Shape, Transformation, and Energy: Critical Resources for Thinking in Chemistry

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At its heart chemistry is about putting substances together and pulling them apart, synthesizing and analyzing, and about explaining how that takes place. Under some circumstances this coming together and breaking apart is natural in that it occurs without direct planning or intervention on the part of the chemist. In these situation it is the role of the chemist to explain and understand what happened and why. Under other circumstances the phenomenon is planned for in the sense of being designed to meet certain purposes. In these situations it is the role of the chemist to predict, design, and modify what happens and why. What makes chemistry hard to learn and to understand is that both the level at which actions occur and the mechanisms by which they occur is atomic or subatomic. It is not simply that such activity can not be seen but that these molecular activities do not appear at the noticeable human scale. The pathway from atomic level structure to macroscopic features is complex and indirect. In addition, it is not possible to directly manipulate the microscopic features, making it difficult to develop intuition for the connection between the microscopic and macroscopic scales (Harrison & Treagust, 2004).

Chemistry is distinct from the other sciences (geology, biology, physics) in that it concerns itself with atoms and molecules thus concerning itself with issues intermediate between physics and biology. It is a domain that is partly reductive and partly descriptive. On the other hand it is a discipline of hyphens: bio-chemistry, geo-chemistry, physical chemistry precisely because it overlaps both in technique and fundamental inquiry the ranges of these other sciences. It is an enormously significant discipline for issues that range from environmental problems and their solutions to understanding medical mysteries such as HIV and finding weapons to attack them. It is a pragmatic discipline that has given us modern dye technology, silly putty, and plastics. It is home to the display of physical beauty inherent in crystal structures and it is this exciting and elegant world that the student is invited into by studying and learning chemistry.

Chemistry has proven to be a challenging subject in the school curriculum (Erduran, S. & Scerri 2004; Gilbert et al, 2004). No doubt this is for many of the same reasons that other sciences are challenging: it relies on mathematics, it has a unique and specialized vocabulary, it requires extreme attention to small distinctions, it operates at a non-human scale, it problematizes the world in a non obvious and non trivial manner. But there are intuitive resources for learning chemistry as well, chemistry and its fundamental ideas are manifested all around the young student. Water commonly exists in three states of matter: liquid, solid, and gaseous. Its crystal form of snowflakes hints at its underlying chemical structure. It is the role of education to support the question of how? Bicycle chains rust, aluminum screens oxidize, and the student has witnessed chemical combustion – it remains for the teacher to support the answers to the questions of why? The cook slowly stirs a sauce with eggs or corn starch and as if by magic the mixture suddenly thickens and takes on a new consistency. What is happening and why was heat needed?

Even with the existence of a set of examples from which to build and intuitions which can be nurtured there are some serious and rather unique challenges to the teaching of chemistry. Some of these challenges have been studied in carefully controlled research studies Harrison & Treagust, 2004), others are inferred from what we know about learning in other scientific fields (Hunt & Minstrell, 1994; Lehrer et al, 2000). We focus on three here and will return to them throughout the rest of the paper. First, the scale of processes both in terms of size and time is both below the human eye and not quite within the realm of easy imagination; twirling electrons linking things together is unlike most common experiences of joining and separating, the action is at the individual molecular level but the recognition is at the macroscopic level leaving the connection slippery indeed some have suggested teaching only within the molecular level to deal with this issue (Tabor & Coll, 2004). Second, keeping track of which of many levels is the targeted one for a particular action or state -- locating a pointer into the complex system in terms of time and action is tricky. Finally, the specific mathematical ideas of chemistry: the multiplicative structures of ratios and intensive quantities that are so elusive even to adults in medicine and engineering and that require careful understandings of the units that begin and the units that complete an action, dimensional analysis, is complex.

Our goal in this paper is to argue for several deep concepts in chemistry that can provide accurate and honest leverage to ideas throughout chemistry but which are accessible in some sense from the beginning. This means simplifying for younger students can not be done in a way that must be undone at a later time. The proposed concepts are **shape and structure**, **transformation**, and **energy and motion**. We are not arguing that these concepts are exhaustive but rather that they do an enormous amount of work in thinking about and in the domain. We are also arguing that these ideas be thought of as conceptual resources to be built up rather than learning objectives to be met. We arrived at this position by considering both what the activities of chemists actually are and what chemists do when thinking through a problem carefully before thinking about formulas or even principles.[1]

The rest of the paper examines what chemists do and how we might think about the overall organizations of chemistry drawing heavily on some recent work that contrasted chemistry texts with scientific discoveries as reported in the popular press and with Nobel prizes awarded in the last half century (Evans et al, 2004). We present some of the most common activities of chemistry and give a brief overview of conceptual resources. We then go into considerable detail about each of the resources: what they are, how the actions of chemists use these resources, what natural resources for learning are and where the challenges exist, we provide a few examples , and then link the ideas in the resources to national standards and some texts. We conclude the paper with a chemistry scenario and some thoughts concerning for critical features for immersion activities that might develop these resources. Throughout we provide examples of what we are discussing and ground each examination in the substances of water, plastic, and gold to provide a familiar anchor for considering these ideas.

<u>What Chemists Do</u>

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[1] We consider the idea of periodicity to be also of fundamental importance as an explanatory and organizational feature of chemistry. We did not choose it for two reasons, first it is already well represented in most chemistry instruction; second, it has moved from its venerable position in the Nineteenth and early Twentieth Century as an explanatory tool to an object of explanation from the atomic structure and the Schroedinger equations.

In our previous contrast between work in chemistry and discussions in texts and standards we asserted that there was a serious disconnect between the sequence and emphasis of ideas in most texts, curricula, and even standards and what the essential aspects of chemistry actually appear to be (Evans et al, 2004). In this paper we expand that idea to include an analysis of essential ideas within the field of chemistry and a set of anchored examples that span grade levels.

Chemists *analyze* matter to determine its composition, they *synthesize and design* new combinations for particular purposes, and they *explain* the actions and reactions of molecules at the atomic and macroscopic levels. To do these activities they make use of a variety of tools. Instruction in chemistry has focused considerable attention on the tools and on appropriate use of tools. But current investigations into learning and remembering has emphasized that knowledge of devices or procedures, such as tool use, tends to be easily forgotten and be unavailable for use in a circumstance other than the one in which it was learned (Greeno, 1997) If it is taught as a separated set of skills to be later assembled or put to use. Further, our own investigation into what exactly was reported on in terms of chemistry results or findings and what was rewarded in terms of Nobel prizes showed an emphasis on *synthesizing or design* activities, *analytic* activities, and *explanatory* activities. If these are the action systems of chemistry then our proposed resources must support and aid this type of chemistry understanding. Tools need to be taught within the context of their use, not as a set of disconnected skills that will be needed at some distant time.

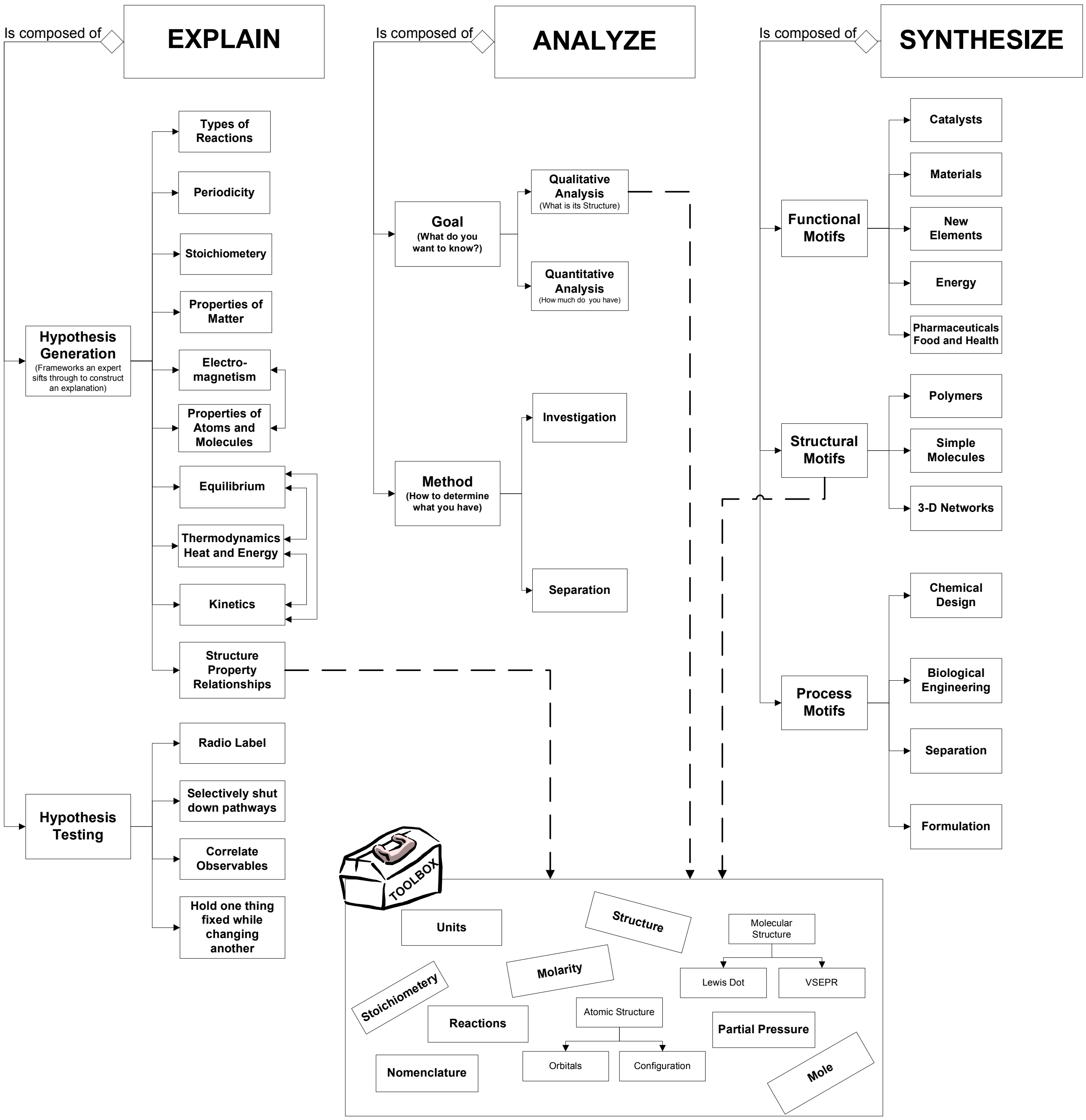

Figure 1: Activities adapted from Evans, Karabinos, Leinhardt and Yaron (2004)

Figure 1 displays the main activities of chemists. It is derived from the figure reported in Evans et al (2004). The activity of *designing and synthesizing* refers to the construction of new materials with desired properties. The design process is comprised of the desired function of the material, the structure used to achieve this function, and the process used to create this structure. Each of these design activities falls into general patterns that we refer to as motifs. Functional motifs include such things as catalysts, materials, new elements, energy, and drugs – they are the motivations or goals for the design activity. Structural motifs include polymers, simple molecules, and 3-D networks – they are structures that the chemist believes may exhibit the desired function. Process motifs include chemical design, biological engineering, separation, or formulation – they are processes or transformations that lead to the desired chemical structures. Taken together the constellation of actions associated with designing and synthesizing are how chemists make things.

The activity of *explaining* refers to the manner in which observations are interpreted and accounted for by chemists either when they are responding to something new and unknown or when they are intentionally developing something to behave in a particular way. In explaining chemists generate plausible hypotheses at the level of observation of phenomenon (macro-properties, reactions) in coordination with what is known at the level of chemical operation (micro) and then set about testing those with the set of tools that are appropriate. Some of the chemical level knowledge that supports the generation of hypotheses includes: types of reactions, periodicity, properties of atoms and molecules, kinetics, equilibrium, kinetics, thermodynamics, and structures. In constructing explanations chemists make extensive use of several representational systems to demonstrate the logic and sensibility of their results.

The activity of *analyzing* refers to the process by which chemists determine the make up of materials. Analytical goals include determining both the structure of the chemical components (qualitative analysis) and their amounts (quantitative analysis). The processes used in analysis include various means for separating mixtures into their chemical components and means for determining the structure of molecules. The processes of isolation or separation for the purposes of analyzing a chemical mixture link closely with the separation processes used for the synthetic goal of extracting a useful molecule from an available mixture.

These are the activities that comprise the work of chemists. They allow chemists to seek answers to a specific set of questions: What is it, what does it do, and what is it good for? This is the set of questions that provoke chemical analysis. How can I build it or improve it? Is the question that provokes the activity of design and synthesis. How do I know and why is it so? Provokes the activity of explanation. To engage in these activities chemists make use of a powerful set of conceptual resources. Figure 2 displays the conceptual resources that we consider to be especially significant. By conceptual resources we mean a type of intellectual touchstone that serves the core activities of chemistry. We consider these resources in terms of the actions of chemists. The three conceptual resources on which we are focusing are ***shape and structure***, ***assembly and transformation***, and ***energy and motion.***

Conceptual Resources

		Shape and Structure	Transformation and Assembly	Energy
Activity	Synthesis and Design			
	Explanation			
	Analysis			

Figure 2: Chemical activities and resources

Conceptual Resources Examined

Shape. ***Structure and shape*** is a core idea in chemistry because it provides one of the main explanatory and manipulative frameworks for the field. By structure we mean the arrangement of atoms in a material. These arrangements in turn effect the known properties of a substance allowing for both prediction and explanation. Chemists have a developed a variety of notational systems at the atomic and molecular level, orbitals, configurations, Lewis Dot, VSEPR, that support the description and manipulation of structural information. These notational systems have the advantage of allowing one to directly operate on the representation itself and quickly and intuitively explore and communicate structural ideas. The properties of a system are viewed as emergent from the structure, so that structure is the defining characteristic of a chemical system. Structural information spans a hierarchy from atomic structure to molecular structure to the structure of three dimensional assemblies. Atomic structure refers to the configuration of electrons within an atom, which establishes the number of bonds it would like to form with adjacent atoms (its valency). Molecular structure refers to the arrangement of atoms within a molecule. These molecules form three dimensional structures that can be either well defined (crystals) or more amorphous (glasses) and dynamic (liquids, gasses). Organic chemistry introduces an intermediate level of hierarchy, the functional group (alcohol, aldehyde, carboxylic acid), that consists of a few atoms arranged in a specific manner. Functional groups convey specific properties and behaviors onto the parent molecule. Envisioning a large molecule as being composed of functional groups (as opposed to atoms) therefore provides a useful means for understanding its properties and behaviors.

The notion of chemical structure goes well beyond shape to encompass a variety of features that results from the arrangement of nuclei and electrons. For instance, refined notations of shape include the spatial location of groups such as hydrogen bond donors and acceptors that influence the way molecules interact with one another and so help establish the structure of assemblies. In rational drug design, chemists optimize a drug by examining molecules whose structures are "similar" to those of a molecule with known drug activity.

Measures used to define "similar" give insight into how the domain envisions chemical structure. Such measures include the overall size and shape of the molecule, the absolute and relative spatial position of various functional groups, and the location of electron rich and deficient regions. Beyond shape, are aspects of a system that are "obvious" to a chemist based on its structure, but do not directly relate to shape. For instance, the presence of an –SH group means the molecule will have a pungent odor. Or the structure of ozone implies that it is highly reactive.

Structure plays a central role in the construction of *explanations*, with molecular structure typically taking center stage. Certain properties, such as reactivity or color, can often be understood directly in terms of molecular structure. Other properties, such as hardness, boiling point, and malleability are properties of the assembly. However, arguments still typically begin with the molecular structure and bridge to the assembly through the way in which structure influences the interactions between molecules. A sensible goal for instruction, one that meshes with all current standards, is to have student be able to explain observations and the basis for their predictions—in chemistry, understanding at some level the idea of structure permits such explanations to join the larger 'family' of chemical explanations. But as a considerable quantity of research has shown positioning students so that they can and do learn and use these processes of accountability to the field in their explanations is by no means trivial. (Lehrer et al 2000, Schwart & Martin, 2004). One difficulty in constructing an explanation from structure is that what appears at the collective level (reduced volume when colder, for example) does not take place at the molecular level – molecule do not shrink they pack closer (Bodner & Herron, 2004).

Molecular structure also plays a central role in *design*, since synthetic chemistry gives direct control of the placement of atoms in a molecule. The central location of activity is at the molecular level leaving the total 3-Dimensional assembly as more of an emergent property. When the target of the design is a particular assembly, the manipulation still occurs at the molecular level. The intent is that features conveyed on the molecules will cause them to assemble into the desired structure.

The target of a chemical *analysis* is the type (qualitative analysis) and amount (quantitative analysis) of all chemical substances in a given sample. Type is essentially defined in terms of molecular structure, since two molecules are considered identical if they have the same structure. The viewpoint of molecules as being constructed from functional groups is a key aspect of qualitative analysis, since many analytical techniques (spectroscopy) suggest the presence of a particular functional group and/or give information on its proximity to other functional groups. Senses such as taste and smell are often also sensitive to the presence of functional groups and this is why, for example, both sugar and saccharine both taste sweat.

A challenging aspect of building up an understanding of ***structure*** is that one must move flexibly between the various levels/scales of structure. Atomic structure determines the preferred number and arrangement of bonds around an atom, thereby establishing molecular structures. Molecular structure, in turn, determines the interactions between molecules and so establishes the structure of molecular assemblies. Explanations regarding properties of the assembly must move between the molecular structure itself, the manner in which this structure can influence interactions with other molecules and then the nature of the resultant assembly. A similar process occurs in design, since one may need to make a molecular structure that infers a particular property onto the assembly. Macroscopic properties are therefore "emergent properties" of molecular structure that are very nontrivial to predict.

The difficulty of trying to predict the macro behavior from the micro organizations is present at the forefront of the domain. For example, in the design of polymers that will lead to plastics with desirable properties chemists must place their bets based on deep understanding of the shape and structure of what is already known. Learning the domain in part means acquiring intuitions such as: "small spherical molecules will tend to be gaseous", "long stringy molecules will tend to form plastics", and "small polar molecules will tend to form tight crystals". Naturally, students will not have all of these ideas of structure immediately available from the beginning. The point here is that building from rather simple notions of structure students can begin to make use of the concept as a resource in explaining, analyzing, and synthesizing. Structure in and of itself is a highly intuitive notion that supports the concept of agency in chemistry. As Schauble and Lehrer have pointed out the idea of agency is particularly crucial to scientific and mathematical understandings in young students (Lehrer and Schauble, 2004).

Crossing between the various levels of the hierarchy is made especially challenging by the need to invoke different argumentation or explanatory frameworks at each level. The levels do not combine like a set of Russian dolls. At the atomic level, one argues in terms of the arrangement of electrons in atomic orbitals. At the molecular level, one argues in terms of both the arrangement of nuclei in the molecule and the behavior of the electrons moving among these nuclei. Molecular structure is sufficiently rich that chemists have evolved a number of notational systems. In some cases, such as Lewis-dot vs. bond diagrams vs. Fisher diagrams, the different notational systems focus attention on different aspects of what is essentially a single model of the molecule. In others, such as Lewis-dot vs. molecular orbital diagrams, the notational systems represent different models of the system that are complimentary but occasionally hard to reconcile.

Water provides an exemplar for how molecular structure, in this case a bent molecule that can both donate and accept two hydrogen bonds, leads to the emergent properties of ice, liquid water, and water vapor/clouds. On a more refined level, structural arguments can account for water having the unique property of being less dense as a crystal than a liquid, thus water when it is cold enough to form a solid takes up more space than when it is warm enough to be a liquid, an “exception to the rule” that makes ice float and therefore plays an important role in everyday life. The inertness and malleability of gold provides another example of how structure can account for properties. In this case the relatively simple structure of stacked spheres leads to an easily deformable material.

Structure and shape also provides an inroad to understanding the principle activities of practicing chemists. In both the pharmaceutical and polymer industries, chemists take advantage of the structural diversity of organic molecules by designing molecules to perform certain tasks. An important aspect of rational drug design is the tuning of structure--add a group here, remove a group there—to obtain a drug that binds tightly to the target protein. This lock and key vision should be elaborated to a deformable lock and key, but the centrality of structure remains. Highly deformable proteins such as HIV's integrase make the search for the correct drug structure (the key) harder, but the process remains one of hunting for the structure that will stick most strongly to integrase.

The polymer industry discovers and optimizes materials by working at multiple structure levels. Varying the repeat unit of the polymer leads to gross differences in properties, from the foam cup of polystyrene to the slick surface of Teflon to the clear properties of polyX (plexiglass). But keeping the repeat unit the same and changing the structure of the assembly by promoting more close-packed structures or building chemical bonds between polymer chains (cross-linking) is also a powerful design approach. For instance, the plastic used to build lawn chairs and that used for (some application of high density polyethylene) are both based on polyethylene. But the process is not always one of intentional design. Both conducting polymers and Kevlar were discovered while their inventors were in search of materials with other properties.

Developing the ideas of structure as conceptual resources will assist in meeting a variety of national and state standards.[2] Standards in the early grades emphasize knowing

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[2] We include an appendix that shows in greater detail the ways in which the developing of these resources would support advancement in learning state and national standards objectives.

many of the ideas but not necessarily understanding the way that they act within the activities of chemistry. For example, middle school standards frequently require students to describe substances in terms of properties that are structural in nature. Students are also required to explain changes in terms of underlying characteristics of materials (Middle School: Wisconsin D.4-8.1-2; California 8th grade section 3; Pennsylvania 3.4.7A; Colorado 2.1; Atlas 4D. High School: Colorado 2.1; Pennsylvania 3.4.10.A, 3.4.12.A; Wisconsin D.12.-2.5.8; California 9-12 Chemistry Sections 1-2; Atlas 4D).

Thus, we are arguing that a target for instruction be a set of activities that bring increasingly sophisticated ideas of chemical structure to the fore. Notational resources should only be built up in the service of one or more of the identified activities. Structure in and of itself is reasonably clear but the understanding of the relationship between the micro –atomic or molecular structure and the observed phenomenon and the fact that it is not recursive makes the idea difficult.

Transformation. Structure accounts for the arrangement of electrons, atoms, and molecules. ***Transformation*** focuses on the processes that can lead to structural change. Conservation of matter dictates that such transformations involve only rearrangements of the atoms and not the magical addition of new matter. The type of transformation that takes place relates to the level of the structural hierarchy at which the transformation takes place. Rearrangements of molecular structure, through the breaking and formation of chemical bonds, correspond to chemical changes. Chemical changes are typically associated with gross changes in a system’s properties and are difficult to reverse.

Rearrangements of molecules to change an assembly, for instance by melting ice or dissolving sugar in water, correspond to physical changes. In a physical process the chemical bonds of the molecule remain intact and it is only the interactions between molecules that are altered. We point this out because so many texts and even standards introduce the idea of physical versus chemical changes at very early levels and tend to treat them as if they were both quite simple to understand and not subtle with respect to chemistry itself; we do not agree.

Both chemical and physical ***transformations*** make use of classes of transformation as a basis for *explanation*. Chemical transformations occur through chemical reactions. Reasoning about reactions is done in terms of general classes such a redox, acid-base, or displacement reaction. Associated with each of these reaction types is a substantial framework that supports predictions of a reactions spontaneity, energetics and speed. For instance, half-cell potentials support predictions of the spontaneity of redox reactions, and acid dissociation constants do likewise for acid-base reactions. Physical transformations also fall into general classes such as changes of state (melting ice), dissolution (dissolving sugar in water), or precipitation (making rock candy from a sugar solution). Each class again has a predictive framework. For instance, phase diagrams provide a notational formalism for organizing data on changes of state and using the data to make predictions.

Explanations based on transformations are typically constructed by first attempting to fit the observed phenomenon into one of the known general classes, which then brings the explanatory framework of that class to bear on the system. The process by which one classifies a new phenomenon is essentially reasoning by analogy with known and well studied reactions or physical transformations. Obtaining the correct match can be quite subtle and will typically lead only to a hypothesis which then must be tested through various analytical means. Even the classification of a process as chemical or physical can be difficult from simple observations. Hammering a piece of gold into gold leaf is clearly a physical transformation since the material retains is chemical character. However, consider the heating of water and Mercuric Oxide. In both cases, a gas is formed that, on cooling, reforms the initial material. That the first is a physical transformation and the second is chemical transformation requires experiments that reveal the character of the gas being formed. The classification is then typically based on rules of thumb: when heating of a substance leads to reversible formation of a gas, it is most likely a physical (evaporation) transformation. Such rules allow one to select the most likely hypothesis.

Structure is the means for specifying the target of a chemical *design*. ***Transformation*** is the means of achieving that target. Indeed, molecular synthesis can be viewed as the use of chemical reactions to create a molecule of interest. In the twentieth century, chemists developed a wide range of reactions that allow construction of essentially any molecule of interest. Much less advanced is our ability to arrange molecules in specific patterns. The predominant means is to construct molecules that will spontaneously form the desired structure. This spontaneous formation of structure, driven by the shape of the molecule, is called “self assembly”. Directed assembly is in its infancy, with elegant demonstrations such as the use of metal tip to push argons atoms on a surface to, for instance, give the smallest known writing of the letters *IBM*.

Transformations are important tools for *analysis* of chemical samples. Analysis of complex samples typically begins with a separation of a mixture into its molecular components, a physical transformation. In qualitative analysis, the substances with which a molecular will react provide keys as to its identity. An example is the classic experiments where students identify unknown ions by measuring which solutions, when added, will induce precipitation reactions. In quantitative analysis, transformations lie at the heart of titrations. In a titration, the amount of a substance is determined by slow additions of known amounts of a reactive species. At the endpoint of the titration, the reactive species has completely transformed the substance to a different structure. The amount of reactive species that must be added to reach the endpoint is a measure of the amount of substance present before the titration.

Transformations are a routine part of everyday life, as such they form the basic foundation for an array of intuitions with which the student and teacher can work. The physical processes of molding gold or plastic into a new shape, dissolving sugar in water, and boiling water contrast with the chemical processes of combustion, the rusting of a nail, the yellowing (oxidation) of plastic, and the solidification of an egg when cooked. Seeing and beginning the explanation of these phenomenon support the extension of intuitions into solid explanations.

The national and state standards emphasize the significance of ideas of combination that lead to changes at the molecular level. In middle school the emphasis is on knowing that these things occur while in High School the emphasis is on understanding and explaining through analysis and synthesis; we noted that several standards seemed to skip ideas of transformation and move directly to consequences or attributes of such transformations. (Middle School: California Grade 8 section 5; Colorado 2.3, Wisconsin, D 8.4.7, D8.3; Pennsylvania 3.4.7A/4; Atlas 4D/7; NSES 5-8

PS A/24D/4. High School: California Grade 9-12 sections 3, 7, and 8; Wisconsin D.12.4.2,4,6,10; Pennsylvania 3.4,10.A and 3.4.12A, Colorado 2.1 and 2.3, Atlas 4D/7)

<u>Energy and Motion</u>. ***Energy and motion*** are core concepts in chemistry (Gilbert, et al, 2004). The flow of energy in a system plays an important role in determining how and why certain processes occur. Controlled flow of energy is also often a goal of chemists, as in the design of fuels or batteries. Energy and motion are also a central component of our visualizations of the microscopic world; the structure of a material is not static, but rather molecules and atoms are continually moving. The timescales on which this motion occurs forms the basis for spectroscopy, perhaps the most powerful tool for analyzing chemical samples.

Energy appears as both the kinetic energy of heat and the potential energy of chemical bonds. Heat is the energy associated with random, undirected motion of atoms and molecules. Temperature is a measure of the energy stored in this random motion. The formation of bonds releases energy in the form of heat while breaking bonds requires energy such as heat or light. During chemical transformations, energy flows between the potential energy of bonds and the random kinetic energy of heat this means that chemical reactions can consume or release heat.

The random ***motion*** associated with heat occurs at all levels of the structural hierarchy, and different formalisms and representations are used to visualize or account for these. For motion at the molecular level, it is useful to envision chemical bonds as springs, which are continuously vibrating. Chemical transformations involve the breaking of some springs and creation of new ones. These processes of breaking and making bonds are typically accelerated by increasing the temperature and thus the degree of random motion in the system.

Motion at the assembly level can be used to understand the states (gas, liquid, solid) of matter. In gases, molecules are moving freely as individual particles, undergoing occasional collisions with one another and with the walls of the container. This microscopic picture accounts for gasses tendency to expand to fill the available space and for their low density. In liquids, the molecules are in close contact with one another but can nevertheless slip by one another with relative ease. In solids, the molecules are trapped at specific points in the material; they can vibrate about this position but can not move over long distances. Both liquids and solids are dense, since the molecules are packed closely together, but only liquids flow, since the molecules in a solid are not free to slip by one another. The physical transformation between states is associated with the random motion of heat. When a solid is heated to its melting point, the random motion associated with the heat is sufficient to break apart the solid lattice and let molecules move about more freely. When a liquid is heated to its boiling point, the random motion is sufficient for molecules to break free of one another and move about in an isolated manner.

Chemists have developed a number of refinements on the energy concept., most notably, free energy and activation energy. These refinements bridge energy to transformations. A transformation is possible if it goes downhill in free energy. Note, however, that the introduction of free energy is a nontrivial extension of the energy concept—energy is a consequence of the first law of thermodynamics whereas free energy is a consequence of the second law. Activation energy is also a nontrivial extension of the energy concept. It can be visualized as barrier or mountain over which a system must climb to achieve a transformation. The activation energy connects energetics to the speed of a transformation with low activation energies being associated with fast transformation.

Light-matter interactions provide a direct probe of the motions occurring in a material. The oscillating electric field of the light interacts with motions that occur at the same frequency/speed as the light. Microwaves interact with rotational motions of molecules, infrared radiation interacts with bond vibrations and visible/ultraviolet light interacts with the motion of electrons. Magnetic resonance imaging (MRI) operates at the extreme low-energy side of the electromagnetic spectrum, using radio waves to reorient a nuclei's magnetic moment in an applied magnetic field. At the high-energy extreme, X-rays and gamma rays are emitted by nuclear transformations or are absorbed by molecules leading to the breaking of chemical bonds.

The notion of ***energy*** in chemistry is that of thermodynamics, which is considerably different than the mechanical energy of Newtonian physics. The most accessible exemplar of chemical energy is heat, but heat has a number of known conceptual difficulties. It is not a physical entity, as in Lavoisier's phlogiston, but yet can flow between substances. Heat is an object whereas cold is not—cold does not transfer to an object but heat does. Cold is the loss of heat or energy. For the student and the early scientists alike this is not an obvious idea (Goedhart & Kaper, 2004).

The interplay between the potential energy of chemical bonds and the random kinetic energy of heat is also known to be conceptually hard. The language of "storing energy in chemical bonds" brings up a false notion that breaking a bond somehow releases energy. (A misconception present even in beginning graduate students in chemistry.) The nature of chemical energy storage is considerably more subtle. It also takes energy to pull two bonded atoms apart and thereby break a bond. In combustion of wood, for instance, it takes energy to break the carbon-carbon (C-C) and carbon-hydrogen (C-H) bonds. However, the formation of the combustion products of carbon dioxide and water involves forming very strong carbon-oxygen (C-O) and oxygen-hydrogen (O-H) bonds. The energy released on the formation of the C-O and O-H bonds is much larger than the energy needed to break the C-C and C-H bonds, so there is a net release of energy. Chemical energy storage then operates by forming weak bonds that can later be exchanged for strong bonds.

The motion of chemical systems brings in another challenging issue of scale. Microscopic motions occur on time scales that are beyond the realm of everyday experience. For instance, it takes about 10^{-14} seconds for a bond to vibrate, corresponding to 10^{14} vibrations each second. Rotations are about 100 times slower, which is still outside the realm of everyday experience. However, an intuitive notion can be developed for relative time scales—in the time it takes a molecule to go through one full rotation, its bonds vibrate 100 times. Similarly, in the time it takes for a bond to vibrate once, the electrons will have orbited tens of times.

The framework developed for describing flow of ***energy*** in a system are powerful resources in the construction of *explanations*. For instance, this resource allows the release of heat during combustion to be linked to structural notions of bond strengths. Free energy enables predictions of whether a process can occur. Activation energy connects energetics the speed at which a transformation occurs. Motion is also important in *explanations*. For instance, motion is essential for understanding the proclivity of a gas to fill the available volume or the fluid nature of the liquid state.

In chemical analysis ***energy*** is often a target of the analysis but is rarely a useful tool for performing an *analysis*. For instance, analysis may reveal the energy given off by a reaction and so help characterize the potential of a material to act as a fuel or energy storage material. However, measurements of the energy are rarely used to identify an unknown substance. ***Motion***, on the other hand, is one of the most powerful tools of modern chemical *analysis* since it can be directly detected by light through spectroscopy. For instance, functional groups have specific frequencies at which their bonds vibrate and these can be detected with infrared spectroscopy. These frequencies then serve as fingerprints for identifying the presence of that functional group in a molecule, supporting molecular structure determination (qualitative analysis). The amount of light absorbed gives information on the amount of the molecule that is present (quantitative analysis).

In chemical *design* ***energy*** may be an important target as in the creation of energy storage materials for batteries. Energy also plays into the design process. For instance, bond strength considerations can help determine whether a certain structure is likely to be stable. Free energy considerations can help determine whether a transformation needed to create the desired material is indeed possible. Design may also pay attention to the motions occurring in the material to achieve certain desired properties. For instance, in liquid crystal displays (LCDs) some molecular motions are designed to be liquid-like while others are designed to be solid-like.

Heat is one of the best instantiations of chemical energy since it is so much a part of our everyday experience. Chemical combustion is our primary source of heat and energy generation. We are also concerned with removing heat from a system whether it is the state change of a liquid to a gas as in the way in which air conditioners usually work or by melting ice to cool a glass of water. Chemical bonds mediate energy flow in the biosphere, with animals consuming the hydrocarbons and gain energy through controlled combustion (calories!) releasing CO2 in water that plants later combine with sunlight and water. These examples provide a base from which to nourish a student's understanding of the interplay of energy and heat in chemical systems.

The national and state standards emphasize the significance of energy and the specific ideas around heat, flow and reaction. The standards seem to emphasize a series of specific pieces of knowledge without the functionality and sense of role that we have tried to provide. In middle school the emphasis is measuring quantities associated with energy and energy transfer. In High School the emphasis is on linking phases of matter with the appropriate kinetic and molecular theories. The work on the development of the resource associated with energy and motion described here connects to the following standards most directly. (Middle School: California Grade 8 3d,e, 5c; Colorado 5-8 2.2, 2.3; Wisconsin, D.8.4,6,8,9; Pennsylvania, 3.4.7B; Atlas 4D/3-4. High School: California Grade 9-12 chemistry section 7,8; Wisconsin D.12.3,7; Pennsylvania, 3.4.10B 3.4.12B; Colorado Grades 9-11 Section 2.2,3; Atlas 4D/4, 4D/9)

A Concluding Example

We think that our analysis of three of the conceptual resources and the scientific activities of chemists allows us to consider the nature of activities that might be of use in the classroom. We start with some assumptions. First, students have intuitions that can be stretched, molded, and built upon that are useful in developing these resources (Schwartz & Martin, 2004). Second, one task of instruction is to share with the student the ways in which the chemists problematize the world around them and a good approach to doing that is to make use of observed, or observable familiar phenomenon (Lehrer & Schauble, 2004). Third, by starting with something simple and yet provocative we can 'hang onto' a few examples that are revisited over the grades we can both make the ideas more subtle and complex and develop and increasingly sophisticated notion of agency. In the example that follows we emphasize building up the conceptual resource of ***structure and shape*** in order to engage in the activities of *explaining, synthesizing*, and *analyzing*.

Real and Wet. Water and oil provide a setting from which to explore chemical structure and physical transformations. For example, comparing the states of the pure substances gives a sense of their underlying structure. Frozen water is a hard crystalline solid while frozen oil is a more plastic solid. This can be understood in terms of water being a small molecule that solidifies with a well-defined structure while oil consists of flexible chain molecules that solidify by collapsing into a spaghetti-like mass. The molecular ***structure*** is reflected also when water and oil are liquid, with the chain structure of oil leading to a more viscous liquid than water. Finally, oil vaporizes at a higher temperature than water because the larger size of the molecules requires more heat energy to launch them into the gas phase than is needed for the smaller water molecule.

Addition of a salt lowers the freezing point of water and raises its boiling point. These colligative properties can also be understood at a molecular level. The salt interferes with the formation of the ice lattice, lowering the temperature at which the lattice begins to form. The interaction between salt and water is stronger than that between water itself, so salt makes it harder for water to break free from the liquid into the gas phase. This accounts for salt raising the boiling point.

The solubility of other molecules in water versus oil provides an opportunity for students to use notions of ***structure*** to make predictions and *explain*. That oil and water do not mix gives insight into the fundamental rule of solubility: like likes like. Oil and water are very different structurally and so do not mix. Substances will be soluble in liquids that are structurally similar. Sugar, with its many O-H bonds, is structurally similar to water and so dissolves preferentially in water. If sugar is shaken in a mixture of water and oil, it will choose to reside in the water layer. Capsin, the substance that makes red pepper, is structurally more similar to oil than water and so, when shaken in a bottle containing both oil and water, it will choose to reside in the oil layer. Ideally, we can identify a number of substances that dissolve in oil or in water to various degrees, so that the partitioning between the oil and water layers is easily visualized.

The difference in solubility between oil and water provides a powerful means for separating molecules. In the chemical technique named extraction, a substance is shaken in a container with water and oil, or any other two immiscible solvents. In this manner, the oil soluble substances can be "extracted" from the mixture by pouring off the oil layer and leaving the water soluble substances behind. This technique would allow students to use ***structural principles*** as resource for *analyzing* samples, for instance, by separating the salt from the oil in a puree of potato chips. Such separation are also a common process in chemical *synthesis*, allowing one to, for instance, extract or caffeine from tea or coffee.

The resources developed through activities relating to solubility can be brought to bear on *explaining* the mechanism of soap or the nature of biological membranes. Both rely on phospholipids, molecules that have a water-loving head attached to an oil-loving tail. Soap washes away substances that aren't usually soluble in water because the phospholipids arrange themselves in a sphere with their heads pointing into the water and their tails pointing inside the sphere to form an oil environment in which the dirt is soluble. These spheres are referred to as micelles. Reverse micelles make water soluble substances soluble in oil by pointing their tails out into the oil and their heads into the solute. A biological membrane is formed by making a double layer, with the heads pointing both outside the cell and inside the cell, such that the inside of the membrane consists of tails arranged end to end.

Virtual and Dry. There is enormous power, we believe, in using an apparently simple set of circumstances as the basis for a real investigation that can be developed over a long time and with increasing levels of sophistication as is the case with water and oil. However, the issue of the conceptual difficulty posed by moving from the microscopic reality which is unseeable and mysterious to the macroscopic visible one remains. The location of action in chemistry is molecular and the location of observation is molar.

Computer simulations may help overcome some of the conceptual challenges in connecting the microscopic to the macroscopic. As discussed earlier, this connection is difficult not only because of the large changes in scale, but because of the indirect means through which structure manifests at the macroscopic level and the lack of a direct means to manipulate and visualize the microscopic. A number of tools exist for visualizing molecular structure. Such tools can make the three dimensional structure of molecules quite vivid and are perhaps the best way to convey the immense complexity of a biological molecule such as hemoglobin. However, such visualizations leave the student in the microscopic scale and do not help bridge to the macroscopic.

Simulations can also provide animated images of molecular motion. For instance, simulators are available that show the molecules of a gas moving quickly through space and colliding with each other and the walls of the container. Students can control variables such as the temperature, allowing an exploration of the effects of temperature on molecular motion. These simulations also allow the connection between motion and macroscopic properties to be developed. For instance, the pressure of the gas can be connected to the collisions of the molecules with the walls of the container. The rate of reactions can also be partially understood in terms of the frequency with which two molecules collide and so have the opportunity to react. One can envision extending these simulations to include physical transformations such as the melting of ice or boiling of water.

The ideal simulation would be one that provided a learning environment in which students develop and use the resources of ***structure, transformation***, and ***energy*** to pursue *explain, analysis* and *design* activities. The development of such an environment is by no means obvious. To build notions of structure, a desirable feature is the ability to directly manipulate molecular structure and see its macroscopic consequences. The challenge is that the connection between structure and properties is an unachieved target of modern chemistry and so can not yet be simulated in a general manner. Plastics may provide an opportunity for a limited simulation in which the structural diversity resulting from choice of monomer, molecular chain length, and degree of cross linking is sufficiently narrow to be amenable to a simulation while still giving students a wide latitude in terms of structural choice. If the simulation produced quantities such as density, melting point, brittleness that are of importance to construction of chairs, combs or other objects, then students could engage in a design process where direct manipulation of chemical structure is used to pursue a macroscopic goal.

In this paper we tried to identify the key conceptual resources of chemistry and the ways in which they are used by chemists. We consider the resources to be broad ways of envisioning the microscopic world and how that world interplays with the macroscopic. As such, they provide overarching themes that can be introduced early to students and developed as students move through the curriculum. The educational task that remains is not to make students into little chemists but to help them share some of the chemists world view. This means that we need to find effective means of supporting students as they learn to problematize the world around them in ways that are familiar to chemists, as they develop a sense of agency or mechanism that resonates with that of the chemists, and as they begin to explain things in a way that is consistent with that of the chemist.

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Conceptual Resources

		Shape and Structure	Transformation and Assembly	Energy
Activity	Synthesis and Design			
	Explanation			
	Analysis			

Figure 2: Chemical activities and resources

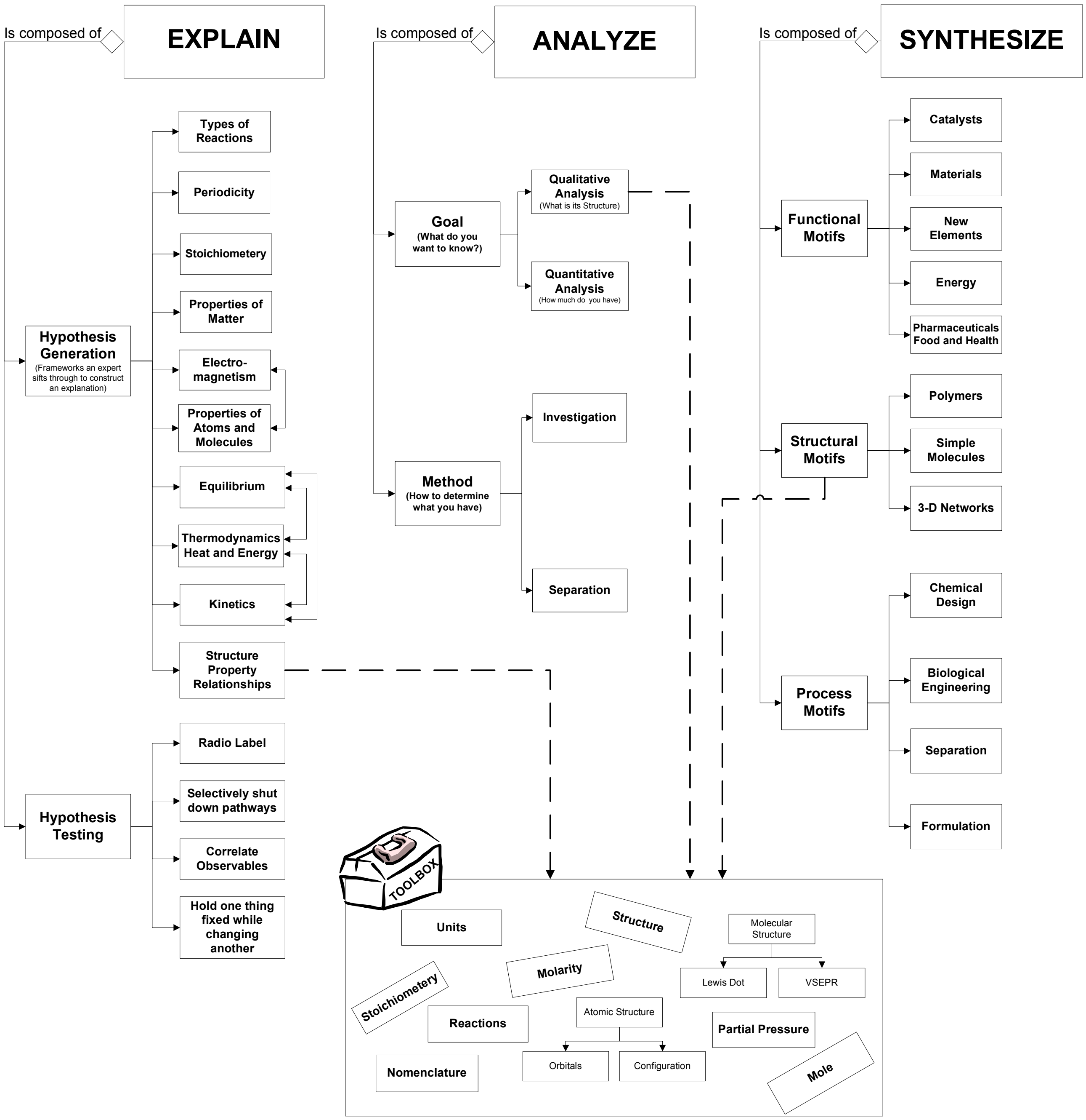

Figure 1: Activities adapted from Evans, Karabinos, Leinhardt and Yaron (2004)

Appendix Table I Middle School correlation with State and National Science Standards

	California Science Content Standards Grade 8	Pennsylvania Academic Standards for Science and Technology	Colorado Model Content Standards in Science Grades 5-8	Wisconsin Model Academic Standards 8th Grade Science	Project 2061 Benchmarks for Science Literacy Grades 5-8
Structure					
Atomic structure	3a	3.4.7.A/1	2.1/3	D.8.1	4D/1
Periodic trends		3.4.7.A/3	2.1/2	D.8.1	4D/6
Molecular structure-properties relationships	3c, 3e		2.1/4	D.8.2	4D/1
Transformations					
Rearrangements of molecular structure	5a	3.4.7.A/4	2.3/4	D.8.3	NSES 5-8 PS-A/2*
Rearrangements of molecular assembly	3b, 5d			D.8.7	
Conservation of matter	5b		2.3/3		4D/7
Energy and Motion					
Energy transfer a physical or chemical process	5c	3.4.7.B/3	2.2/2	D.8.4	4D/3
Molecular motion	3d, 3e	3.4.7.B/1	2.3/1-2	D.8.6 D.8.9	4D/4
Interactions of matter with electromagnetic radiation				D.8.8	

Appendix Table II High School correlation with State and National Science Standards

	California Science Content Standards: Chemistry Grade 9-12	Pennsylvania Academic Standards for Science and Technology	Colorado Model Content Standards in Science Grades 9-12	Wisconsin Model Academic Standards 12th Grade Science	Project 2061 Benchmarks for Science Literacy Grades 9-12
Structure					
Atomic structure	1d, 1e	3.4.10.A/1	2.1/1	D.12.1, D.12.2	4D/1 4D/2
Periodic trends	1a, 1b, 1c, 1g	3.4.10.A/2	2.1/2 2.1/3	D.12.5	4D/6
Molecular structure-properties relationships	2a, 2b, 2c, 2d	3.4.10.A/5 3.4.12.A/4		D.12.8	4D/8
Transformations					
Rearrangements of molecular structure	3a, 3g	3.4.12.A/2	2.1/4 2.3/1	D.12.4, D.12.6	4D/7
Rearrangements of molecular assembly	7c		2.1/4 2.3/1	D.12.1	
Conservation of matter	3e	3.4.10.A/6 3.4.12.A/7	2.3/2, 2.3/4	D.12.10	
Energy and Motion					
Energy transfer a physical or chemical process	7b. 7c, 7d, 8d	3.4.10.B/3 3.4.10.B/4 3.4.12.B/1	2.2/1, 2.2/2	D.12.3 D.12.10	4D/4
Molecular motion	4a, 4b, 4e, 4f, 6b, 6e, 7a, 8a, 8b	3.4.10.B/4 3.4.12.B/4	2.3/1-2	D.12.7 D.12.11	4D/9
Interactions of matter with electromagnetic radiation	1j	3.4.12.C/1		D.12.9 D.12.12	

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