students apply their notions of substance and CI, which can be analyzed for a progression of sophistication.

Implications for teaching

Value of the CSI Survey for teaching

Discussions with teachers about the CSI Survey and the types of data produced led to the conclusion that this survey is best suited as a tool for uncovering student thinking rather than assessing chemistry content knowledge. In other words, the open-ended nature of the questions elicited many ideas, so the pilot responses and the teachers' expectations of how their own students would respond were not easily evaluated for sorting whether students understood particular chemistry topics (e.g., stoichiometry, types of bonding, particulate nature of matter). Rather, the teachers and researchers agreed that the structure of the survey would prompt students to reveal chemical thinking, i.e., their reasoning and problem solving using chemical knowledge (Sevian & Talanquer, 2014). Because there are multiple sets, the CSI Survey could be used at different points in a unit or a year to assess progress students make in their chemical thinking. The use of the CSI Survey is not restricted to teachers using the Chemical Thinking curriculum (Talanquer & Pollard, 2010); other reform-based chemistry curricula, such as the IQWST curriculum (Krajcik, Reiser, Sutherland, & Fortus, n.d.), also include concepts related to CI in their units. As described previously, however, CI thinking is foundational in many aspects of

chemistry (e.g. nomenclature, see Table 3-1 for additional examples). Thus, the CSI Survey can be used as an activity to assess CI thinking within many curricula that may not specifically target CI knowledge.

The teachers consulted during the CSI Survey development emphasized the importance of using data collected from the implementation of this instrument to design rubrics and scoring guidelines. This will allow teachers to utilize this instrument with their classes and then easily interpret student responses. These will be developed once the learning progressions within each CI theme have been analyzed, so that the rubrics can be empirically validated and incorporate the findings from the large-scale implementation of the CSI Survey. A rubric with instructions for interpreting the most common student responses to the CSI Survey has been included in the Appendix, along with examples of student responses.

Outside of diagnosing chemical thinking, open-ended assessments like the CSI Survey offer a range of benefits. Students, as well as teachers, are often uncomfortable with open-ended questions where there is not one single correct response. Use of this instrument could allow students practice with applying their chemistry knowledge in ways they are not familiar, and can send a meta-message (Roberts, 1982) to students that there are many ways chemistry can be applied to answering authentic questions. Teachers need to respond to the disciplinary substance of students' thinking (Coffey, Hammer, & Levin, 2011). Doing so requires eliciting a variety of ways students might think in a chemical context so that teachers can make sense of it in order to make instructional decisions (Robertson, Scherr, & Hammer, 2016). This dependency creates a critical path task, in that allowing teachers to be

more responsive to their students' thinking depends on having classroom formative assessment tools that can expose this thinking.

Implications of chemical identity themes for teaching

Knowing that students can exhibit different ways of thinking about chemical identity can be useful for instructors. The eight themes can be used to characterize the different ways students are applying chemical identity thinking when solving problems in chemistry. Students may exhibit a tendency to rely on one way of thinking about CI, which can inhibit other more advanced ways of considering CI from being considered. Instructors can provide feedback to students on the appropriateness of the CI thinking they have applied in their reasoning, and expose students to additional ways of solving problems while considering CI.

The CI theme most commonly observed in students' responses was *tests and experimental values*. Since this is a popular way of classifying and differentiating substances, instructors can discuss with students the types of experimental values and tests that are appropriate for questions of CI. Many of these tests and values students are already familiar with, such as boiling point, density, and pH. Intensive properties such as these that can be reliably used to identify substances were called response properties in the hypothetical learning progression developed for CI thinking (see Figure 2-1). Allowing students to explore both physical and chemical response properties through experimentation can help students understand which response properties are appropriate for determining CI. Additionally, this establishes the necessity of analysis to determine the CI of a substance, and encourages students to use more than one CI theme in their thinking.

Based on the prominence of one theme over the others in students' responses to specific CSI Survey questions, it can be inferred that the prevalence of certain themes is context dependent. The link between context and student responses has been investigated by other researchers (Broman & Parchmann, 2014), and this dependence is likely present in students' CSI Survey examples. For example, it was noted that *composition and structure* thinking appeared more frequently in the CSI Survey questions corresponding to the second core question of CI (how is this substance different from other substances?). It appears that differentiation questions are more likely to prompt *composition and structure* thinking than classification questions. This dependence of CI thinking on context means that instructors may be able to predict the chemical identity themes students are likely to include in their responses. Additionally, instructors can create their own questions designed to uncover students' thinking within a specific theme to observe and help refine the range of students' ideas or to see if student thinking changes across the semester.

Implications of chemical identity for teaching and learning biochemistry

As indicated by the expert biochemists, CI knowledge is particularly relevant when learning about molecule and protein identification and separation, determination of intermediates in metabolic pathways, and biochemical laboratory techniques such as gel electrophoresis and liquid chromatography. From the responses to the creative exercises, it is apparent that the themes of *composition and structure*, *class*, and *tests and experimental values* are more prevalent than other themes of CI thinking in the biochemistry problems that were tested with the participants. Since these ways of thinking were not explicitly probed for by the

contexts, it can be inferred that students are more comfortable relating these chemical identity themes to biochemical contexts than others. Instructors may be able to increase how frequently students apply CI knowledge by explicitly linking it to the content covered in class.

The value of creative exercises greatly depends on how instructors make use of them. Creative exercises can serve as an activity to determine what previously learned chemistry knowledge students think is relevant to a new concept or big idea before moving on to a new unit. Creative exercises can also be used as an assessment to examine how students are linking material learned earlier in the course with new material. Instructors may also use creative exercises as an activity to promote students linking content material themselves, and by receiving credit for these linkages, students are rewarded for this type of learning behavior that connects previously learned material to new contexts picked by the instructor. The creative exercises designed in this study may be used for any of these purposes, in addition to assessing the themes of CI knowledge students bring forth to biochemical contexts.

Suggestions for building chemical identity thinking

A more gradual development of the notions students have of substance and chemical identity could result in a better understanding of these concepts. Two studies (Canac & Kermen, 2016; Voegelzang, van Berkel, & Verdonk, 2015) have indicated the importance of chemical language in relation to students' understanding of substance. Their findings indicate that students struggle with chemical language concerning substances and have markedly different interpretations of the words chemists use to infer meaning about substances (e.g. mixture, compound, molecule).

The instructional model proposed by Vogelezang et al. (2015) offers a gradual method for building student understanding about substances that allows them to empirically develop meanings associated with the chemical language used to talk about substances.

In order to incorporate CI into the traditional chemistry curriculum, instructors must deliberately foster the connections students make between substances and CI. There are many traditional chemistry concepts where CI can be naturally included (e.g. redox reactions, reproduced in Table 3-1 below), but instructors must direct students to not only explain and predict the properties of substances but to consider how these properties can be used to classify and differentiate substances. Providing opportunities for students to explore explicit extensive vs. intensive properties of substances and their utility in comparing and contrasting substances will help students independently determine which properties are useful for establishing CI. These activities can assist in illuminating the limitations of certain concepts of substance and certain types of properties, and in doing so can promote a shift in student thinking from *intuitive* to *transitional*. Guiding students to probe implicit properties and emergent behavior can facilitate moving students to *normative* thinking, where they have a systems-level understanding of substances. Simultaneously developing students' conceptions of substance and their knowledge of properties for differentiation will build a more cohesive understanding of substances and chemical identity.

Table 3-1. Examples of concepts in a typical chemistry curriculum where CI is relevant (reproduced from chapter 3)

Typical chemistry concept	Relevance to chemical identity
Acid-base reactions	When considering reactions, students must be able to classify substances as acids or bases in order to determine types of reactions and whether or not they will occur.
Intermolecular forces	To determine the types of intermolecular forces that might exist between substances on a molecular level, students must understand the chemical identity of a substance and be able to think in general terms about how the composition and structure (which are related to chemical identity) lead to the types of interactions that may exist between molecules.
Mixtures vs. pure substances	Most of the matter encountered in daily life is part of a mixture, and students in chemistry must first understand the differences between mixtures and pure substances in order to properly assign chemical identity. Mixtures are made of multiple substances with unique chemical identities, which can be used to separate and identify the components.
Nomenclature	In chemistry, nomenclature is used to reveal information about the identity of a substance. In order to properly assign nomenclature, students must first understand how to classify substances. For example, a substance must be first identified as ionic or molecular before it can be named.
Solubility	When asking questions of solubility, students need to classify substances (e.g. ionic vs. molecular) in order to determine whether a substance will dissolve in another substance, and to what extent.
Redox reactions	Chemical identity is involved when identifying oxidizing agents and reducing agents in order to decide what kinds of reactions might be possible with particular reagents.

Concluding remarks

This thesis has attempted to define and more thoroughly characterize chemical identity thinking. Existing literature on conceptions of substance and CI was used to produce a hypothetical learning progression for CI. The prior research was carefully used to inform the development of an instrument, the CSI Survey, which was

administered with 460 students at a range of educational levels with the intent of eliciting their CI thinking. The data collected using the CSI Survey were analyzed following established procedures for content analysis. This analysis revealed eight common themes (*change, class, composition & structure, function, organism effect, sensory information, source, and tests & experimental values*) for students' CI thinking in responses to the CSI Survey. These eight themes for CI thinking can be used to characterize students' CI thinking within the classroom, and instructors can help students to access productive ways of identifying and differentiating substances in different situations. Exposure to these themes of CI thinking can help students learn to determine the contexts where a particular CI theme is relevant, and instructors can help foster these connections by giving students opportunities to classify and differentiate substances. This thesis has provided a foundation for future research concerning students' conceptions of substance and CI, and next steps include the analysis of learning progressions within each theme of CI thinking.

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Appendix

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1. Expert feedback questionnaire (distributed as a Google Form)

Introduction:

This instrument is designed to probe the ideas of chemical identity students use from grades 8 through the end of college. Chemical identity encompasses the concepts associated with identifying and differentiating substances. Each item in the instrument seeks to answer one of the two core questions associated with chemical identity: 1. What is this substance? 2. How is this substance different from others? By collecting data with the instrument when it is fully developed, we seek to elucidate students' ideas about chemical identity and determine how those ideas are used in student reasoning. We expect that students' chemical identity ideas will change with increasing chemistry education, based on our hypothesis of a chemical identity learning progression that we recently published (Ngai, Sevian & Talanquer, 2014).

1. Approximately how long did it take you to complete this instrument?
2. Which question was the easiest to answer? Why?
3. Which question was the most difficult to answer? Why?
4. Was the phrasing of any of these questions confusing? If so, how might it be improved?
5. What chemistry knowledge or expertise did you draw on to answer these questions?
6. Do you have any recommendations for alternative substances that can be used or alternative questions to ask?
7. Do you have any other suggestions to improve this instrument?

2. CSI Survey Sets

CSI Survey Set A

1. Your friend's favorite earring is made of a light gray metal. How would you be able to determine if this is silver? Please explain your response.

2. Your friend's mother tells you this earring is made of pure silver. Your friend accidentally lost her earring and you found it a few months later. You noticed that it was no longer shiny and that it was now a dark gray/black color. Is the earring still made out of silver, or is it a different substance? Please choose your response below.

_____ Still Silver

_____ Different Substance

Please explain your response. What evidence do you have that the earring is made out of silver or a different substance?

Is there any further information you would like to know in order to make a decision? If so, what is it? How would this information help you make a decision?

3. You have been assigned a school project where you have to explain what chlorophyll is to other students in your class. You decide to create a poster that has the title: "What is chlorophyll?" What would you put on this poster, and how would it help you explain what chlorophyll is to the other students?

4. Chlorophyll can be isolated from the leaves of a tree growing in the forest and from algae growing in a pond. Is the chlorophyll from the leaves of the tree the same or different as the chlorophyll from the algae in the pond? Please choose a response below.

_____ Same _____ Different

Please explain your choice. What evidence do you have that the chlorophylls are the same or different?

Is there any further information you would like to know in order to make a decision? If so, what is it? How would this information help you make a decision?

CSI Survey Set B



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1. You have a cup of an unidentified liquid in front of you. How would you determine whether or not this is water?

2. You heat a pot of water over a stove and it begins to boil. What is in the bubbles that are rising to the surface?

Please justify your response. How do you know what is in the bubbles?

Is there any additional information you would like to know in order to determine what is inside the bubbles? If so, what information? How would this information help you make a decision?

3. In its natural state, oxygen is a gas. If you had an unlabeled cylinder filled with gas, how would you determine if it is oxygen? Please explain your response.

4. Carbon dioxide also occurs naturally as a gas. How would you tell the difference between carbon dioxide and oxygen? Please explain your response.

Is there other information you would like to know in order to tell the difference between carbon dioxide and oxygen? If so, what information? How would this information help you tell the difference between carbon dioxide and oxygen?

CSI Survey Set C

1. You meet someone who has never heard of caffeine. What would you say or do so that this person could recognize caffeine in the future?

2. Caffeine is present in many plant seedlings and acts as a pesticide to discourage insects from eating the unprotected plants. Is the caffeine found in seedlings the same as the caffeine found in energy drinks, such as Red Bull, or is the caffeine different? Please select your answer below.

_____ Same _____ Different

Please explain your choice. How do you know that the caffeine is the same or different? What evidence do you have?

Is there any additional information you would like to know in order to determine if the caffeine is the same or different? If so, what information? How would this information help you make a decision?

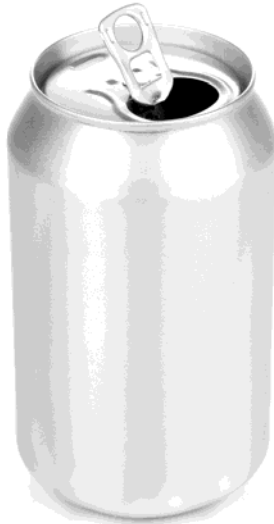
3. What could the object below be made out of? How would you know this?



[Iulia Bycheva] © 123RF.com

Is there other information you would like to know in order to determine what the object above is made of? If so, what information? How would this information help you determine what the object is made of?

4. Could the object below be made of the same substance as the object in the picture you saw previously? Please select your response below.



[serezniy] © 123RF.com

_____ Same Substance

_____ Different Substance

Please explain your choice. How do you know that the substance is the same or different? What further information would you like to know, and how would this help you make a decision?

CSI Survey Set D

1. There are white, crystalline granules on the table in front of you. How would you be able to determine if this is sucrose (also known as table sugar)? Please explain your response.

2. Let's assume the white granules are sucrose (table sugar). You take the sucrose and heat it over a flame until it turns from a solid into a liquid. The liquid now has a brown, caramel color. Is the liquid still sucrose, or is it a different substance? Please select your choice below.

_____ Still Sucrose

_____ Different Substance

Please explain your choice. How do you know whether it is still sucrose or a different substance? What evidence do you have?

Is there any additional information would you like to know to help you make a decision? If so, what information? How would this information help you determine if the brown liquid is sucrose or not?



[andrewkuzmin] © 123RF.com

3. You have a cup of an unidentified liquid in front of you. How would you determine whether or not this is ethanol?

4. You heat a pot of ethanol and it begins to boil. What is in the bubbles that are rising to the surface?

Please justify your response. How do you know what is in the bubbles?

Is there any additional information you would like to know in order to determine what is inside the bubbles? If so, what information? How would this information help you determine what is inside the bubbles?

3. CSI Survey with example student responses:

The following pages contain sets A-D of the CSI Survey along with example student responses. The responses have been chosen so that they reflect some of the most common ideas students used when answering this survey. Student responses have been left unedited. Code names indicate educational level and student number within that educational level. For example, 823 is the 23rd student within the set of 8th grade students who participated in the data collection using the final version of the instrument. The educational levels were:

Middle and High School		Undergraduate	
Indicator code	Educational level	Indicator code	Educational level
8	8 th grade	F	General chemistry
10	10 th grade	O	Organic chemistry
AP	AP Chemistry	P	Physical chemistry

CSI Survey Set A

1. Your friend's favorite earring is made of a light gray metal. How would you be able to determine if this is silver? Please explain your response.

[823]: I would look at the color, because I know silver is usually a shiny gray metal.

[AP1]: You can test the density of the earring - different substances have different densities.

2. Your friend's mother tells you this earring is made of pure silver. Your friend accidentally lost her earring and you found it a few months later. You noticed that it was no longer shiny and that it was now a dark gray/black color. Is the earring still made out of silver, or is it a different substance? Please choose your response below.

_____ Still Silver

_____ Different Substance

Please explain your response. What evidence do you have that the earring is made out of silver or a different substance?

[1017]: Different substance. Because silver does not rust

[AP8]: Still silver. If it is the same earring, then it should still be made out of silver. The dark gray portion would be different substances that had reacted with the silver over time.

[O9]: Different substance. The earring reacted with something in its environment and it changed the composition of what was silver to a new substance. Just as rust is a different substance than iron, the black color could be the result of such a reaction. Or the earring could just be dirty because something black got on it.

Is there any further information you would like to know in order to make a decision? If so, what is it? How would this information help you make a decision?

[835]: I would like to know how much the earring weighed before and after it was lost because it can help decide if it is the same substance.

[865]: I would want to know where the earring is found so that I could know what made it a different color because it could be dirt or something that wore away at it.

3. You have been assigned a school project where you have to explain what chlorophyll is to other students in your class. You decide to create a poster that

has the title: “What is chlorophyll?” What would you put on this poster, and how would it help you explain what chlorophyll is to the other students?

[1047]: Chlorophyll is the green coloring in leaves and plants that help absorb sunlight so that plants can create food from carbon dioxide and water.

[F69]: My poster would include a diagram (drawing) of chlorophyll, which includes a close up image, and one or more reference images (where it is in the plant). It would also include an image of actual chlorophyll as seen via microscope. For my own personal understanding of the world, context, physical location, and abundance is EXTREMELY important for my understanding of the subject. I would include a summary of the steps which converts light to energy through chlorophyll, the form that energy takes, where it is sent, and how it is used.

4. Chlorophyll can be isolated from the leaves of a tree growing in the forest and from algae growing in a pond. Is the chlorophyll from the leaves of the tree the same or different as the chlorophyll from the algae in the pond? Please choose a response below.

_____ Same _____ Different

Please explain your choice. What evidence do you have that the chlorophylls are the same or different?

[1010]: Different. It's different because it's taken from different substances. One from a leaf and another one from the pond.

[813]: Same. The chlorophyll for any plant has the same use for the plant.

[O16]: Same. The chlorophyll is the same because chlorophyll is just a substance that is found in chloroplasts. Both Algae and tree leaves can perform photosynthesis so chlorophyll is necessary for both.

Is there any further information you would like to know in order to make a decision? If so, what is it? How would this information help you make a decision?

[1062]: Maybe more in depth research at observing what chlorophyll looks like on a microscopic level. This would help me make a decision because then I would be able to see if they really do differ or remain the same.

[P8]: A qualitative and quantitative comparison of the chlorophylls. With this information one can say whether the chlorophylls are the same or different.

CSI Survey Set B



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1. You have a cup of an unidentified liquid in front of you. How would you determine whether or not this is water?

[828]: One can determine if the liquid is water by smelling it, tilting the cup, or even tasting it to see if it smells, moves or taste like water.

[1060]: I would look at its ph level, and if it were 7 ph then it would be water

[F31]: To determine whether it is water or not, boil it to see if it reaches the boiling point of water

2. You heat a pot of water over a stove and it begins to boil. What is in the bubbles that are rising to the surface?

[878]: Hot air.

[1046]: H₂O particles

[O21]: Water vapor.

Please justify your response. How do you know what is in the bubbles?

[878]: The water is heated, therefore the bubbles should be hot inside too, but is filled with air due to the evaporation.

[1046]: Because when water is together the Hs and Os link but when they are boiled the heat separates compounds from one another

[O21]: I know the bubbles are water vapor because the water is transitioning from a liquid state to a gaseous state when it is boiling

Is there any additional information you would like to know in order to determine what is inside the bubbles? If so, what information? How would this information help you make a decision?

[1038]: Is there anything else in the pot of water?

[O41]: The temperature that these bubbles are rising at. If it's at boiling point of water, then it is most likely water and nothing else. I wouldn't need any other information since I was specifically told that there was only water in the pot.

3. In its natural state, oxygen is a gas. If you had an unlabeled cylinder filled with gas, how would you determine if it is oxygen? Please explain your response.

[812]: I would determine if the unlabeled cylinder filled with gas is oxygen or not by seeing if it helps me breathe

[1034]: I would weigh the container. Then I would release the gas and then weigh the container again. I would also measure the volume of the container. Then I would subtract the final cylinder mass from the initial to obtain the mass of the oxygen alone. Then I would look up how much oxygen weighs per volume of gas and compare that with the mass of the oxygen I obtained.

*"I don't know" was a common response for this question.

4. Carbon dioxide also occurs naturally as a gas. How would you tell the difference between carbon dioxide and oxygen? Please explain your response.

[104]: You'd be able to tell the difference because oxygen has two atoms and carbon dioxide has 3. You'd also be able to tell because oxygen feeds a fire, carbon dioxide puts it out. There are a variety of tests you can do to figure out the difference. Lastly, we breathe oxygen, not carbon dioxide.

[P10]: Carbon dioxide is the most oxidized form of carbon. In two separate jars, one containing CO₂ and one containing O₂, a match will only burn in the one containing O₂

Is there other information you would like to know in order to tell the difference between carbon dioxide and oxygen? If so, what information? How would this information help you tell the difference between carbon dioxide and oxygen?

[AP72]: Mainly the weight of the cylinder and the conditions that the gases are given to me. I can do calculations from there.

[P7]: If you can not burn the samples, then knowing the densities, the mass of each sample, and the volume of each sample would allow you to distinguish between the two because you can just compare the calculated densities

CSI Survey Set C

1. You meet someone who has never heard of caffeine. What would you say or do so that this person could recognize caffeine in the future?

[1030]: Caffeine is most commonly found in coffee and tea. It energizes a person and helps them feel awake. If a person drinks too much of it, they might feel very hyper and alert. They could also crash and become exhausted after a few hours of having ingested it.

[AP75]: I would tell them about all of the items which caffeine can be found in, such as coffee and certain soft drinks. I would tell them about the uses and purpose of caffeine, and the effects it can have on humans.

2. Caffeine is present in many plant seedlings and acts as a pesticide to discourage insects from eating the unprotected plants. Is the caffeine found in seedlings the same as the caffeine found in energy drinks, such as Red Bull, or is the caffeine different? Please select your answer below.

_____ Same _____ Different

Please explain your choice. How do you know that the caffeine is the same or different? What evidence do you have?

[1021]: Different. I think it is a different kind of caffeine because having an energy drink with caffeine in it doesn't necessarily ward off insects. IF it were the same, then everyone would drink caffeinated drinks during the summer to keep mosquitoes away.

[AP45]: Same. A chemical with a certain name gets that name based on the structure it has. The name would change if the chemical was different.

[AP74] Same. I think the caffeine would be the same. however, to different organisms they would have different effects, but the elements involved would be the same. They could be arranged in different ways and thus serve different purposes. And at distinct ratios there could be differences in the concentration and lethal dose.

Is there any additional information you would like to know in order to determine if the caffeine is the same or different? If so, what information? How would this information help you make a decision?

[1023]: I would like to know what the caffeine is made out of in order to figure out if they are the same or not. This will help me because if they are the same, they will be made out of the same elements.

[O6]: Whether the caffeine is synthesized in a lab or extracted. Also, knowing the impurities that may be present in the synthesis or extraction of caffeine

3. What could the object below be made out of? How would you know this?



[Iulia Bycheva] © 123RF.com

[821]: I think the object is made out of silver because the color of it is silvery and it looks like a the material a silver necklace would be made out of.

[P31]: The object clearly looks like it is be made out of some metal..i discerned this from the shiny/metallic appearance, and the rough edges and what look to be maybe tool markings on the surface - all typical characteristics of metal. I could further narrow it down based on its silver-ish color...but that still leaves many different metals and I can't say its a pure metal- it could be some alloy. Looks can be deceiving...I pretty positive based on the surface texture and markings that this is a piece of some metal or metal alloy.

Is there other information you would like to know in order to determine what the object above is made of? If so, what information? How would this information help you determine what the object is made of?

[830]: Where it was found, how old it is and what kind of environment it was found in.

[1057]: The molar mass, it would help me determine the substance based on the periodic table.

[P14]: What does it feel like? Does it conduct electricity? Is it pliable? What is it density? If it conducts electricity that supports it being a metal. Seeing if its density matches any density of a known atom. If not it may be a composite of different types of materials

4. Could the object below be made of the same substance as the object in the picture you saw previously? Please select your response below.



[serezniy] © 123RF.com

_____ **Same Substance**

_____ **Different Substance**

Please explain your choice. How do you know that the substance is the same or different? What further information would you like to know, and how would this help you make a decision?

[853]: Same substance. It could be the same substance because of the texture and how it looks like before it was deformed. The can has the same color and same look to it like the substance before.

[AP64]: Different substance. Although the appearance of the metals are the same, it's commonly known that cans are made from aluminum. I guessed that the previous object is iron, so they are made up of different substances. The chemical formula would help determine what elements make up the can.

[O36]: Same substance. Similar color and luster are the most immediately apparent. The fact that it was malleable enough to mold into that shape also lends itself to the fact that it's a metal, like the first picture. There could be some slight differences, considering that the product above likely had to go through some purification processes in order to be safe for food usage, but those are likely minor differences.

Density and melting point would once again be useful, seeing as how if they matched the first material, then they're extremely likely to be the same compound.

CSI Survey Set D

1. There are white, crystalline granules on the table in front of you. How would you be able to determine if this is sucrose (also known as table sugar)? Please explain your response.

[810]: I would taste it or add it to something to see the difference if its sweeter than before it has to be sucrose.

[1032]: If you want to determine if this is sucrose, the overall thing you want to make sure is that it is able to be dissolved since sugar is soluble. What you can do to test this is add cup of room temperature water so that it can unsolidify the crystals. It is known that sugar can dissolve in water so if it is the case that this is table sugar, it will dissolve. If it is not, than it wont and we will have to find another way to test what substance can be.

2. Let's assume the white granules are sucrose (table sugar). You take the sucrose and heat it over a flame until it turns from a solid into a liquid. The liquid now has a brown, caramel color. Is the liquid still sucrose, or is it a different substance? Please select your choice below.

_____ **Still Sucrose** _____ **Different Substance**

Please explain your choice. How do you know whether it is still sucrose or a different substance? What evidence do you have?

[825]: The substance is still the same because I didn't add any other substances to the sugar. All I did was melt it using fire.

[1036]: Still sucrose. It is still sucrose however a phase change has occurred from a solid to liquid. Phase changes do not involve chemical changes, they just affect the way the molecules are bonded together. Sucrose in a liquid form has less intermolecular bonds.

[F128]: Different substance. The chemical bonds are broken up and the sucrose chains are broken into smaller bonds which cant be formed back to sucrose, the larger molecule is broken down to smaller molecules

Is there any additional information would you like to know to help you make a decision? If so, what information? How would this information help you determine if the brown liquid is sucrose or not?

[1037]: Knowing the formula of the brown liquid would help, if it is different from that of the sucrose then it is a different substance.

[P32]: I would like to know more chemical properties of the caramel liquid such as melting point, boiling point, and IR information.



[andrewkuzmin] © 123RF.com

3. You have a cup of an unidentified liquid in front of you. How would you determine whether or not this is ethanol?

[1015]: I would determine whether or not this is ethanol by the smell of it because I know it has a powerful chemical odor to it

[AP7]: I would burn it because ethanol is an alcohol and alcohols burn. If it burns I can at least conclude that it is an alcohol and not water.

[P19]: Determine its boiling point and compare it to known ethanol boiling points assuming this a pure sample.

4. You heat a pot of ethanol and it begins to boil. What is in the bubbles that are rising to the surface?

[852]: Air particles are in the bubbles that are causing it to rise, I don't even know what ethanol is.

[1022]: Hydrogen gas and oxygen gas and carbon gas.

[O43]: The bubbles contain vaporized ethanol that has reached its boiling point and is escaping the pot.

Please justify your response. How do you know what is in the bubbles?

[852]: A liquid can't just start floating in the air, without something to lift it.

[1022]: I know most alcohols are made up of carbons, hydrogens and oxygen.

[O43]: when a substance in the pot is boiled it will vaporize and move from the heated source to the air.

Is there any additional information you would like to know in order to determine what is inside the bubbles? If so, what information? How would this information help you determine what is inside the bubbles?

[822]: I would like to know what ethanol contains altogether so I can find what it reacts to.

[F19]: what elements or compounds that are in ethanol would help to determine what is inside the bubbles, because then i could determine what would be on the product side, and i will get a gas on that side of the equation.

[P19]: If this is a pure substance of ethanol? The actual BP of ethanol.

4. Rubric for the CSI Survey

Purpose: This rubric is intended to be used with all sets (A, B, C, D) of the CSI Survey. The rubric is structured to help teachers identify students' chemical identity thinking in their responses to the CSI Survey. This rubric has been evaluated by practicing chemistry teachers who have used the CSI Survey in their classrooms. These teachers are not using the chemical thinking curriculum in their classrooms, and still found the CSI Survey to be of value for their teaching. Teachers can use this rubric to help achieve three possible goals: 1) to perform a self-evaluation of their teaching and whether it influences students' chemical identity thinking, 2) to get a "snapshot" picture of individual students or an entire class with regard to chemical identity thinking and reasoning, and/or 3) to track progress in chemical identity thinking and reasoning for individual students or an entire class over time. The CSI Survey and rubric have been designed to provide information on students' current chemical identity thinking; future publications will provide information on pathways students might follow when progressing from novice to advanced chemical identity thinking and suggest methods to develop students' chemical identity thinking.

Step 1: Identify the cues or properties used in the students' responses.

To begin, it is useful to determine the cues or properties students are using when considering the chemical identity of a substance. The cues or properties that students use in these responses tend to be what the students consider to be important when solving questions of chemical identity, and from these cues, instructors can infer what chemistry knowledge the students are applying to the problem. The table below contains some of the more frequently used cues or properties, and can be used to help identify the cues or properties students are using in their responses. The appropriateness of the cue or property that has been used is often dependent on the student's response as a whole. Experts and novices could use the same cue but for very different reasons.

Explicit extensive-intensive properties	Explicit-implicit intensive properties	Composition	Structure
- appearance - hardness - volume - mass - shape	- melting point/boiling point etc. - flammability - viscosity - reactivity - pH	- indication of components, from differentiation of mixture and pure substance to consideration of submicroscopic components (e.g. atoms, molecules)	- indication of arrangement of components, from bond connectivity to overall molecular shape, generally on the submicroscopic level

Step 2: Evaluate the quality of the supporting arguments.

When responding to these questions, students should justify why the cue(s) they chose will help them to determine the chemical identity of the substance in the question. Their justification, or reasoning, can be assessed for its complexity. More complexity is not always required to provide a sufficient justification and does not always indicate a greater understanding of the chemistry concepts; however, the complexity of students' reasoning can be tracked over time or examined across questions.

Descriptive	Relational	Linear Causal	Multicomponent
Descriptive types of reasoning typically focus on the most salient feature of the system and use it to make a decision or judgment without indicating a cause or reason, and often repeat information from the problem or context.	Relational types of reasoning establish a correlation, or relationship, between the noticed feature and the phenomenon or effect. A phenomenon is often reduced or overgeneralized to a single agent or variable, and no mechanisms are proposed.	Linear causal types of reasoning present a mechanism by which the variable or feature causes the effect or phenomenon. The mechanism is the underlying cause(s) that explains the phenomenon at hand, which are often particulate in the context of chemistry problems. In this type of reasoning, a number of agents or effects may be reduced to a single chain of events.	Multicomponent types of reasoning involve more than one variable or feature. The relationships or interactions between these variables are considered.
Ex. I know that bubbles are filled with air.	Ex. There was water in the pot before, so there must be water in the bubbles.	Ex. The stove provides energy to the water molecules, and some of the water molecules have enough energy to spread out and enter the gas phase.	Ex. When the water molecules reach a certain energy level, they can spread out into the gas phase. The water molecules in the gas phase form a bubble that rises to the top because it is less dense than the liquid water.
Ex. Oxygen is a gas, so the gas in	Ex. If the gas is odorless, it is	Ex. Since all substances have a	Ex. I know that oxygen is an

the cylinder is oxygen.	oxygen.	specific density, if you can determine the density of the gas in the cylinder and it matches the known density of oxygen gas, you can find out if it's oxygen.	odorless and colorless gas and that it is flammable. If this gas matches all of those properties, then it is possible that it is oxygen.
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Step 3: Look for evidence of assumptions that may be guiding student thinking.

Identification of some of the following assumptions in students' responses may help teachers understand student thinking, although the assumptions might not characterize all of students' chemical identity thinking. Similarly to the cues and the reasoning, there are contexts when specific assumptions are more appropriate to apply than others. Assumptions do not always lead to "correct" or "incorrect" thinking; rather, each assumption may be of value depending on the situation. Students' reliance on assumptions to guide their thinking may be tracked over time or across questions.

Functional usage - Purposes that substances serve in daily life are used to classify them (e.g. chemicals are for cleaning). Additionally, the ability of a substance to perform certain actions may be used to classify or differentiate substances (e.g. liquids can be poured).

- Ex. Oxygen is used for breathing, so if the gas helps me to breathe I know it is oxygen.
- Ex. Chlorophyll is what plants use to produce food from sunlight.

Surface similarity - The tendency to pay attention to perceptual cues or perceivable properties (e.g. shape, color, smell) to classify or differentiate – this can lead to a belief that these observable characteristics stem from an essence or inner structure common to substances with similar characteristics.

- Ex. The object is made of silver because it looks hard, like a metal, and it has a silvery appearance that reminds me of silver jewelry.
- Ex. You would know if the liquid is water if it looks like water and moves like water when you pour it out of the glass.

Historicality - The origin or history of a substance is used to determine a substance's chemical identity or to tell if the identity has been lost as a result of a change (e.g. if a substance is made by two different processes, different chemical identities result).

- Ex. The chlorophyll in the leaf is different than the chlorophyll in the algae because they come from different types of plants.

- Ex. The caffeine in Red Bull is different than the caffeine in the plants because the caffeine in the Red Bull went through a process in the lab that changed it.

Substantialization - Properties are separable from substances, and can be added or removed without a change in chemical identity (e.g. a substance's ability to burn can be "used up," at which point it ceases to burn but retains its original identity).

- Ex. Even though the earring has changed color, it is still silver. It can change color but still be the same metal.
- Ex. The caffeine in Red Bull is synthesized in a lab and its effect as a pesticide is removed before it is put into Red Bull.

Additivity - Properties of a substance result from an additive combination of its components' properties, and thus can be added or removed in conjunction with the components (e.g., CH₄ has one part carbon-like properties and four parts hydrogen-like properties).

- Ex. The bubbles in the water are either hydrogen gas or oxygen gas, in a 2:1 ratio, because that is ratio of hydrogen to oxygen in water molecules.
- Ex. If a substance has the same number of carbon atoms, hydrogen atoms, and oxygen atoms as a molecule of sucrose, then it is the same as sucrose.

Elementalism - A component of a substance (usually an atom, bond or functional group) is the carrier of a specific property (e.g., an aldehyde present in a molecule has the property of an IR absorption peak between 1740 and 1690 cm⁻¹).

- Ex. The oxygen in the carbon dioxide makes carbon dioxide flammable, because oxygen by itself is flammable.
- Ex. The hydrogen atoms in the water molecules make them able to go into the gas phase.

Structuralism - Differentiation using models based on specific composition and molecular structure that can be applied across different classes of substances, and recognition that substances share similarities in structure at the particulate level.

- Ex. The caffeine in the Red Bull might be geometrically arranged in a different way than the caffeine in the coffee. It might have the same components, but these might be put together in a different way, which could explain its different effects.
- Ex. Chemicals are named based on the specific structure they have, so since it has the same name that means the substances have the same structure and are the same.

Emergence - The interactions of components of a substance on a subatomic, atomic, or molecular level emerge as properties of that substance, and can be used to identify or differentiate substances.

- Ex. When the sucrose goes from a solid to a liquid state, the intermolecular forces in between the molecules of sucrose are broken but it doesn't change the identity of the molecules of sucrose.
- Ex. Chlorophyll appears green because the interaction of light with the molecule of chlorophyll, so if the color is not green this can indicate a difference in the composition or structure of the molecule, making it different from chlorophyll.

5. General protocol for follow-up interview after completion of CSI instrument

1. Ask participant to verbally explain his/her written response - see if there is more detail in the verbal than the written response
 - Give the participant a chance to elaborate on answer
 - Ask for an alternative method of identification
2. Have participant define any terms that might be interpreted differently - i.e. chemical, change, what it's composed of, properties
3. Double check what further information participant would like to know, and ask how that information would help participant identify the substance or make a decision about its identity after a process
4. Ask participant if any of the questions were confusing
5. Ask if there is anything the participant was thinking about when completing the instrument that he/she did NOT write down or talk about in our interview, if so, ask why it was not recorded

6. Categories

First-level categories

- Identify the change taking place in the bubbles in order to identify substance
- Type of reaction or change determines the identity of the metal - focus is on interaction of metal with something else
- Use observations of substance in bubbles to identify
- Assign metal to a category (metals, elements) and associate properties of that category to the metal in order to determine what can and cannot occur
- Associate caffeine with a broader classification of things
- Caffeine is a specific molecule, compound, or chemical and are the same in energy drinks and plants - assignment of caffeine to a specific category
- Determine identity of substance in bubbles based on knowledge of what can exist as a gas
- Same name means caffeine are the same
- Use the chemical structure to determine if it is caffeine
- Caffeine's identity is determined by its composition - a change in composition = new identity
- Carbon dioxide is a larger molecule than oxygen, which gives it different properties
- Composition is what determines identity of metal
- Determining the composition of the gas will help identify if it is oxygen
- Figure out composition of earring to determine if it is made of silver
- Use composition of gases to differentiate
- Substances in bubble are dependent on composition of original substance
- Use substances already present to figure out identity of substance in bubbles
- Consider the effect of heat in order to determine what happens to the identity of the substance
- Presence or lack of external influences can be used to decide if identity of metal has changed - overlaps with continuity, history, and type of reaction
- Assignment of affective impression to caffeine as part of identity
- Consider effects on humans, use experience with these substances
- Differentiate based on effects from breathing in gas
- Identify caffeine by the effects it has on your body
- Living organisms need oxygen to breathe, use effects of breathing gas to determine if it is oxygen
- Observe effect of earrings on human to determine what they are made of
- Since it has the same effects or characteristics, the caffeine are the same
- It is the concentration of caffeine that is different in seedlings vs. energy drinks, not the caffeine itself
- Determine if a solute is present in the liquid
- Caffeine can be produced naturally or synthetically and be the same
- Caffeine in energy drinks has been modified, while caffeine in seedlings is natural - this makes them different
- Caffeine originates from specific sources, use source to identify it

- Comparing sources of caffeine in other products - caffeine in other products also comes from a plant, so it is possible for caffeine to be produced by a plant as a pesticide and be the same caffeine
- The same caffeine can originate in plants and then be used in other products (i.e. coffee or energy drinks) - separating source from uses
- Add a substance to the gases to see the reaction or product formed (substance is specified)
- Mix earring with another substance and use observable change or reaction to identify
- Mix gas with known substance and observe reaction and or product
- Observe chemical interactions when liquid is mixed with another substance
- Modifications may be made to substances that alter them in some noticeable way without changing their chemical identity, a substance can have multiple forms
- Presence of something else (color, compound) or reaction does not affect underlying identity of silver - silver takes precedence - could be part of continuity strategy
- Caffeine can affect different organisms differently, but still be the same caffeine (one substance can have multiple functions)
- Carbon dioxide is needed for photosynthesis in order for plants to survive, while oxygen is not
- Describe purpose or function of caffeine
- Different functions = different substances
- Caffeine is IN the object - caffeine can be identified by the objects it is in
- Caffeine IS the object - caffeine can be identified as objects
- Identify things caffeine is in
- Labels can be used to identify caffeine
- Carry out general, unspecified tests and compare to silver
- Change environmental conditions (P,T) and observe effect on gas
- Convert the gases into a liquid or solid and observe or measure their properties in this state to differentiate
- Determine molar mass of the gas and compare it to molar mass of oxygen
- Determine the density of the gas and compare it to the density of oxygen
- Determine the mass or density or use tests that utilize mass or density to identify the liquid
- Differentiate gases based on mass, weight, molar mass, density
- Distinguish gases based on property of flammability (oxygen is flammable, carbon dioxide is not)
- I know they oxygen and carbon dioxide have different properties but I'm not sure how to differentiate them
- Identify liquid based on pH (pH of water is 7)
- Measure a physical property of the metal earring and compare it to known values of silver's properties
- Oxygen is flammable, so test flammability (burnability) of gas using various methods
- Physically manipulate the liquid and observe its behavior
- Test a chemical property of the metal and compare it to reference values or established outcomes
- Use an instrument or test (not always specified) to identify gas based on measurable or observable property (also not always specified)
- Use an instrument to identify the liquid
- Use an outside source to tell you whether or not the earring is made of silver
- Use general properties to differentiate gases

- Use phase change characteristics to identify liquid
- Use qualitative tests of liquid's properties to identify
- Caffeine can be detected by measurable or observable salient properties
- Identification based on physical senses
- Identify gas based on appearance
- Qualitatively compare liquid to water and other liquid substances
- Use observable characteristics (appearance, taste, feel) of the earring to determine if it is silver
- Use smell to determine whether or not the gas is oxygen
- Use the change of appearance to determine if the silver has changed identity

Second-level categories

- By determining what type of change or process is occurring (chemical, physical, or even more specific) can determine the identity of the final substance
- By placing a substance in a more general category, the properties or features associated with that category can be used to aid in identification of the substance
- Chemical structure determines the chemical identity of a substance
- Molecular components of or within a substance can be used to establish identity
- Composition of the initial substance or presence of other substances can be used to determine the identity of the final substance after undergoing a process
- Concentration of a substance or presence of other substances in a mixture can explain differing effects of a substance in two different contexts
- Establish if the system at hand is a mixture or single substance
- External forces can act on a substance to change its identity, so identifying the external forces present and how they influence the substance is important
- How a substance affects humans or other living organisms can be used for identification
- How a substance is produced or processed - natural or synthetic - impacts its identity
- Knowing the source of a substance can help identify it
- Mix a known substance(s) with the unknown substance and observe if there is an interaction or reaction
- Rely on past experience with substance for cues about its behavior or contexts it could be found in order to help identify it
- Substances have an essential quality or component that gives it its chemical identity, so if that remains, other parts of the substance can change while identity is maintained
- The purpose or function of a substance can be used for identification or differentiation
- Type of object or material associated with a substance can be used to determine identity
- Use senses to identify substance (appearance, smell, taste, texture)
- Use some property or test of the substance to identify it through comparison to an ideal or known value

Third-level categories

- History

- Change
- Purpose and effect upon use
- Composition and structure
- Object that it's in
- Experimental/measurable values

Refined third-level categories

- Change
- Class
- Composition and structure
- Function
- Organism effect
- Sensory information
- Source
- Tests and experimental values

7. CSI Codebook

The following table and compilation of coded student responses were created during the coding process for the CSI Survey data. The codebook served as a way to define the codes in order to ensure consistency. The codebook can be used by researchers and instructors to interpret their own students' responses to the CSI Survey.

Category	Student thinking	Examples
1. Source <ul style="list-style-type: none">- Knowing the source can help identify it- Substances have an essential quality or component that gives it its CI, which could come from its source	<ul style="list-style-type: none">- nature vs. chemical activities, origin plays a role in chemical identity- mixtures may assume the chemical identity of one component in the mixture- chemical identity is based on more than just appearance	847: It is still sucrose because even though it change forms and colors, it is still from the sucrose. 1028: I hypothesized that the caffeine probably is the same because I know that the caffeine in coffee comes from the coffee beans which is comes from an organism. If the caffeine in coffee is found in the plants then it is probably the same caffeine as the

<p>Defining characteristics</p> <p>Novice ideas:</p> <ul style="list-style-type: none"> - Source impacts the chemical identity of a substance, student typically does not indicate what specifically changes, has a general concept of CI that could be interpreted as an essence, even if this is not stated (e.g. not microscopic) - Substances have an essence or quality that contributes to its identity, and this essence can last through processes or changes that occur to the substance, thus preserving its CI <p>Advanced ideas:</p> <ul style="list-style-type: none"> - although source does not impact the chemical identity of the substance, some may still feel it is useful to know sources of this substance 	<p>one found in plant seedlings.</p> <p>1053: I would put where chlorophyll came from, and how it came to be, as well as what it actually is. This would help other students understand what chlorophyll is because it would help them understand its origin and how it came to be, which is essential when discussing what something is.</p> <p>1049: The reason why the caffeine found in seedlings is the same as the caffeine found in energy drinks because caffeine has to come from somewhere, one source. If the caffeine in energy drinks was not the same as the caffeine found in energy drinks then where would that caffeine from? Much like the cocoa powder found in chocolate is the same as the cocoa seed.</p> <p>F87: still silver because and element retains its most basic units regardless of influences.</p> <p>AP71: It is very possible that silver reacted with air and oxidized or there were other chemical reactions that slightly changed the composition. The majority of the substance should still be silver though.</p> <p>O18: the dark grey and black color can be remove with robbing alcohol. the substance on it doesn't mean its not pure metal anymore</p>
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<p>2. Change</p> <ul style="list-style-type: none"> - How a substance is processed impacts CI - Focus on type of change occurring to substance, characterization of the context or process (“this is what happens when...”) - Effect of external agents on CI 	<ul style="list-style-type: none"> - processes affect the chemical identity of a substance - the type of reaction determines whether the CI of a substance changes - comparison to what students already know: rusting changes CI (or it doesn't), this must be similar to rusting - the force or agent might implicitly guide students to think about type of reaction 	<p>P34: because at the boiling point. water begin to transfer their condition from liquid to gas. so the bubbles is one of the way that water can transform into gas. also boiling water mean put in some more energy and mean more work. so it have to release the work out to keep balanced the boiling point.</p> <p>875: To change it to something other than pure silver, it would have to undergo a chemical reaction, which would most likely alter the shape of the earring.</p> <p>1046: Because when water is together the Hs and Os link but when they are boiled the heat seperates compounds from one another</p>
<p>Defining characteristics</p> <ul style="list-style-type: none"> - By identifying the type of reaction, process, or change that is occurring, students can infer whether the CI of the substance changes (e.g. phase change vs. oxidation) - Students might describe the mechanism of this process at either the macro or micro level - The focus could be on an external agent or force that indicates the type of process or change that is happening OR simply the presence of specific agents could indicate that the CI changes or stays the same - Students focus more on describing what did or could have happened to the substance rather than talking about the reactivity of the substance (which would make it 8. Tests) 		<p>835: A substance cannot change unless you add multiply sources of heat or other factors.</p> <p>F116: When water is heated, the molecules of water are moving quickly creating bubbles that cause evaporation.</p>

<p>3. The organism effect</p> <ul style="list-style-type: none"> - Use effect of substance on living organisms to determine CI 	<ul style="list-style-type: none"> - in differentiation, organism is the variable OR substance identity is the variable - affective impressions of substances can be used to identify them (e.g. good vs. bad for humans) 	<p>F6: I would start breathing and if I start to get light headed or unable to stay awake then I would know that its CO2 and that I should probably stop breathing that bad air in. If Im doing fine then it must be oxygen</p> <p>1056: If it was the same caffeine acting as a pesticide, we would not be able to consume it. That is why it is not the same, I have no evidence to prove it.</p>
<p>Defining characteristics</p> <ul style="list-style-type: none"> - The “test” involves how the substance impacts a living organism (primarily humans), the result of this test or its effect (or lack of an effect) on organisms can be used to identify substance - The action of a substance on humans (e.g. caffeine makes humans more alert) is used as a defining characteristic (*need to consider how to separate this from function/purpose/object) - At a more advanced level, this could involve arguments about toxicology 		<p>871: When caffeine is entered into the human system, it causes an increase of energy.</p> <p>F65: There are no harmful effects of breathing the bubbles. If it was Hydrogen gas I would assume it would be harmful. O2 obviously is not.</p> <p>F83: You could tell if it was silver, by the way it reacts with her skin.</p> <p>AP65: The last thing I would add is how chlorophyll affects humans when we eat greens and other food substances with chlorophyll.</p>
<p>4. Sensory info</p> <ul style="list-style-type: none"> - Use info gained from senses 		<p>P24: the first thing I would do is to look at the color of the earring. the second thing is to touch it with my</p>

<p>Defining characteristics</p> <ul style="list-style-type: none"> - Info about the substance is obtained by using the senses, and this information is the sole or primary basis for determining CI - Is often used as a cue for other tests that indicate other CI info about the substance 		<p>hands if it is silver.</p> <p>1029: I would examine it physically and identify its properties. Is it clear? Is the liquid thick? Thin? Is there anything within it? What color is it? What does it smell like? From the information I have obtained, if it matches the criteria of being clear and odorless, I would assume that it is water. If it doesn't, it is not water.</p> <p>823: I would look at the color, because I know silver is usually a shiny gray metal.</p> <p>F82: color of the gas and smell of the gas would help me determine what gas it is</p> <p>Ex. You know it is chlorophyll if it is green</p>
<p>5. Composition and structure</p> <ul style="list-style-type: none"> - Chemical structure - Chemical components 	<ul style="list-style-type: none"> - if the components are the same, the substances are the same - arrangement of components does not impact chemical identity - the differing components of a substance contribute to properties or qualities that can be used to distinguish them 	<p>F93: Caffeine would be different based off of common knowledge of other ingredients. For example, there is more than one type of sugar. It is still sugar/caffeine, but the way it's chemically structured may be different.</p> <p>AP61: Caffeine has a specific chemical structure. Its presence in different solvents does not change its chemical identity.</p> <p>AP74: I think the caffeine would be the same. however, to different</p>

Defining characteristics <ul style="list-style-type: none"> - The components or structure (arrangement) of a substance is considered for its CI - Most of this thinking occurs on the molecular level, but some students might reason about components of substances on the macroscopic level - Components or structure are specified or named, vs. when comp/structure is used for classification it is typically more generalized 		organisms they would have different effects, but the elements involved would be the same. They could be arranged in different ways and thus serve different purposes. And at distinct ratios there could be differences in the concentration and lethal dose. F75: This metal is still silver, a possible outcome of the metal being a darker gray is through oxidation where water has affected the metal. Since it is pure silver the metal is composed of only the element silver, therefore it is still silver.
6. Class <ul style="list-style-type: none"> - Classification of a substance to infer CI 	<ul style="list-style-type: none"> - all substances in the same class exhibit similar behaviors or properties 	1035: Caffeine is a chemical, so regardless of where it came from the caffeine itself will be identical.
Defining characteristics <ul style="list-style-type: none"> - By placing a specific substance into a more general class or category of substances, behaviors typical of that class can be used to infer the identity of the specific substance, or whether it belongs to that class - Separation of pure substances vs. mixtures can be used to reason about CI - <i>When students say "substance x is a..." is this automatically a classification? (e.g. oxygen is a gas, so therefore...)</i> 		F82: Because oxygen is a gas and the bubbles are gas bubbles 1041: Metals rust being exposed to factors like rain, wind and other stuff which it could have come in contact with while it was lost. P20: Most earrings are not made of 100% pure materials; they are often a mixture of two or more to make the work of the jeweler easier giving a desired shape. So, it is normal that the earrings get a little oxidized, but they can get cleaned and shine again.

<p>7. Function</p> <ul style="list-style-type: none"> - Use object or material commonly associated with substance as ID - Purpose or function of substance can be used as ID 	<p>- Everyday experience can be relied upon (association heuristic?) to provide a context in which the identity of the substance can be placed</p>	<p>AP56: Caffeine is a chemical that makes you awake and alert for a long period of time. It is commonly found in coffee and some sodas. Many people consume it in the morning and it can cause a crash later on. It is addictive but there are not many withdrawal symptom.</p>
<p>Defining characteristics</p> <ul style="list-style-type: none"> - Focus is on how the substance is used (typically informally, not in a lab), and its use is typically associated with an object of which the substance may be a part 		<p>AP75: I would tell them about all of the items which caffeine can be found in, such as coffee and certain soft drinks. I would tell them about the uses and purpose of caffeine, and the effects it can have on humans.</p> <p>AP38: They (caffelines) are doing different things. One is acting like a pesticide which stops insects from eating and killing crops. While the other is a common substance found in energy drinks, soda, coffee, etc. One kills and repels insects while the other one gives you a lot of energy.</p> <p>Ex. Chlorophyll makes a plant green OR Plants are green because of chlorophyll</p>
<p>8. Tests & experimental values</p> <ul style="list-style-type: none"> - Test or observe properties of a substance, compare to known values - Use characteristic reactivity of substance to determine CI 	<p>- these values or properties will not change and can be reliably used to determine the chemical identity of substances</p>	<p>O25: in a very safe place i would try to put make fire using the gas, if it is oxygen i will get fire.</p> <p>AP52: I would determine if it is water by conducting an experiment. Because water has certain boiling point and freezing point, I would boil and freeze the liquid to the temperature for water's boiling point and freezing point. Also, I would use a pipette to drop little droplets of the liquid</p>

<p>Defining characteristics</p> <ul style="list-style-type: none"> - Participants suggest using a test or the results of a test (can be general or specific) to obtain information that will be used to determine CI of substance, generally by comparison to a known value - students may or may not explicitly make the connection between the results of the test and subsequent identification or differentiation - This can occur on both the macroscopic and microscopic levels 	<p>to determine if it is water because water's surface tension causes the water droplet to spread out when it comes to contact with surface.</p> <p>1029: I would conduct a chemical reaction that involves oxygen. For example, I could conduct a synthesis reaction with aluminum and oxygen to form aluminum oxide. If aluminum oxide has formed, then it would confirm that the unlabeled cylinder filled with gas is oxygen.</p> <p>P17: I would first test to see if the white crystals dissolved in water. If they did not, then I would immediately be able to tell that they were not sucrose.</p>
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Distinguishing reasoning and cues:

Reasoning – main factor contributing to a student’s line of thinking or argument about the chemical identity of a substance

Cue – factor or characteristic that contributes to or leads to the major reasoning, a cue cannot stand on its own, can have multiple cues contributing to the same reasoning

Examples of coding

Key: Student code number appear first (CSI Survey question in brackets): Student response in normal font [**coding in bold and separated into primary reasoning, prop, and short explanation of assignment**]

1053 (silver earring question): I believe that the earring is made out of a different substance because if it were silver , I do not think it would be able to change colors at all. [**prop: 2. Change, primary: 1. Essence – there is something that keeps the earring silver and would prevent it from changing color**]

F39 (silver earring question): The oxidation of the metal [**prop: 2. Change**] indicates that the material used is not silver based on its periodic properties. [**primary: 6. Class – substances can be put into classes based on periodic properties**]

P15 (silver earring question): Pure silver would not naturally change to a different color [**primary: 6. Class – pure vs. not pure imparts specific behavior**]. A

chemical change would have to take place. Therefore, I'm assuming the earring was probably silver plated and over time the silver faded and the metal underneath started to erode and/or was oxidized by oxygen in the air [**primary: 2. Change – this mainly contributes to the argument of class, because it supports reasoning that pure substances behave differently**].

AP24 (silver earring change): I know personally that real silver jewelry can still turn dark gray or a black color over time from wear and water and other effects [**prop: 2. Change – wear and water and other effects can change silver**]. You can clean that off and have it retain its old color [**primary: 4. Sensory info – the “old color” = part of identity of silver**] by making a reaction by mixing baking soda with white vinegar and boiling water. [**prop: 1. Source – the essence of the silver, its color, is maintained throughout these changes**]

AP51 (silver earring change): Certain metals have the potential to be oxidized [**prop: 6. Class – classification as a metal that could be oxidized**], in which their chemical formula is changed [**primary: 5. Composition – chemical composition changes as result of oxidation**], thus their physical appearance changes as well [**prop: 4. Sensory info – the color change is indicative of the composition changing**]. For example, iron and copper experience rust, in which their color changes from grey to orange-brown, or brown to green, respectively. This occurs once the metal is oxidized, or oxygen molecules interact with the metal atoms, forming FeO or CuO₂ [**prop: 2. Change – explaining the type of change, oxidation, going on and how it impacts the composition**]. Therefore, because there is evidence that the silver changed in physical appearance, and the fact that silver is a metallic substance, it is reasonable to say that the silver is now a different substance, after it has been oxidized. [**summary sentence with all the props and primary reasoning**]

F148 (silver earring change): because, silver reacted with the atmospheric Oxygen and rusted. the rusting does not change the nature of the metal. [**prop: 2. Change – the type of process occurring is rusting, and rust does not change the CI, primary: 1. Source – there is some essence or component that stays the same throughout the rusting process that allows the silver to retain its “nature” or chemical identity**]

104 (carbon dioxide vs. oxygen): You'd be able to tell the difference because oxygen has two atoms and carbon dioxide has 3. [**primary: 5. Composition – differentiation based on types of atoms making up substance**] You'd also be able to tell because oxygen feeds a fire, carbon dioxide puts it out. there are a variety of tests you can do to figure out the difference. [**primary: 7/8 daily use and possibly tests – it depends on how student is viewing the ability of oxygen to feed a fire and CO₂ to put out a fire – if it is the typical use of these substances then it is 7, if this is a property that these substances have that we can test it is 8**] Lastly, we breath oxygen, not carbon dioxide. [**primary: 7. Daily use – this is how we use these substances when we breathe and exhale**]

O44 (water bubbles): I would think that helium is definitely one of the gases because just like a helium balloon, the balloon rises. I would also think that oxygen is in the water because there is air in the bubbles and oxygen is in air. Lastly I would think that carbon is in it because I would feel like carbon is in air. **[primary: 6. Class – is deciding what substances the gases are based on the thinking “all things that are/do this... are this...”]**

AP64 (caffeine source): It is the same type of caffeine but the use is different because insects react differently to the caffeine. One substance can have many uses. The caffeine is the same because coffee has caffeine and coffee is a plant seedling. **[primary: 1. Essence – by stating that a substance can have many uses, the student implies that there is something beyond its use that gives caffeine its identity]**

107 (water bubbles): I think the bubbles rise to the top because the carbon needs to be released **[primary: 2. Change – focus is on the rising action of the bubbles, and the need of the carbon to be released is the mechanism of this change]**

AP52 (water bubbles question): Since the boiling process is not a chemical reaction but rather a phase change **[prop: 2. Change – student uses the type of reaction occurring to cue thoughts about composition]**, bubbles should be composed of the elements in water **[primary: 5. Composition – the elements in the original substance determine the elements and thus identity of the substance in the bubbles]**. Boiling process breaks bonds in water molecules so it is plausible that bubbles are composed of the elements that are in water. **[prop: 2. Change – is explaining the mechanism of the change to illustrate why the main line of reasoning about composition is correct]**

O36 (metal chunk question): The luster **[prop: 4. Sensory info]** and lack of definite crystalline structure **[prop: 5. Structure]** would imply that it's some sort of metal **[primary: 6. Class – cues on specific features to place substance in class of metals]**. Seeing as how it appears to be in open air and isn't violently reacting **[prop: 8. Tests & Experimental Values – uses (non)reactivity to exclude it from a subclass of metals]**, it's pretty safe to assume that it's not a Group IA or IIA metal **[primary: 6. Class – getting more specific with the type of class the substance belongs to]**. With those in mind and the color, if I had to guess, I'd say it's aluminium. **[primary reasoning: uses the props to make judgments about the class of substances the metal belongs to in order to narrow it down to a specific substance]**

P17: I would first test to see if the white crystals dissolved in water. If they did not, then I would immediately be able to tell that they were not sucrose **[primary: 8. Tests & Experimental Values – uses a solubility test]**. If they did dissolve, I would perform a flame test, as I know that sucrose is an organic compound and should not produce a colored flame **[prop: 8. Tests – uses a flame test to determine belonging to a class, primary: 6. Class – is it an organic or inorganic compound?]**. If a

colored flame was produced, I would be able to say that the compound was not sucrose. If The flame was not colored then I would take an IR spectrum of the compound (dissolved in some inert solvent) and compare it to the structure of sucrose (which I'd have to look up). **[prop: 8. Tests – use an instrument to get the IR spectrum, primary: 5. Composition & structure – info from the IR test tells you about the structure of the crystals, which can be compared to the known structure of sucrose]**

1033: It is still sucrose because, it's only table sugar that has been melted. The table sugar is turning into a solid to liquid phase. **[prop: 2. Change – considering the type of change, a phase change]** Only it's shape is changing, not its molecular structure . It's like water. If you freeze water, the molecular structure for water is the same. It's only in a different form. **[primary: 5. Composition – uses knowledge of the type of change occurring to reason that the molecular structure, which is linked to the CI, is not affected during a phase change]**

874: it's still sugar because it didn't get mixed with another substance **[prop: 6. Class – this is pure and not a mixture]** for a chemical reaction to happen so it still is sugar **[primary: 2. Change – a chemical reaction needs to happen to change identity, and you need another substance in order to have a chemical reaction]** plus if u taste it, it still taste like sugar **[primary: 4. Sensory info – taste remains the same]**

F17: It will still be sucrose because when it is heated, it melts and becomes a liquid at a certain temperature. **[prop: 2. Change – is focusing on the heat and infers that when it melts it becomes a liquid, would be 8. Experimental & Tests if student focused on the temperature it melted at and not the process, primary: 1. Source – there is something about the sucrose that enables it to retain its chemical identity, despite the heating process]**

P19: Color change is usually an indicator of a chemical reaction **[prop: 4. Sensory info, primary: 2. Change – using color to infer reaction type]**, in this case sucrose is a multiple carbohydrate structure and it is held together with an ester bond **[prop: 6. Class – classifying the sugar as made of multiple carbohydrates, primary: 5. Composition & structure – using the class to talk about the composition of the sucrose]**. when heated it is likely that this bond broke and the smaller sugar subunits were oxidized **[primary: 2. Change – explains what happened on the molecular level when heat was applied to the sucrose]**.

8. Biochemistry expert survey (administered online via GoogleForms)

Introduction

Hello! The purpose of this survey is to collect information from biochemists about their work and how it relates to identification and differentiation of substances. By participating in this survey, you agree to let us use your responses in our research. All responses will be kept anonymous and will inform education research. We greatly appreciate your participation, and any questions may be directed to the PI of this work, Dr. Hannah Sevian (hannah.sevian@umb.edu), or the graduate student working on this project, Courtney Ngai (courtney.ngai001@umb.edu). You may withdraw from this study at any time.

Survey questions

1. Please describe briefly what your biochemistry-related work (e.g., research, applications, product design, regulatory) is about (e.g., characterization of a specific protein, purification of proteins).

2. We are exploring the extent to which the identification of chemical substances is relevant in biochemistry work. We consider the question of “chemical identity” to involve categorization of substances into classes of substances, and collection and analysis of relevant information to enable substance identification and differentiation. If you can, please give one example from your biochemistry-related work of a problem in which you answer questions of chemical identity. Describe the problem, why it is important to identify and/or differentiate the substance(s), and how you do so.

3. To what extent do you consider answering questions of chemical identity to be significant in your biochemistry work?

- It is a major part of my biochemistry work.
- It is essential to my biochemistry work, but not the majority of my biochemistry work.
- It is sometimes relevant to my work, but not often a concern of my biochemistry work.
- It is not very relevant to my biochemistry work.

If you wish to provide further explanation for your choice above, please include it here.

Demographics

We have included a few demographic questions to ensure a variety of fields are represented in the responses.

Please mark the answer(s) that best represents the sector(s) in which you work:

- Academia
- Pharmaceutical industry
- Biotech/Biopharma industry
- Clinical or medical research
- Forensics
- Medical products and instruments
- Home/health products industry
- Food or agriculture industry
- Chemical products industry
- Government (federal, state, investigatory) sector
- Other

Are you affiliated with any professional societies related to your biochemistry work (e.g. American Chemical Society)? If so, please indicate the society, as well as the division or branch of that professional society (if relevant).

What are the top academic journals that are most relevant to you?

In what academic disciplines and specialties do you have terminal degrees and/or technical certifications?

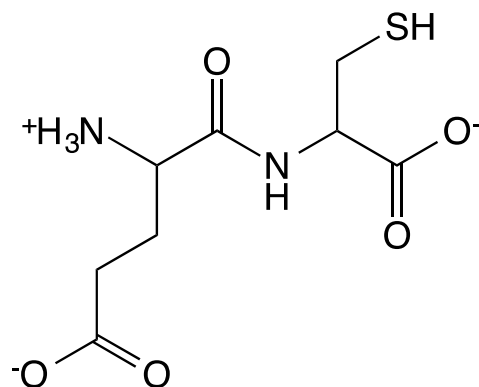
Where are you located?

- In the U.S.
- Outside the U.S.

9. Creative exercises

CE1 – Dipeptide (this heading was not included in student version)

Write down as many **correct, distinct, and relevant facts** you can about:

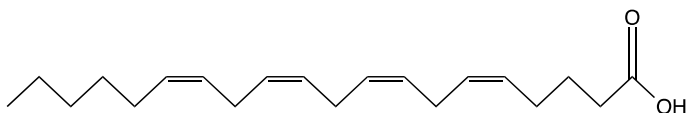


Ten (10) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in a chemistry course, including general chemistry, organic chemistry, and any biochemistry courses. All other outside information, combined, will only count as one distinct fact towards the correct responses.

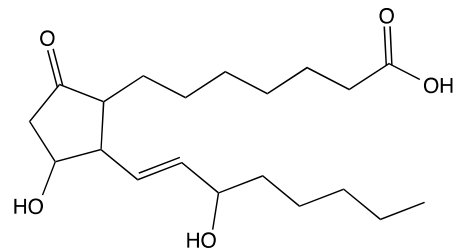
CE2 – Fatty acids (this heading was not included in student version)

Write down as many **correct, distinct, and relevant facts** as you can about **both molecules**:

Molecule A



Molecule B



Five (5) statements will get you full credit for the problem, which is worth 5 points. Recall the information you use should be information you learned in a chemistry course, including the general chemistry, organic chemistry, and biochemistry courses. All other outside information, combined, will only count as one distinct fact towards the correct responses. You may list more than five statements.

CE3 – DNA (this heading was not included in student version)

Write down as many **correct, distinct, and relevant facts** as you can about:

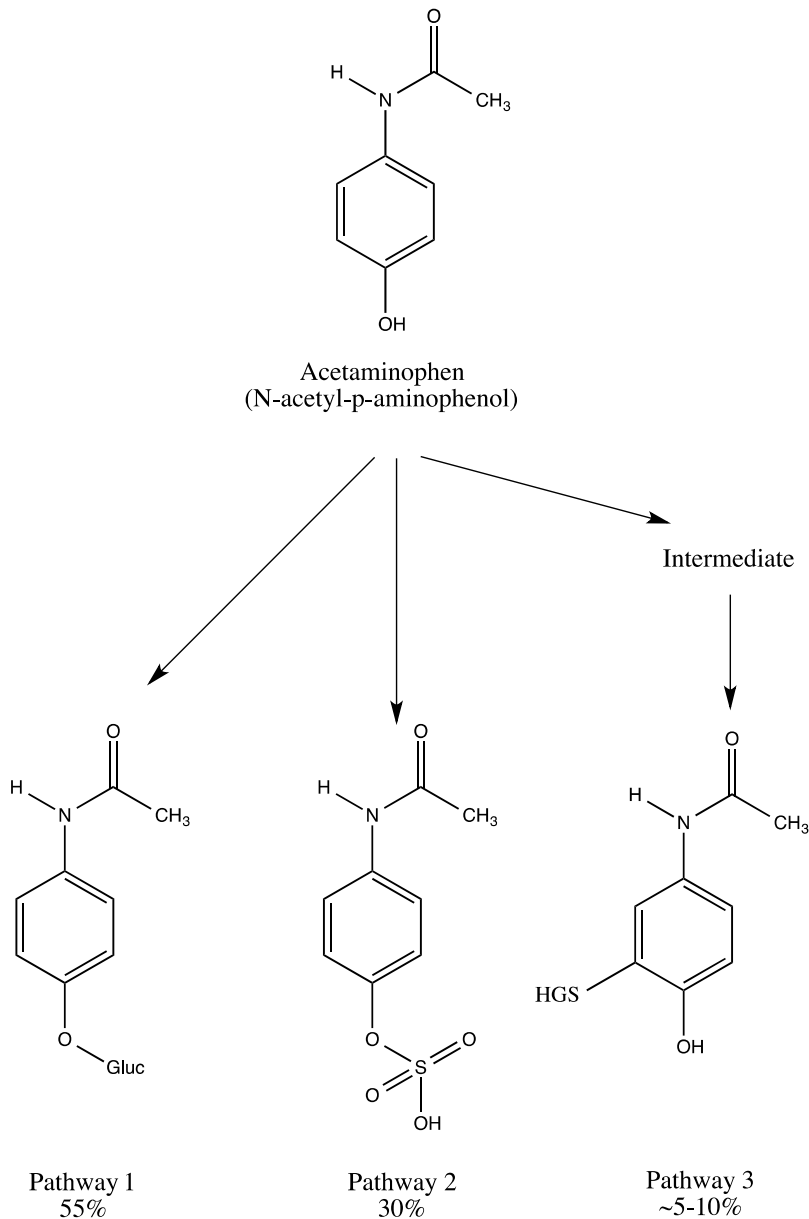
You have two solutions of DNA fragments purified from bacterial cells. In one solution, the DNA is purified directly from healthy bacterial cells. In the other solution, the purified DNA has been damaged by exposure to UV radiation for 10 minutes.

Five (5) statements will get you full credit for the problem, which is worth 5 points. Recall the information you use should be information you learned in a chemistry course, including general chemistry, organic chemistry, and biochemistry courses. All other outside information, combined, will only count as one distinct fact towards the correct responses. You may list more than five statements.

CE4 – Acetaminophen metabolism (this heading was not included in student version)

Write down as many **correct, distinct, and relevant facts** as you can about:

Acetaminophen metabolic pathways for excretion



Prescott, L. F. (1980)

Key: Gluc - sugar, HGS - glutathione

Five (5) statements will get you full credit for the problem, which is worth 5 points. Recall the information you use should be information you learned in a chemistry course, including general chemistry, organic chemistry, and biochemistry courses. All other outside information, combined, will only count as one distinct fact towards the correct responses. You may list more than five statements.