A Tagmemic Semiotic Analysis of Chemical Representations

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A semiotic analysis of chemical formulas and reactions using tagmemic theory discloses many features relevant for semiotic structure. Among these are the etic/emic distinction; the presence of units, hierarchy, and specific system contexts; the relevance of particle, wave, and field perspectives; contrast, variation, and distribution in units; filler, prominence, and function in the hierarchy. In chemical representations, a principal hierarchy of three levels is spelled out: (i) the level of the smallest units, which includes the signs for the chemical elements, (ii) the level of the formulas for molecular compounds, and (iii) the level of equations for chemical reactions. Further, it is argued that chemists use not one but four distinct kinds of semiotic systems in describing these three levels: (a) formulas like H_2O to describe molecules; (b) descriptions using special technical vocabulary; (c) stick diagrams in two dimensions; and (d) three-dimensional models with balls representing the atoms. There are also hybrid descriptions that use resources from more than one of the four distinct systems. The analogous structural features that belong to chemical formulas, on the one hand, and natural languages, on the other hand, show that such a semiotic analysis of chemical formulas is appropriate and fruitful.

Keywords: chemistry, content, emic/etic, hierarchy, perspective, reference, sign system, tagmemic theory

1. Introduction

What kind of semiotic structure belongs to the notations of chemistry? The aim of the present investigation is to confirm that such notations of chemistry can be fruitfully analyzed using the tools of *tagmemic theory* (Pike 1967, 1982), showing extensive structural parallels between natural language and the notations of chemistry.

Chemists and students of chemistry talk and write about issues in chemistry using natural languages, which are clearly semiotic systems (e.g., Zlatev et al., 2023). So, in an obvious sense there could be an analysis of chemistry as a part of natural language. But such a generic analysis would not distinguish chemistry from any other topic of communication. Charles S. Peirce contemplated a new field that he called "phaneroscopy" (Peirce, 1906, p. 1; Tursman, 1989, p. 453), which he considered to be comparable to chemistry. His idea was to use bonding and valence in chemistry as an analogy for the bonding of thoughts or "phanerons" in the mind. In this respect, Peirce referred to chemistry by way of a playful analogy, using it as an inspiration for a general semiotic of the mind. More pertinent for the present approach are his wide-ranging explorations of diagrammatical thinking and icons (Ambrosio, 2023; Bellucci and Pietarinen, 2020; Peirce, 1931-58, 1.54, 1.369, 2.599, 2.778, 2.782, 3.419). But the task of this article is narrower: to demonstrate semiotic structure in the specific technical notations of chemistry.

What might distinguish chemistry from the point of view of semiotics is that elementary chemistry has a special system of signs in addition to natural language and technical vocabulary. It has the symbols for the chemical elements, often arranged in the "periodic table of the elements" (Németh, 2013), shown in Figure 1.

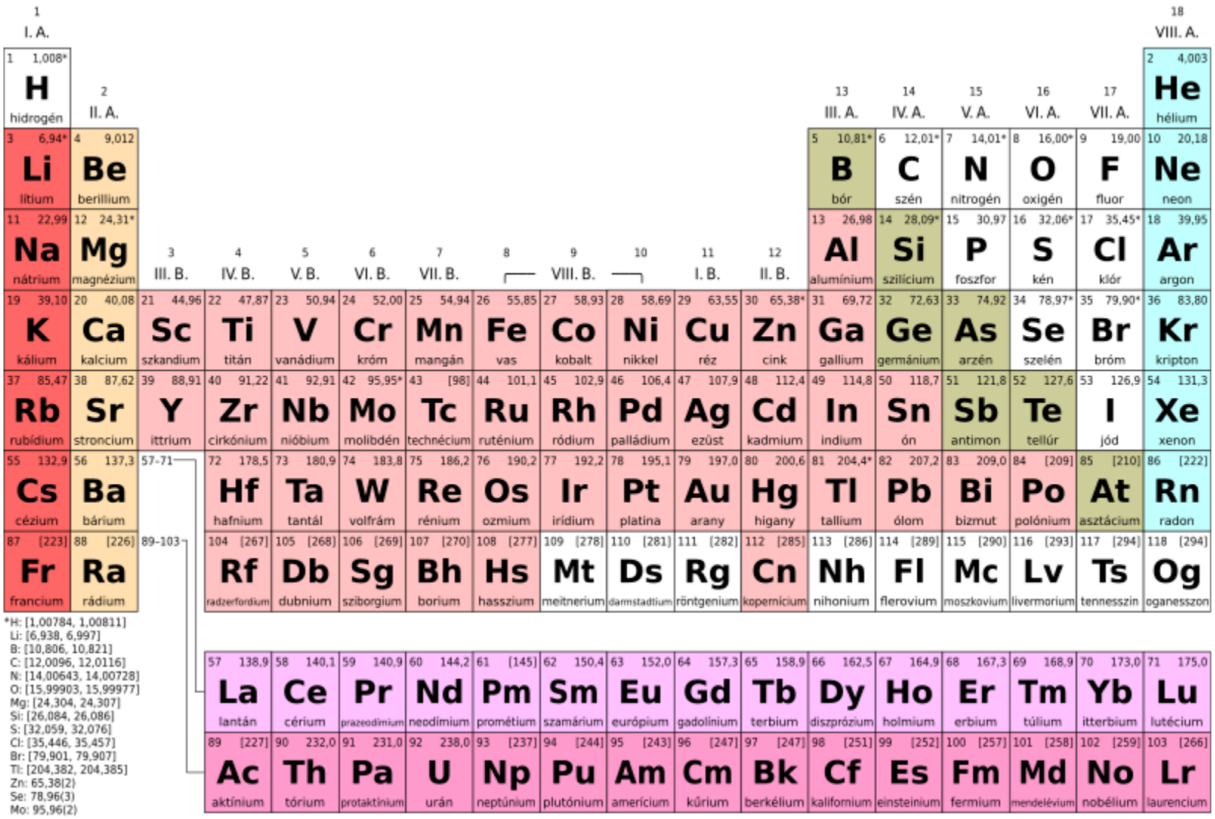

Figure 1. The periodic table of the elements
https://commons.wikimedia.org/wiki/File:Periodic_table_simple_hu.svg

According to the normal order of presenting the period table, the first entry is *H*, standing for hydrogen. Each chemical element has its own distinctive standard symbol, functioning as a *signifier*, in the sense of (Saussure, 1998 [1916]), representing the element hydrogen as a *signified*. Taken together, they form a *sign system*, where meaning is determined partly by the relations between the signs. The signifiers make up a distinct subsystem, a graphological subsystem, which supplements the normal graphological system of any natural language. The signifieds together make up a distinct subsystem. As emphasized in Saussurean semiotics, the relation between these subsystems is predominantly conventional.

Tagmemic theory belongs to this tradition of semiotics, but develops it considerably, as I will show in the following sections. Each of the following sections presents a specific aspect of tagmemic theory and then applies it to chemical representations. Section 2 focuses on the emic/etic distinction and the triad consisting in unit, hierarchy, and context. Section 3 focuses on three analytical perspectives (particle, wave, field), while Section 4 on the features of contrast, variation, and distribution. In Section 5, I discuss how adjusting the threshold for finer-grained analysis reveals structures like isotopes, isomers, and stereoisomers. This leads us to the key proposal to distinguish between four semiotic systems in chemical representations in Section 6 (formulas, technical terms, stick diagrams, and 3-D diagrams), and to see how they function in relation to different semiotic subsystems: expression, organization, and content, in Section 7, 8, and 9. Finally, I conclude that the tagmemic analysis of chemical representations reveals features shared with other semiotic systems, such as language, as well as differences, and touch on the difficult question of reference.

2. Tagmemic theory and chemical representations

While tagmemic theory (Pike, 1967, 1982) is best known as a framework for linguistic analysis, it is deliberately structured in such a way that it can be applied to any system of signs. One of its strengths as a semiotic theory is that it devotes explicit attention to what linguists have called *surface structure*, the visible or oral or perceptible aspect of communication of meanings (Pike, 1982, p. 111). As I will demonstrate, there are several alternate chemical notations. and each of these is a distinct sign system.

Tagmemic theory has also incorporated specifically the *emic/etic distinction*. The emic is the "insider" point of view, while the etic is that of an outside analyst (Headland, Pike & Harris, 1990; Mostowlansky & Rota, 2023; Pike, 1967; Poythress, 2009). This is important in differentiating between chemists' understanding of their notations (emic) and analysts' discussion of how chemical notation compares to other semiotic systems (etic), one of which is English as a natural language; but the scope of possible comparisons is enlarged by the tagmemic framework itself, due to its aim of characterizing semiotic systems of all kinds. Tagmemic theory also explicitly incorporates the discussion of multiple possible analytic viewpoints, each chosen by the observer or analyst (Pike, 1982, p. 3). This observer choice comes to the fore in considering how chemists can choose to introduce finer distinctions within a normal emic unit consisting of a single element, or an emic unit consisting of a molecular formula.

According to tagmemic theory, semiotic systems may be expected to be organized in terms of units, hierarchies, and contexts (Pike, 1982). Units are fixed "pieces" within a semiotic system, recognized as distinct by users of the system. For example, the word *dog* is a distinct unit in English. Hierarchies are organizations of smaller pieces into larger and larger structures. The two words *the* and *dog* can be composed together into a larger-sized unit, the phrase *the dog*. Third, contexts are larger frameworks of associations that influence the interpretation of any one piece. For example, the word *dog* functions within the graphological subsystem in contrast to neighboring related words like *hog* and *bog* and *cog*. It functions with the subsystem of signifieds in contrast to words designating other animals. As shown in this section, this kind organization also occur with chemical formulas.

2.1. Units

Each signifier for a chemical element is a *unit* in the semiotic system of chemical notation. It is, in fact, a minimal unit: the smallest emic unit in a hierarchy of units; it is a ground-level unit (Pike, 1967). Normal participants in conversations about chemistry have an emic point of view. A semiotician stands outside the conversations in order to analyze them. But the semiotician may investigate the chosen field of study either to determine *emic* units, as perceived by the insiders, or to see universal properties in relation to many semiotic systems, implying an *etic* point of view.[1]

2.2. Hierarchy

Hierarchy occurs in chemical formulas because chemistry includes not only signifiers for individual elements, but signifiers for compounds. For example, H_2O is the chemical symbol for water. It is composed of three ground-level "symbols", namely *H, 2*, and *O*. Taken together, these three ground-level signifiers and the corresponding signifieds make up a single unit at the next higher level of a hierarchy (Pike, 1982; Weaver, 1985).

The ground-level signs are thus comparable to single-morpheme words in a natural language. They cannot be further decomposed in meaning. The next higher level, which is used to designate molecules, is like the phrase level in a natural language. Each phrase is composed of a string of words, according to certain rules of composition. Likewise, each signifier for a molecule

[1] Here, I use these notions in this restricted sense, without entering the larger debate about social-scientific methods that sprang from the distinction (Harris, 1976; Headland, Pike, and Harris, 1990)

like *H_2O* is composed of the word-like ground-level *H, 2*, and *O.* All the ground-level signifiers in this semiotic system are of three kinds: either a single capital letter (such as *H*), or a sequence of two letters, with only the first capitalized (such as *He* for helium), or a numeral (such as *2*). The letters come from the standard roman alphabet. From the point of view of chemistry, the signifier *He* for helium is not further decomposable. It is a ground-level emic unit within the special semiotic system for the chemical elements.

There is also a *syntax* for the notation for molecules. In the formula for a molecule, a numeral can only occur immediately following a signifier standing for an element. The numeral *1* is not used but instead is indicated by the absence of any numeral. So *H_2O* would have the same meaning as H_2O_1, if the latter were allowed by the syntax of the system.

Is there a level of hierarchy above the phrase level? In this semiotic system, the next level with special symbols is the level of equations for chemical reactions. We may use as an example the equation describing the reaction of hydrogen molecules and oxygen molecules together to form water, as shown in example (1).

(1) $2\ H_2 + O_2 \rightarrow 2\ H_2O$

This level of hierarchy can be thought of as analogous to the clause or sentence level in a natural language. It makes a "statement" about how molecules interact. For the benefit of non-chemists, this particular equation says that two molecules of hydrogen (H_2), each of which is composed of two atoms of hydrogen (H), combine with one molecule of oxygen (O_2), composed of two atoms of oxygen (O), in order to form two molecules of water (H_2O).

We therefore have three sizes of units. The smallest or ground-level size is the signifier for an element. The subscript numerals that may attach to the chemical symbols also count as units of the smallest size. The next larger size is the phrase size, made up of a sequence of minimal units. The next larger size after the phrase size is the sentence size, to describe chemical reactions. These three kinds of unit form a hierarchy. Within the hierarchy, each unit is composed of units of the lower sizes below it.

As in language, there can be "level skipping". Just as some phrases in English, like *it*, are composed of a single word, some molecules in chemistry are composed of a single atom of an element. The element argon (Ar), for example, can occur in gaseous form, in which no one atom of argon is bonded to another atom. So a single molecule of argon is represented with the phrase *Ar*, which is also the word-level or ground-level sign for the element argon. Or in other words, the sign *Ar* functions as both a word and a phrase, simultaneously filling a role on two levels of the hierarchy.

2.3. Contexts

The third key aspect of the theory is that of context (Pike, 1982, p. 107). Each unit, and each structure within a hierarchy, functions in relation to multiple contexts. There is, of course, a large context of communication among human beings about chemistry (Schummer, 1994, 1997). There is the context of the world of chemical reactions. But there are also contexts closer to the inner aspects of the semiotic system. As emphasized already by Saussure, each sign in the system functions in contrast to all the other signs in the system. And all the signs together form a field of relations.

In fact, the periodic table itself shown in Figure 1 is a two-dimensional diagram of salient relations between elements. Any two adjacent elements in the horizontal direction have a relation in which the right-hand element is the next one up in a natural order. The first element in a new row is the next one up after the last element in the previous row. The new element has one more proton in the nucleus than its predecessor, and neutral atoms have one more electron than those of the preceding element. Any two elements in the same vertical column have a relation of sharing the same valence, at least roughly speaking. And it is valence that is a main factor in what molecular compounds the atom will naturally join.

As an example, consider column 1 (the left-most column) in the table. It contains the alkali metals, lithium, sodium, potassium, rubidium, and cesium, with valence +1. These elements have an electron shell structure such that they can easily "donate" a single outer electron to a nearby atom. They easily make compounds with elements of valence −1 like fluorine and chlorine. There is therefore a natural affinity between all the elements in this single vertical column. This affinity belongs not only to the technical details of electron shell structure, but to the *kind* of chemical reactions into which they enter, and the kind of molecular structures in which they participate.

In using the periodic table, chemists show that they ascribe multidimensional meanings to the chemical symbols for the elements. Each signifier, such as *O* for oxygen, exists not only with a distinct signified (one chemical element), but in relation to the signifieds of neighboring signifiers in the two-dimensional array of the periodic table. For example, *O* has a special relation to *S* (for sulfur) and *Se* (for selenium), because the latter two elements belong to the same column of the periodic table and therefore share a meaning-component with O, namely the valence −2.

One might say that the periodic table is a kind of chemical analog to a multi-dimensional table constructed for a natural language, classifying types of sounds or types of morphemes in the language. For example, personal pronouns in English can be classified in three intersecting dimensions: (a) singular or plural; (b) person (first, second, or third person); and (c) grammatical function (subject [*I*], object [*me*], possessive [*my*], predicate possessive [*mine*]).

3. Contexts and perspectives

The element of *context* discussed in the previous section leads naturally to a discussion of three main perspectives employed in tagmemic theory: the particle perspective, the wave perspective, and the field perspective (Pike, 1959, 1982). Each of these three is a perspective on the *whole* of a semiotic system, and they are thus complementary rather than competitive. The particle view analyzes a semiotic system as broken into stable "chunks"; the wave view treats the system as processes; the field view treats the system as a network of associations or relations. For example, the word *dog* is a chunk. It is a stable emic whole that can be reidentified in each occurrence. At the same time, in actual use it is a process. It is transmitted or received as a temporal sequence of letters d-o-g in writing or phonemes in oral discourse. In typescript the letters are completely discrete. But in script writing they flow into one another, and the exact shape of one is influenced slightly by the preceding or succeeding letters. Similarly, in oral communication the exact character of the sound of individual phonemes is influenced by neighboring phonemes, before and after.

3.1. The particle perspective

With respect to the semiotic system of chemical notation, the particle perspective treats a whole system as a system of discrete units, as Section 2.1 and 2.2. This perspective is usually the most common and natural one for naive users of the semiotic system.

3.2. The wave perspective

The wave perspective treats the whole system as a system of processes (Weaver, 1985 p. 299, tenets 2-3). Oral communication has a natural wave structure, because it is spread out in time. One sound leads into another. In chemistry, the processes in communication can be either oral or written. Each act of communication can be viewed as a process, starting with the beginning of the discourse and traveling to the end. It is analogous with processes in the world to which the chemical notations refer. These processes are chemical interactions and reactions, which are symbolized by reaction equations. Atoms of an element do not "stay put" forever, but rather interact with other atoms. In fact, it is only through interactions that chemists can identify which atom belongs to which element. Chemists are aware of these processes, as is demonstrated by their use of reac-

tion equations. It seems natural to think of the atoms as more "basic" than the processes in which they participate. Likewise, the chemical symbols for atoms are more "basic" than the reaction equations that represent chemical process. Yet for a chemist, the processes are in fact more basic than the elements when it comes to identifying and understanding what is what. The significance of a particular element is that all its atoms can participate in the *same* processes.

In chemistry in its earlier "classic" phase, the focus was on processes involving interactions with other atoms of other elements. In the present day, small quantities of material can be analyzed spectroscopically. In such an analysis, the interaction is not a direct chemical interaction with other atoms, but an interaction mediated by light. But such an interaction is still a process. Processes reveal the capabilities of the elements. In chemistry, the processes represented by reaction equations, are the clues to identifying the particle-like units, the atoms,

3.3. The field perspective

The field perspective analyzes a semiotic system as a system of *associations* or *relations*, in multiple dimensions (Pike, 1982; Weaver, 1985, tenets 1, 9). As we have already seen, the periodic table is a two-dimensional representation of a two-dimensional system of natural relations among the elements. The periodic table reveals a natural field aspect belonging to chemistry.

In fact, the understanding of any one element, as a particle, depends not only on processes ("waves") but on relations (a field structure). To see what an element can do, one explores how it combines with *other elements*. How does it enter into *relations* with these elements, especially in molecular compounds? Even if there were no periodic table, relations between atoms and between elements would play a key role in our understanding of the capabilities of each element. The capability of an element is revealed in relations. So also when it comes to the signs of the semiotic system of chemical formulas. The meanings of the signs are revealed in the relations of co-occurrence and contrast with other signs.

Moreover, for compounds, characteristics like color, hardness, and solubility cannot be accounted for merely by naively averaging the characteristics of the elements that make up the compound. For example, at room temperature hydrogen and oxygen are gases, but the compound H_2O (water) is liquid. The characteristics of waters are, as it were, *relational* characteristics. They are a product of the established relations between two elements within the compound H_2O. The properties of water arise neither from hydrogen alone, nor from oxygen alone, nor from averaging the properties of hydrogen and oxygen (as might be achieved from simply mixing the two gases together without a chemical reaction). Taking into account the bonding *relation* between hydrogen and oxygen is essential for understanding the behavior of the compound. This is also the case with chemists' understanding of the meaning of the signs in the system.

4. Contrast, variation, and distribution

According to tagmemic theory, each emic unit enjoys contrastive-identificational features (or contrast, for short), variation, and distribution. These three aspects derive respectively from the use of the particle, wave, and field perspectives (Poythress, 1982a), described in the previous section. We may illustrate once again using the example of the word *dog*. The word contrasts with other words like *hog* and *cog*. It has two variant forms, namely singular *dog* and plural *dogs*. And it can be used to refer to a whole spectrum of entities in the world, dogs of various breeds, ages, and sizes. This spectrum of reference shows the existence of *variation* in the word. Finally, the *distribution* is the cluster of typical contexts in which the word *dog* occurs. It occurs as a noun at the head of a noun phrase. It occurs in communicative environments in which people want to talk about dogs. It is straightforward to show that emic units in the notation of chemistry possess these three aspects.

4.1. Contrast and variation

Each unit contrasts with other units. And it has *identifying* features that function to identify it positively and to serve as a contrast negatively with other distinct units. So, for example, the signifier *H* for hydrogen contrasts graphologically with signifier for other elements, such as *O* for oxygen and *He* for helium. Likewise, there is corresponding contrast in the signifieds: hydrogen, contrasts to oxygen, helium, and molecular compounds.

Each unit can undergo *variation* and still be identifiable as the *same* emic unit. Different occurrences of the signifier *H* count as variants of the same type. Correspondingly, each new atom is a variation in comparison with the atom type.

4.2. Distribution

Distribution is the framework of expected contexts, both grammatical and topical, in which a particular unit is expected to appear. The idea of valence in chemistry is closely related to distribution. In the world that chemists discuss, elements with valence +1 (alkali metals) form compounds in those situations in which they can donate a single electron (as symbolized by the valence of +1) to a molecular complex. Their *distribution* is the complete set of molecular frames within which the donation of the one electron completes an electronic shell. Similarly, in the system of chemical notation, the distribution of the signifier for a given element will correlate with its valence: the signifier appears in the context of notations for molecules with appropriate valence relations.

An example may illustrate. In the world of atoms, the radical -OH, the hydroxide radical, needs one extra electron to complete the outermost election shell of 8 electrons in the oxygen atom. Sodium (Na), an alkali metal with valence +1, has a single loose electron to donate. So it easily forms a molecule NaOH, sodium hydroxide. The radical -OH is thus part of the distribution of Na. These limitations on the way chemical compounds are formed are then mirrored in the way the chemical symbols are used together. Correspondingly, in the relations among signifiers, *Na* for sodium will be found to group together with *OH* into *NaOH*, which is a phrase-like whole at the next level of the semiotic hierarchy.

5. Thresholds for focus

We have treated the chemical symbols for the elements as minimum-size emic units. In much of the usual work of chemistry, the focus of attention does not travel below a certain minimum, or "threshold" (Pike, 1967, pp. 111, 129–130). But in special situations chemical analysis finds it important to differentiate more minutely. It is possible for a chemist to shift the threshold of attention to distinguish isotopes *within* a single chemical element. This shift illustrates the power of the observer/analyst, in this case the chemist, to differentiate more minutely and to create new emic units within the old undifferentiated unit (a single chemical element).[2]

From the standpoint of tagmemic theory, isotopes (Section 5.1), isomers (Section 5.2), and stereoisomers (Section 5.3) are three different illustrations of the possibility of expanding a semiotic system to focus explicitly on variations that were initially considered etic variations on the same emic unit. The choice of threshold of attention is up to the chemist, depending on his or her focus.

[2] The units are *emic*, since they are described with specific standard notation, within the subculture of chemists interesting in the study of isotopes.

5.1. Isotopes

In the case of elements, one of the interesting variants is isotopic variation. The same element can have instances with distinct masses, depending on the number of neutrons in the nucleus. For example, there is variant form of hydrogen called *deuterium*, which has one neutron in the nucleus in addition to the one proton. It is called an "isotope of hydrogen". Correspondingly, a notation has been developed to have a regular way of unambiguously identifying these variants: the signifier ^{1}H designates ordinary hydrogen, with one proton and no neutron in the nucleus. The superscript 1 preceding the letter *H* indicates the total number of nucleons, that is, protons plus neutrons. The signifier ^{2}H designates deuterium, with one proton and one neutron, for a total of two nucleons, and correspondingly, the ^{3}H designates tritium, which has one proton and two neutrons. Carbon (C) has three naturally occurring isotopes, carbon-12 (^{12}C, the most common, with six protons and six neutrons), carbon-13 (^{13}C, with six protons and seven neutrons), and carbon-14 (^{14}C, with eight neutrons, which is radioactive).

From the standpoint of normal elementary chemistry, these isotopes are variants of one emic unit, namely the element carbon, signified by *C*. All three isotopes form the same molecular compounds and enter into the same chemical reactions. Consequently, much of the notation for chemical analysis does not distinguish between isotopes of the same element. For example, the formula for water, H_2O, does not specify any particular isotope of H (hydrogen) or O (oxygen). But a chemist has the choice of introducing an emic distinction when he or she makes a transition to focusing on the specific chemistry of isotopes. Within the context of a universe of discourse dealing with isotopes, each distinct notation for a distinct isotope then becomes a distinct emic unit. There are still variations among the different instances of this emic unit, but they are variations in the location in a text. In the world of chemical reactions, in the actually bonding of the unit, the variations are variations in bonding, not within the internal structure of the unit.

5.2. Isomers

The distinction between etic and emic points of view comes up not only because of variations in the number of neutrons (isotopes), but subtle variations in molecular structure. The same chemical formula for a molecule can sometimes be realized in more than one shape. The distinct shapes are called *isomers*. For example, butane, C_4H_{10}, has four carbon atoms and ten hydrogen atoms. It occurs in two distinct isomers: a branched form and an unbranched form. The same formula C_4H_{10} applies to both forms equally. To distinguish them, one must employ not a formula but a two-dimensional diagram that shows the connections, as shown in Figure 2.

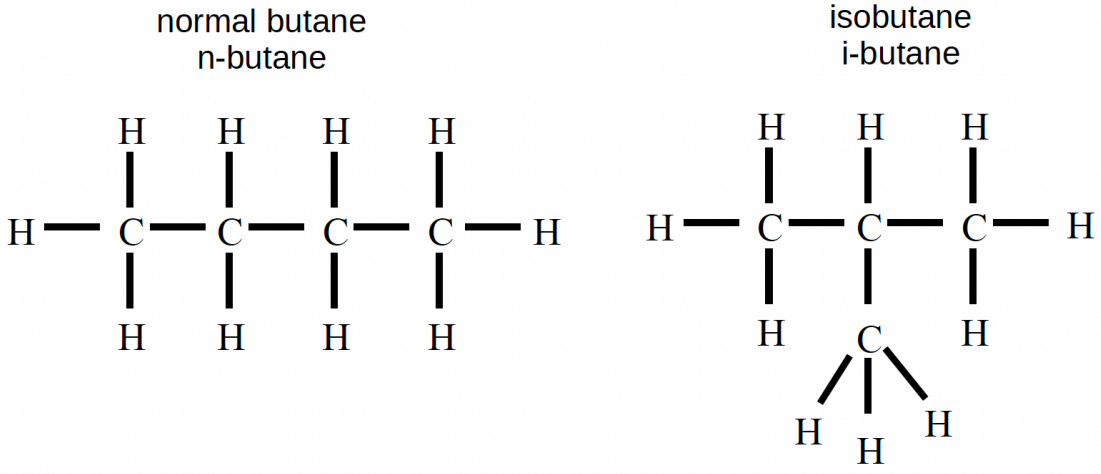

Figure 2. Two different isomers of butane

From the standpoint of the most elementary forms of chemistry, these two isomers are etic variants of the same emic unit, butane, C_4H_{10}. [3]This unit is one member of the phrase level of the semiotic hierarchy in chemistry. The fact that chemists give the same name *butane* to the two variants confirms that, from an elementary point of view, the two are treated as the same emic unit. However, it is possible to differentiate, as the two-dimensional diagrams in Figure 2 demonstrate. And in a more refined naming system, the two isomers receive distinct names, *n-butane* and *i-butane*. Whether the difference is considered etic (and therefore ignored) or emic (and therefore explicitly in focus) depends on the larger universe of discourse, within the field of chemistry. A chemist makes a choice in a particular act of communication as to which universe of discourse he is inhabiting.

5.3. Stereoisomers

The most subtle form of difference in isomers is a difference in handedness, called "stereoisomerism" (Jones, 2023). For example, there are left-handed and right-handed amino acids. Consider the amino acid alaline. It has two stereoisomers: left-handed alanine (L-alanine, where *L* stands for *levo*, 'left') and right-handed alanine (D-alanine, where *D* stands for *dextro*, 'right'). These are not identical in shape, but are mirror images of each other (like a left hand and a right hand in the human body). The two forms have identical chemical bonding (except for handedness) and identical chemical reactions until they participate in a reaction in which they combine with another molecule that *also* has a handedness.

It is well known that normal proteins in cells are constructed from left-handed amino acids, not right-handed, called "homochirality" (AstroAli, 2026; Ozturk Lab, 2026). A combination of left-handed and right-handed amino acids would not have the same functionality. Since the difference between a left-handed and a right-handed amino acid with the same chemical formula cannot be properly represented in a two-dimensional diagram, one needs a three-dimensional model. With complicated biological molecules a three-dimensional model is also needed in order to show the possible bonding interactions between various parts of the *same* large molecule, or to show how an enzyme (typically a protein molecule) has a spatial configuration that enables it to interact precisely in catalyzing a chemical reaction inside a cell.

6. Representations in different semiotic systems

The examination of isomers illustrates the fact that chemists have had to invent several different kinds of sign systems for representing chemical phenomena (Francoeur, 1997; Kozma et al., 2000; McDermott & Hand, 2013).

The simplest and perhaps the most familiar is the use of a *formulas* like H_2O for water or C_4H_{10} for butane, as used in Sections 2, 3, and 5. A second alternative is to use *special vocabulary* that allows unambiguous identification of the most common chemical compounds. This special vocabulary includes the term *butane* for C_4H_{10}, but also the capability of making further distinctions between isomers: *n-butane* versus *i-butane*.

But as shown in Section 5, there is a third alternative, illustrated in Figure 2: a *two-dimensional stick diagram* or graph, showing not only the atoms but the chemical bonds between them. For large molecules, this system of notation is clearer and easier than using technical terminology, showing an advantage of diagrammatic representations (Peirce, 1931-58, 1.54). A practical disadvantage, however, is that it has to employ two dimensions. That may make it inconvenient when one wants to embed the designation within a discourse in writing.

[3] This is *etic* because it is outside the focus on discussion within elementary chemistry. But it is easy later on for a chemist to shift to the more minute descriptions of isotopes. At that point, the distinctions are emic (and recognized as such by fellow chemists).

The fourth alternative is to produce a *three-dimensional model*, with balls to represent the atoms and sticks or snaps of some kind to represent the chemical bonds between the atoms. As mentioned in Section 5.3, this kind of three-dimensional model is necessary in order adequately to represent the difference between stereoisomers. It is also necessary to show the possible three-dimensional configurations of very large molecules. Enzymes may depend on an ability to change their spatial configuration as they catalyze a specific chemical reaction.

The diagrams of molecules used in chemistry textbooks and on the internet sometimes rely on subtle modifications of the bonding lines, in order to signify that one bonding line would in reality come forward out of the plane of the page, and another would go backward below the plane of the page, as shown in Figure 3. There, the wedge-shaped line (joining a *C* to NH_2) represents a bond that comes forward out of the page from the C atom. The dotted line represents a bond that travels from the C atom backward below the page. A representation of this kind is clearly a compromise, due to the resources of a two-dimensional page: it represents in two dimensions a shape that is three-dimensional.

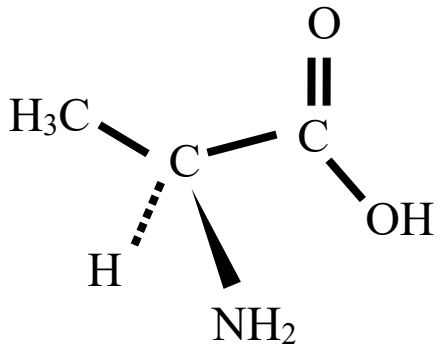

Figure 3. Three-dimensional structure of L-alanine

These four notations used by chemists as supplements to the resources of natural language constitute different semiotic systems, since they consist of (at least somewhat) different signs and relations between them (Zlatev et al., 2023). Each one has its own advantages and disadvantages. The three-dimensional model is clearly the best for the fullest representation of the information about molecular bonds. But it is the least convenient if the medium is oral communication or a quick summary.

We should note also that there are hybrids using combinations of the different sign systems. As mentioned, Figure 3 is mostly a two-dimensional stick diagram. But the use of the wedge-shaped line and the dotted line imitate the ideas belonging to the three-dimensional model. Moreover, rather than fully producing a stick model at every point, it conveniently uses an abbreviated form for some of the minor clusters of atoms. On the left of the figure, H_3C signifies a methyl group consisting of a central carbon atom and three attached hydrogen atoms. Toward the bottom of the figure NH_2 signifies an amine group, with a central nitrogen atom and two attached hydrogen atoms. And to the right, *OH* signifies a hydroxyl group. These notations follow the pattern of the first kind of notation, namely molecular formulas.

The third level of the emic hierarchy, the level of chemical reactions (Section 2.2), is most commonly represented by using formulas, with additional conventional signs like + for bringing two molecules together and an arrow → for the process of reaction. If the reaction is a two-way reaction, one uses a two-way arrow: ↔ or ⇄.

But it is possible, with some effort, to represent a chemical reaction in the notations of the other semiotic systems as well. If we use the technical terms for molecules, the reaction itself is

normally represented using natural language to connect the phrases. Thus we have the description in (2).

(2) *Two molecules of hydrogen plus one molecule of oxygen combine to produce two molecules of water.*

If we use stick diagrams, we can represent each of the molecules in a distinct stick diagram and then connect them using the same signs as in chemical formulas: + and →. If we use three-dimensional models, we can again use the connecting signs + and →. Or, with even more iconicity, we might undertake to produce a video clip that shows the interactions of the atoms as a dynamic process. In this case, we have shifted to a wave perspective (see Section 3.2).

7. Intermediate emic units

Our brief look at representational hybrids in the previous section has exposed another aspect of the structure of emic units in chemistry. There are units consisting in symbolic representations of some *parts* of a molecule. The parts are intermediate in size between single atoms and complete molecules. The methyl group H_3C (often written $-CH_3$), the amine group $-NH_2$, and the hydroxyl group -OH are instances of such parts, or *radicals*. Another such group is the phenyl group or phenyl ring ($-C_6H_5$), consisting of a hexagonal ring of six carbon atoms, joined by single and double bonds. These are clearly *emic units*, because chemists often view them as discrete wholes because their occurrence is so common.

If, then, these radicals are emic units, do they offer us an intermediate *level* of units: a level higher than the level for atoms but still lower than the level for complete molecules? The answer is "no". There are intermediate-size emic *units*, but there is no discrete emic *level* between the word level and the phrase level in chemical notation. To see why, it is helpful to refer to a key article by Pike (1976), which explores the question of levels. It is focused on phonology and levels in phonology, such as a phoneme level, a syllable level, and (in some languages) a phonological-word level that may be manifested in stress groups. Phonology is an excellent test case, because discerning distinct levels is typically more challenging in phonology than it is with respect to a hierarchy of grammatical units. Pike (1976, p. 46) writes:

> A rhythm wave is not always a unit of a phonological level. Specifically, a rhythm wave, or a grouping of smaller rhythm waves, is not a unit of a phonological level unless the entire text of which it is a part can be divided into units of that level with nothing left over. For example, consonant clusters, although rhythmic groupings, are not units of a phonological level because an entire text cannot be divided into consonant clusters only. For the same reason stressed syllables are not a level. An entire text can, in some specific language for example, be completely divided into phonemes, and also completely divided into syllables, and into phonological words.

We may apply this reasoning to the hierarchy of representation in chemistry as follows:

- The *word level* consists of signs for all the elements plus additional subscript numerals to indicate the number of instances of an element within a molecule.
- The *phrase level* consists in formulas for molecular compounds, plus some connectors that make sense only on the phrase level, as symbols that will hold together the phrases at the next level up, the sentence level: + and →.
- The *third level* is the sentence level for describing chemical reactions. This level combines molecular formulas with the extra symbols + and →. Texts in chemistry are composed of ordinary language as well as the special notation for chemical reactions. But the "sentences" for chemical reactions still represent a level *within* the specialized semiotic system that is a

kind of extension of natural language for the purposes of chemistry.

Now we may return to the question of how to deal with radicals such as $-CH_3$ (the methyl group). The radicals do not make up a distinct level of their own, because the entire "text"—in this case, the text for representing a whole molecule—cannot in every sample case be decomposed without remainder into radicals. We can use the language analogy of compound words such as *in-law* or *man-child*. These are emic units in English. They are intermediate in size between the word level (*in* and *law*) and the phrase level (*their in-laws*). But they do not represent a distinct *level*, because whole texts cannot be broken down without remainder into compound words. Likewise, radicals in chemistry do not represent a distinct level.

8. Filler, prominence, and function

The particle, wave, and field perspectives (Section 3), with the related ideas of contrast, variation, and distribution (Section 4), can be applied specifically to the phenomena in the three-level hierarchy. They yield reflections of themselves within the structure of hierarchy, in three interlocking aspects: filler, prominence, and function (Poythress, 1982b). Let us consider whether these can be fruitfully applied to the representations of chemistry.

8.1. Filler

Suppose we focus on two successive levels in a hierarchy. The *filler* is defined to be the class of units at a lower level that fill a fixed empty space in a construction of a unit of a higher level. For example, in the phrase *my neighbor's black dog*, the possessive pronoun *my* is similar to other possessive pronouns such as *your* and *our*. The class of possessive pronouns is the filler of one of the positional slots (a modifying slot) in the phrase as a whole. We can picture the empty slot by having a simple underline: ___ *neighbor's black dog*. It is understood that the empty space marked by the underline is to be filled with one unit chosen from among all the units that belong to the appropriate filler class.

In chemistry, we consider the hierarchical relation between signs at the lowest level and the emic units at the next level, units designating molecular compounds. The lowest level units are either signs for elements or numerals. For example, in the semiotic system of chemical formulas, the chemical symbols, such as *H, 2*, and *O*, combine to form a phrase H_2O. The *O* is a filler for the empty slot in the formula H_2__. The same slot can be filled by other symbols. For example, H_2S is hydrogen sulfide.

8.2. Prominence

In a hierarchy, prominence is defined in tagmemic theory to be the relative weight or centrality of one unit in comparison with the neighboring units on the same level that together fit into a single unit on the higher level. We ask: *Which of the several units on the lower level is the main contributor to the nature of the higher-level unit?* If there is such a "main contributor", it is considered to be the prominent contributor to the next higher-level unit. In the English phrase *my neighbor's black dog*, *my* is peripheral while *neighbor* is the prominent unit. *My neighbor* in turn is peripheral within the whole phrase, while *dog* is prominent in the whole phrase.

It is arguable whether there is a sense of intrinsic prominence with regard to distinct elements that make up a molecule. If there is a central atom around which the other atoms are grouped, and to which they are bonded, that atom would seem to be the most prominent one.

The same principle holds for the representations of chemical molecules, in several of the semiotic systems discussed in Section 6. In the chemical formulas for molecules, the symbols for elements are prominent in comparison to the numerals specifying the number of one kind of element. That relative prominence is intuitively reinforced by the fact that the numerals appear as

subscripts rather than as full-sized numerals. In the formula for methane, CH_4, each of the hydrogen atoms is bounded to the central carbon atom, as shown in Figure 4. The carbon atom is the prominent one in the context of the molecule as a whole. The *C* symbol is accordingly represented as prominent in relation to the H symbol.

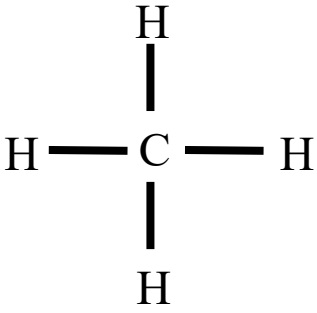

Figure 4. A stick-figure graph representation of C (carbon) as prominent in methane

In a molecule like butane with several centrally located carbon atoms (represented in Figure 2), it might be argued that the entire backbone of carbon atoms is prominent.

8.3. Function

In the tagmemic theory, *function* is defined as the role that a lower unit plays in the structure of the higher unit in which it is embedded. To once again use the familiar example, in the phrase *my neighbor's black dog*, *my* functions as a possessive modifier within the larger phrase structure *my neighbor*. In a chemical formula like CH_4, each element, whether C or H, functions in a bonding relation to the whole molecule. The formula itself does not explicitly specify the nature of these bonding relations. In a stick diagram (see Figure 4), the functions are more explicit. The sticks, that is, the lines connecting the symbols, stand for chemical bonds. C bonds to each of four hydrogen atoms. Within this stick-figure based semiotic system, the fourfold bonding symbolized in the sticks is the function of C in the molecular whole. Each chemical symbol H bonds with a single bond to the central C. Its function is to have a single bond with C. The valences of atoms indicate their *potential* to bond in certain fixed ways with neighboring atoms. But the atomic symbols like H do not actually have a hierarchical function until they participate in a bonding relation. Their function is to bond with whichever other atomic symbols they are bound to.

8.4. Tagmemic formulas

Tagmemic formulas are sometimes written to specify both the function and the filler, with a colon between them. For example, the formula for the phrase *my neighbor* might be given as in (3).

(3) Modifier: possessive pronoun + *Head: common noun

Modifier and *Head* are labels for the functions, while *possessive pronoun* and *common noun* are labels for the corresponding fillers. The asterisk is added to the Head to indicate that it has the more prominent function. So, by analogy, we can write out a tagmemic formula to describe the structure of the chemical formula for a molecule as in (4).

(4) *Participating-atom: symbol-for-an-element +
Number-of-times: numeral *n*(+ Participating-atom: symbol-for-an-element + Number-of-times: numeral)

It is understood that if the numeral is 1, the slot *Number-of-times* is to be filled with a blank. The letter *n* preceding the parenthesis indicates that the structure within the parenthesis may be repeated any number *n* of times.

The tagmemic formula in (4) does not indicate very much. It would be much more complicated, but also much more revealing, if we were to describe the expected rules governing the production of stick diagrams. Here the idea of valence comes into its own. C, with a valence or +4 or −4, is supposed to form four bonds with neighboring atomic symbols. H, with a valence of +1 or −1, is supposed to form a single bond with a neighboring atomic symbol.

In connection with the study of two-dimensional or three-dimensional models, the role of semiotic theory comes to the fore. This is so because semiotics, in contrast with linguistics, studies two-dimensional and three-dimensional structures of hierarchies of signs. To put it somewhat simplistically, a painting is a two-dimensional structure of hues and textures. A sculpture is a three-dimensional structure of hues and textures and shapes. A movie is a two-dimensional spatial representation with structural organization in the time dimension as well. All these cultural products are proper objects of semiotic study (Sonesson, 2026). The more diagrammatic representations of chemistry are clearly a venue worthy of semiotic investigations.

9. Semiotic subsystems

What further analysis may we bring with the help of tagmemics? In the semiotic system natural language, there are three semiotic subsystems: semantic content subsystem, a phonological subsystem for sound (or graphological subsystem for writing), and a grammatical subsystem for internal organization (Poythress, 1982a).[4] Is there something similar for the semiotic systems in chemistry?

There is, at least to some degree. The graphological subsystem for language corresponds to the subsystem of chemical symbols for the various elements. As discussed in Section 2, these symbols serve as signifiers that have to be contrastive in relation to each other, but also to have to have a positive identity so that they can be re-identified for each new occurrence of the symbol. The standard symbols for the elements serve as the members of the minimum-size level of the graphological subsystem for chemical formulas. The content subsystem of language corresponds by analogy to the function of the signified aspect of a chemical sign; the sign as a whole subsystem refers to occurrences of the corresponding chemical elements themselves, as things in "the real world". But note once again that like in most semiotic theory in the structural tradition, in tagmemics these subsystems operate *together* in any specific text, as a "form-meaning composite" (Pike 1982, p. 44).

Likewise, the phrase level, consisting of chemical formulas, can be analyzed in terms of a graphological subsystem and a content subsystem. The graphological subsystem consists in concatenations of letters and subscript numbers, according to the pattern we saw in the tagmemic formula in (4). The content subsystem consists in the function of the chemical formulas to designate molecular configurations in the real world, or in an imaginary world of possible chemical compounds.

Is there a third subsystem for chemical formulas, a subsystem analogous to the grammatical subsystem of a natural language? This is a more difficult question. The content subsystem for chemical formulas is deliberately designed to match as much as possible the realities concerning chemical combinations in the world. And the corresponding graphological system is designed in turn to match the content system. This situation is analogous to the case of "fusion" in tagmemics: single emic units may be fused instances that combine characteristics that at other points in the system are represented by two distinct units (Pike, 1967, Ch. 14). Especially with higher level units, there may be fusion between whole subsystems. In some languages, little distinguishes grammatical and content boundaries at the level of paragraphs and larger sections of discourse.

[4] Pike (1982, Chaps. 9-11) discusses these subsystems in connection with the three levels of the hierarchy.

In the case of chemical formulas, we do see some degree of distinct function for a grammatical subsystem, with respect to the formulas for chemical compounds. We may best illustrate by considering the role of the subscript numerals in a formula like the formula for butane, C_4H_{10}. What is the meaning and function of the numerals 4 and 10? From the standpoint of a semiotic analyst who initially knows nothing about chemistry, the graphological subsystem can still be described and understood, as a subsystem. One may write a tagmemic formula to describe the rules for properly composing a chemical formula. One may do so without understanding what 4 and 10 *mean*. To the outside analyst, they are just numerals, and they occur in subscript position following any one of the set of symbols belonging to the grounds-level words for the semiotic system. So the graphological subsystem can be more or less "understood" internally, while putting into the background the question of meaning.

But the question of meaning has then to be faced, when we come to the content subsystem. The 4, we know, signifies that there are four carbon atoms in a molecule of butane. But it is above all the *arrangement* of the atoms, as shown in a two-dimensional (see Figure 2) or three-dimensional diagram, that most directly expresses the chemical "meaning" of the molecule. The numbers 4 or 10 are a kind of secondary representation, based on counting all the atoms of the same type. But in and of itself, it is not revealing. Thus, it is like a kind of intermediate, grammatical information, useful for the purpose of eventually arriving at meaning and reference, but useful only indirectly. A distinct grammatical subsystem thus reveals itself in the way that these numerals function.

On the other hand, if we use a stick diagram, the reference to molecular structure is much more direct. The structural arrangement of the parts, and their hierarchical connections to each other and to the larger unit (the molecule as a whole), are directly "written into" the diagram. Consequently, the grammatical subsystem is almost completely fused with the content subsystem, within the overall semiotic system of the stick diagrams.

It could be argued, however, that in the system of stick diagrams there is still some faint distinction between the three subsystems. The content subsystem allows chemists to think about meanings. These meanings involve the three-dimensional configuration of atoms into molecular structures. The chemist, in knowing the meaning of the signifier *C*, knows that a carbon atom can form four single bonds. And when there are four distinct bonds, these bonds characteristically exist in a tetrahedral arrangement in three dimensions. So when the chemist sees the stick diagram for methane, as in Figure 4, he or she can imagine a three-dimensional configuration of hydrogen atoms around the central carbon atom, even though nothing in the geometrical layout of two-dimensional diagram hints at it.[5] But the "grammar" of the diagram does not show this three-dimensional information. The "graphology" of the diagram is even simpler. A purely graphological analysis would just say that one can observe lines connected to letter-like symbols spread out in a plane.

10. Conclusions

In this article, I have aimed to show that many of the fundamental concepts of tagmemics can be applied to analyze the representations of chemistry: formulas and graphs. The analysis has shown that not only do these representations constitute semiotic systems, in the sense of particular (kinds of) signs and relations, but systems whose overall structures present familiar features belonging to other semiotic systems, including natural languages. These features include the usual "triads" in tagmemic theory:

- unit, hierarchy and context (Section 2);
- particle, wave, and field perspectives (Section 3);
- contrast, variation, and distribution (Section 4);

[5] I am not considering here the hybrid notation that arises with the use of a wedge or a dotted line to hint at a third dimension, shown in Figure 3.

- filler, prominence, and function (Section 8); and
- content, phonological, and grammatical subsystems (Section 9).

We could also fruitfully employ the etic/emic distinction (Section 2 and elsewhere) and the concepts of threshold of focus (Section 6).

The analysis discloses that the representations used in chemistry can be treated within the overall viewpoint of semiotics. The result is not surprising, in a way, since chemists are communicators, and communication requires semiotic systems. Yet it is valuable to see the effects of the humanity of the chemists operating also within specific technical aspects of chemistry. It is a reminder that scientific work is human work, not merely abstract concepts.

The semiotic analysis of chemistry raises the question of how one might explain the presence of semiotic structure within chemistry. The obvious starting explanation would be that chemists are people, and that chemistry is in part a social endeavor involving communication, as mentioned above. Nearly all forms of human communication involve signs. So any special signs invented in the context of chemistry can be expected to conform to the basic framework used in semiotic analysis. Moreover, the presence of particle-like, wave-like, and field-like phenomena in communication can be aligned with findings in information theory (Poythress, 2013b).

But in the case of chemistry, we may wonder whether there is something more involved. For chemists themselves, communication—though important—is secondary to understanding the world. The four special semiotic systems for chemical representations are indeed designed partly for ease in communication. The first of them (chemical formulas) uses ready-made symbols from the roman alphabet and from the Arabic numeral system. But the semiotic systems are also clearly designed to match the world—in this case, the world of elements, molecules, and chemical interactions between them. The match is clearest when we consider the fourth of the semiotic systems, the system in which chemists build three-dimensional models for molecules. These three-dimensional models are diagrammatic iconic signs, and apart from content, they also point to real or possible *reference* (Sonesson 2026). After all, chemists think that their representations match the structure of molecules in the world.

So why do the molecules and structures "out there" conform to the basic semiotic structures found in the sign systems? That is still an open question. The world itself has structure. But how is it that it is amenable to representation in semiotic form in chemical notation? That question is important, but it is left for another day.

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