

# Orismology (the Science of Defining Words) and the Geometrical Foundations of Chemistry. 5. The Heuristics of Primacy

Seymour B. Elk

Elk Technical Associates, 321 Harris Place, New Milford, New Jersey 07646

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Orismology, the science of defining words, plays a major role in understanding concepts in chemistry. Its effects are so pervasive that how different words are denoted as well as the unstated—but implied—connotations that they carry often influences the direction in which both laboratory and theoretical chemistry research progresses. An examination of the role that synthetic geometry (including graph theory, topology, etc.) plays not only in describing the physical foundations that underlie the organization and description of chemical moieties but also of equal importance in helping us to sort out just what is our perception of these moieties is undertaken. This fifth article of the sequence is an examination of what effect the optimization of two often mutually-conflicting parameters has had in our understanding of chemical structure, taxonomy, and nomenclature.

## 1. INTRODUCTION

This report continues our exploration of how both the denotation and the connotation of the words that we use influence our perception of what is chemical “reality”. In earlier parts of this series, we laid the foundations of the general subject matter<sup>1</sup> and examined the underlying topology,<sup>2</sup> what constitutes a ring,<sup>3</sup> and how these rings may be combined.<sup>4</sup> In each of these reports as well as in many of the seminal studies that we had undertaken both previously and concurrently we often *blithely* assigned primacy to one parameter vs that of a frequently competitive parameter. At this point it is prudent to note that we are frequently called upon to make choices in chemistry that apply to what “the general chemistry community” believes, *at the time*, to be the most common cases. Consequently, in this report we shall first undertake an investigation of which parameters have, historically, been assigned this role of primacy and then re-examine, in light of modern advances, whether such assignments are either necessary or desirable.

As a further word of introduction we observe that neither the concept of primacy nor the desirable heuristic of “simple” is self-evident. In fact, the intermingling of these two concepts is often the driving force that has produced much of our understanding of science. Furthermore, the choice of which of two parameters to consider as **the** primary one in our intuitive concept of what is “simple” is *always* highly suspect.

## 2. CHOICE OF MODULE

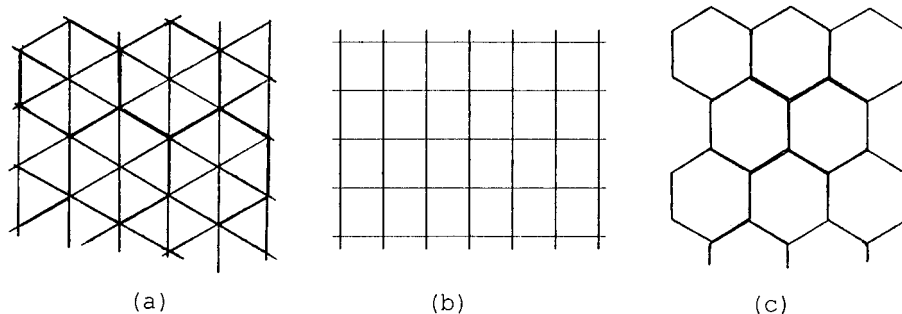
In the formation of a molecule from its component parts, the first and, in many instances, most obvious organization of components are the two disjoint sets of (a) individual atoms and (b) pairwise (linear) connections between atoms, which are assumed to be represented by covalent bonds. The implications of this is that these two sets **alone** are sufficient to describe the relevant chemistry, i.e., that an appropriate graph (where atoms are represented by nodes and bonds by edges) is isomorphic with a chemical molecule. To the

contrary, we note many instances in which there exist higher orders of modules which function as integrated units, i.e., where the old Euclidean axiom “The whole is equal to the sum of its parts” is a major misstatement. Even before it became common practice to apply principles of graph theory to chemistry, chemists had been organizing chemical molecules in terms of larger aggregate “functional groups”; some of which have properties quite distinct from the individual atoms and/or bonds.

At this point, let us turn to the isomer distinction problem of the 1820s. The two silver compounds (cyanate—AgNCO and fulminate—AgOCN) ionize to form two distinct groupings, only one of which involves a single atom (and, by default, is an important functional entity {namely, a group of size 1}). The orismology question ‘Whether we wish to categorize either or both of the (anion) groupings (cyanate or fulminate) as a “functional group”?’ is purely heuristic and, from a pragmatic perspective, is answered by how significant is the synergism of the individual smaller “functional units” as well as to what percent of the time these groupings occur. For the case of fulminate, we suspect most chemists would not consider there to be any great synergism, except in perhaps highly specialized studies, and thus would not place emphasis on this grouping; i.e., fulminate would not, *in general*, be classified as a functional group of *significance*. By contrast, the cyanide grouping, and to a lesser extent the cyanate grouping, is encountered more frequently in nature and in the laboratory; consequently, for several cases the special synergism in either or both groupings MAY be considered as a significant chemical aggregation.

Historically, we note that the term functional group occurs most frequently in organic chemistry<sup>5</sup> textbooks, in contradistinction to its much less common usage in inorganic chemistry texts. Furthermore, organic chemists consider as the smallest functional groups all individual hetero- (non-carbon and non-hydrogen) atoms as well as all multiple bonds between carbon atoms. Next in priority, individual groups are often subordinated to a somewhat larger module (usually one which contains a relatively small number of atoms; e.g., carbonyl). These form the traditional functional

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**Figure 1.** The three regular tessellations of the plane.

groups taught in elementary organic chemistry texts. Continuation of this organization to many levels of coordination is common. For example, when an alkyl group is attached to a carbonyl group, which, in turn, is connected to various other single atoms of small functional groups, such combinations of carbonyl group and the latter atom or group of atoms exhibits sufficiently different characteristic properties so that each of these is designated as a distinct functional group: When combined with a single hydrogen atom, the chemical properties of the carbonyl–hydrogen grouping (called an “aldehyde”) are different from when it is combined with a methyl or other alkyl group (called a “ketone”), which are different from when combined with a hydroxyl group (called a “carboxylic acid”), etc. Each of these larger groupings is ubiquitous enough and has enough characteristic properties to be generally classified as a unit unto itself, rather than just as the linear concatenation of a two smaller functional groups.

From the above, we recognize two major taxonomy problems:

- (1) Where to draw lines of demarcation so as to define the *most significant* “functional groupings”?  
and
- (2) To what extent such a hierarchy should be extended?

One of the more obvious cases where we must answer the question “whether the individual functional groups should be suppressed?” involves the concatenation of double bonds with either single or double bonds yielding the three *drastically different* groups of isolated bonds, conjugated bonds, and cumulenes, respectively. Furthermore, we note that only the first of these three categories is chemically “nearly equivalent”<sup>8</sup> to a single double bond. In the other two cases, the differences in chemical properties are sufficiently great that lumping such compounds into a single taxonomy class creates more confusion and misclassification than it creates order.

Additionally, as well as problems that arise when combining together groups that should not have been so combined we also encounter instances where we have overlooked groupings that should have been grouped. In particular, there exists “bonding” that spans a space. These include hydrogen bonding, tautomerism, etc. Such bondings occur even though we do not assign the same graph theoretical treatment to them that we did to covalently bonded atoms. (See also refs 1 and 3.)

Before leaving the subject of how to choose modules, let us again focus on the observation that the ideal of simplicity is a heuristic one. Because we are interested in concatenation of atoms, we can achieve “simplicity” by concatenation in

an embedding space of one, two, or three dimensions. This corresponds to exactly two, three, or four distinct ligands (bonds) to an atom, respectively. (Note that we have not required homaloidality, just dimensionality!) We believe that for purposes of taxonomy

- (1) the single, chemically most significant choice lies in selecting the simplest module that can exist in a given embedding space  
and
- (2) that such a module will be one that can be further extended so as to tessellate the embedding space.<sup>10</sup>

For a one-dimensional embedding space, this is expressed as a noncyclic chain of identical atoms. (Mathematically no discussion of type of bonding is relevant, even though this will be of significance chemically.) For a two-dimensional space, any of the possible tessellations of the plane might be viable. However, in order for there to exist a situation of static stable chemical equilibrium, it is desirable that identical atoms be positioned at vertices corresponding to regular polygons. (Note that the corresponding choice in the one-dimensional space was the trivial one of identical atoms at the end of each bond.) Such a scenario is mathematically fulfilled by exactly three tessellations of the plane (Figure 1); only one of which, the hexagonal tessellation (with a coordination number of three), is of significance chemically: A triangular tessellation would have six bonds emanating from each atom, while a square tessellation would induce tremendous bond strain of  $sp^3$  hybridized orbitals by trying to extended [4.4.4.4]fenestane<sup>11</sup> beyond a single module. It is presently a purely unsupported speculation as to whether, within some specially prepared environment, some other atom, such as a Group VI element (either 6A or 6B in the older periodic chart or 6 and 16 in the presently accepted version, e.g., sulfur or tungsten), could be induced to form either a three-dimensional array of cubically positioned atoms or a coplanar square array of covalently joined atoms; however, no such organization of molecules is presently known.

### 3. ENUMERATING MODULES

In addition to the problem of choosing modules to describe the various combinations of atoms that form molecules, we also encounter the problem of how do we enumerate these modules. In the simplest case, we may describe the relevant chemistry using a one-parameter system. For such a scenario, the idea of counting items is equivalent to asserting that there exists a one-to-one and onto relationship between the entities being counted and the set of natural numbers.

An example of such a system is the set of unsubstituted acyclic *n*-alkanes. Describing and/or nomenclating an unsubstituted acyclic *n*-alkane is completely unambiguous inasmuch as the set chosen allows for exactly one method of annellating additional modules (single carbon atoms) to the previous aggregation; namely, there is a congruence of products formed by annellation at all of the possible sites (namely the two ends) of the previous aggregation. Consequently, all that is required is a number (or name) stating how many carbon atoms are involved. **However**, whenever the module chosen is more complex (either the unsubstituted, the acyclic, the *n*-, the alk-, or the -ane is not mandated), then the set is no longer unambiguously isomorphic with a single set of natural numbers. At this point, it is important to note that in selected cases it **may** be possible to devise a larger system that is once again isomorphic with a single set of natural numbers; however, often the price paid in terms of both simplicity and historical precedent is daunting. One such set, developed nearly 30 years ago by Matula for the entire set of acyclic alkanes (*n* AND branched)<sup>12</sup> and which we extended first to other sets of one parameter systems<sup>13</sup> and then to ordered multiparameter systems,<sup>14</sup> is sufficiently remote from familiar concepts as to make its acceptance by the general chemistry community **extremely unlikely**.<sup>15</sup>

The more likely alternative for acceptance and the one that has historically been adapted by chemists is to use an ordered set of parameters, each of which is isomorphic with the natural numbers. One major problem with such a scheme is that there **may** not be a logical ordering of parameters. To the contrary, we conclude that the notion of primacy is highly subjective.

Before formulating any math model to be used for purposes of taxonomy and nomenclature, let us examine the arbitrary choices that one makes (some of which are at the unconscious level) in setting up a system of measurement. In addition to the obvious choices of a starting point and a unit length, one must also select a reference on which to make our measurement; i.e., the most fundamental arbitrary choice is what shall be the "measuring reference". Because heuristically the geometrically simplest space is homaloidal and the smallest dimension in which measure is defined is one-dimensional, whenever possible, we opt for straight lines on which to make measurements. Having selected this measuring reference, the second arbitrary choice is some preselected point embedded thereon. In the simplest system this is designated as "zero". (Note that other preagreed upon names such as "one" for a logarithmic scale, etc. could have been chosen.) The third arbitrary choice, a unit measure, creates two more arbitrary choices: (1) Which direction on the measuring reference do we define as increasing (positive) as well as one that we often subconsciously make? (2) What is the functional relationship between the various points on the measuring reference? The answers given to the commonly-used standardized system are as follows: (1) Let the measuring reference be moved so as to lie in a horizontal orientation with + measured to the right. (2) Let the distances between successive integers all be equal; similarly, let equal fractional parts by "uniformly" spaced.

Applying the above to molecules, we first select a single "linear" chain and then assign "locant numbers" to the individual modules (single atoms) in that chain. Note that because of the choice of measuring reference, we have inferred that an acyclic chain be chosen. With such a

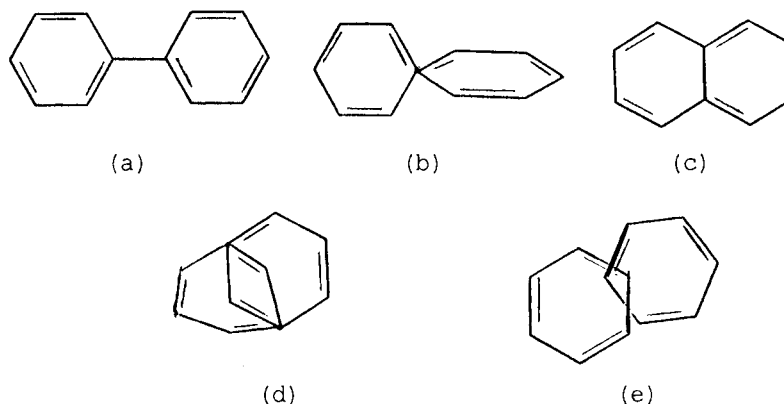
restriction, the next heuristic choice decrees that the longest possible linear chain be selected. However, even in those instances where there does exist a single such chain, rather than a multiplicity of chains all having the same total length, there may still arise questions of primacy. Historically such questions have been established by fiat. For example, in the historically accepted model, which was developed into the standardized nomenclature for organic chemistry by the International Union of Pure and Applied Chemistry (IUPAC),<sup>16</sup> it was decreed that the "primary" chain be limited to carbon atoms only. On the other hand, in some of the many other prominent systems proposed to correct recognized inadequacies in the IUPAC model,<sup>17</sup> such as the scheme referred to as "nodal nomenclature",<sup>18</sup> allowance is made for the "longest" chain to include non-hydrogen heteroatoms. Furthermore, in the IUPAC (standard) scheme, it was next decreed that the "primary" chain be the one which contains a maximum number of multiple bonds, rather than a longer chain having fewer functional groups. In other words, functional groups are of higher priority than chain length in IUPAC, whereas the reverse is true in nodal nomenclature. Also, in the IUPAC system, the degree of "unsaturation" (double vs triple bonds) was subordinated to the number of such unsaturations, with the added inconsistency that, when there were an equal number of multiple bonds in a chain, double bonds were assigned higher priority than triple bonds, etc.

Up until this point, the modules being considered were single atoms, which are well represented by discrete points. Now, we observe that as well as having single atom modules various combinations of atoms may also be chosen as "building modules". At this point, it is important to note the orismological line of demarcation between a functional group and a building module. A functional group is a grouping suggested by the chemistry, whereas a building module is a mathematical abstraction that may or may not correspond to a set of atoms. For example, a single benzene ring is both a very important functional group that has an added stability which makes it stay together as a unit chemically in very many reactions and also is an important building module which is characterized by its regular hexagonal planar shape. Mathematically, the union of two benzene rings could be envisioned in five distinct ways.

(a) They could each be connected to a third mathematical construct, such as a line segment, forming a "biphenyl". Figure 2a is the viable molecule  $C_{12}H_{10}$ .

(b) They could be connected through a single atom, forming a "spiro" compound. This, **HOWEVER**, is unattainable since the spiro carbon would have to have six bonds. Figure 2b would be a fictitious 11 carbon molecule. Note the spiro union of two six-membered carbon rings is chemically viable **IF AND ONLY IF** all four bonds from the spiro atom are single bonds.

(c) They could be connected through a pair of adjacent atoms, forming a "reticular" compound. Figure 2c is a representation of the familiar compound naphthalene,  $C_{10}H_8$ . Note that both rings are not truly benzene any more. By sharing two carbon atoms, there is a deficit in both the number of carbon atoms and in the number of peripheral hydrogen atoms. Clar<sup>19</sup> views this as only one of the rings having a "true" benzene structure and the other ring having a lesser "aromaticity". The



**Figure 2.** The five mathematically possible unions of two benzene modules.

implication of this is that of the three potential topological representations<sup>20</sup> in terms of

( $\alpha$ ) “boundary defined” (union of boundary segments),

( $\beta$ ) “open content-defined” (space enclosed by the boundary but not including the boundary), and

( $\gamma$ ) “closed content-defined” (space enclosed by and including the boundary)

only the open content-defined topology ( $\beta$ ) views such a union as adding two modules. ( $\alpha$ ) and ( $\gamma$ ), on the other hand, like Clar, view this “sum” as less than two modules; namely,  $A \cup B = A + B - A \cap B$ , where the intersection of these two modules, which has been counted twice, is the set of two atoms and one bond.

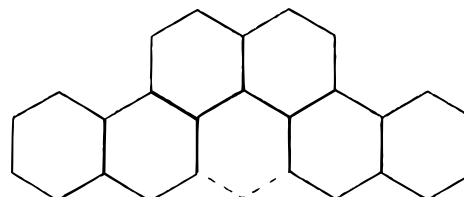
In other words, only in one of the three traditional topological descriptions of a geometric figure larger than a simplex<sup>21</sup> does the union of two hexagons (mathematical modules) strictly correspond to the union of two chemical modules.

(d) The union of two benzene rings at a pair of nonadjacent atoms is precluded chemically by the need for six bonds at each of the two common carbon atoms, in exactly the same manner as for (b). Furthermore, such an arrangement would be mathematically complicated by the conflicting requirement of overlapping and coplanarity of the rings (Figure 2d).

(e) The catenane union of two benzene rings (Figure 2e) is precluded by the space required to thread a carbon-carbon bond through a ring. Frisch and Wasserman<sup>22</sup> advise of theoretical studies that estimate the smallest unsaturated 2-catenane ring to be 18 carbon atoms in length, while the middle ring of a 3-catenane<sup>23</sup> would require at least 26 carbon atoms. Furthermore, the ring size would have to be even larger for any ring containing multiple bonds.

Of these five methods of forming the union of two benzene modules, exactly one is of chemical importance: (c). One other (a), while viable chemically, is, to date, purely a curiosity. Consequently, let us restrict our focus to the reticular fusion of benzene modules.

We are now ready to examine modules that are larger than single atoms and, consequently, can no longer be represented as discrete points in the given embedding space. The previous isomorphism that was possible between linearity and straightness is no longer universally valid. In other



**Figure 3.** A molecule in which linearity and straightness are NOT equivalent.

words, even though we are cognizant of the fact that an *n*-alkane is not geometrically straight,<sup>24</sup> for such a single “backbone” molecule, there DOES exist a simple transformation that is one-to-one and onto between the given molecule and a Euclidean straight line. In Figure 3, on the other hand, we observed that now “linearity” implies a nonoverlapping union of connected line segments passing through the interior of each molecule, in contradistinction to our heuristic idea of “straight”.<sup>25</sup> In fact, for this particular example, the heuristics include the existence of a phantom module in a five-module long straight chain vs the six-module long “linear” chain. Furthermore, as we had observed when the module under consideration is pentagonal (or any other odd number of sides for a regular polygon), rather than hexagonal,<sup>26</sup> the difference between linearity vs “straightness” is even more evident, and that the standardized technique for drawing modules developed by Patterson<sup>27</sup> is grossly flawed.

Additionally, using the benzene module as the counting reference, we had earlier noted the counting problem in most pericondensed arrays of benzene module.<sup>28</sup> Namely, because chemists wished to maintain the pre-eminent position of the benzene module, there is inconsistency in counting rings: By fiat there are seven rings in coronene (i.e., the simply-connected model is chosen; **however**, in other circulenes, including circumpolyenes, the multiply-connected set of benzene rings is selected, and the enclosed ring is relegated to outside the boundary.

The analogous extension in three-dimensional embedding space to polymantanes, using the adamantane module, is *relatively* straightforward. Although there is a wider set of possible combinations of two adamantane modules than there is for benzene modules, we introduce no fundamentally new mathematical chemistry ideas that need to be probed.

#### 4. REVISITING SOME SPECIAL QUESTIONS OF PRIMARY VS SIMPLICITY

Not only are there primacy problems in choosing and enumerating the modules to be used in describing the relevant

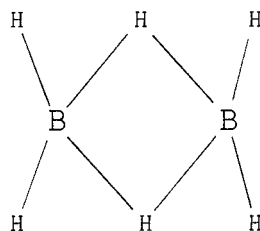


Figure 4. Diborane.

chemistry but also there are ambiguities which arise as a consequence of internal inconsistencies in the definitions of some of the words we use in both the chemistry and the mathematics itself. This section is a potpourri of three extensions and refinements of earlier applications. First, we re-examine a special orismological question that was raised during the early evolution of modern graph theory. Next, we reconsider how primacy affects a fundamental topology problem we had analyzed earlier. And finally we tie in our recent study in which we delineate when a nomenclature is synthetic vs analytic.

**4.1. Graph Theory of a Cycle.** Reiterating from Part 1 of this series, we noted that in the late 1960s, major controversy arose as to whether the minimum size of a cycle was three nodes (as expounded by followers of Harary<sup>29</sup>) or whether loops and multiple edges also constituted cycles (as asserted by the earlier school of thought, represented by Nash–Williams<sup>30</sup>). In our earlier report on the orismology of the word *ring*,<sup>3</sup> we alluded to, but did not actually spell out, what we now believe to be the difference in primacy that proponents of these two schools of thought allocated to the fundamental definitions to be used in graph theory. It is our present contention that a major part of this difference in perspective as to “what is a cycle?” is predicated on the heuristic implied by the adjective “simple”, especially when this adjective is combined with the concept of figure. The question we had raised “Did *simple* imply homaloidality ala Harary or was constant curvature sufficient ala Nash–Williams?” is equivalent to asking which parameter is given primacy when designating simple figures. In other words,

- (a) Do we consider that a triangle is the simplest figure in a plane inasmuch as all of its segments are points sets which utilize the reference curvature of zero—despite that we require three such segments?

or

- (b) Do we consider that both the lune and the circle are “simpler” since they require fewer segments—even though these segments deviate from the reference and thus are, from a curvature perspective, more complex?

Further usage of Nash–Williams’s perspective, that we did not explore in Part 1, might be of more than passing interest; namely, it would be perfectly consistent to consider a lone pair of electrons on an atom as being a self-loop (one-cycle). Whether such a treatment will lead to either interesting or fruitful applications awaits further study.

Continuing this same type extrapolation to an even smaller number of more complex modules, one could consider not only double bonds as two-cycles but also, because a single covalent bond is viewed as the “product” of two electrons, we may envision that a single bond has two halves—which form a “specialized two-cycle”, akin to the three-atom, two-electron bonds encountered in diborane (Figure 4) By such

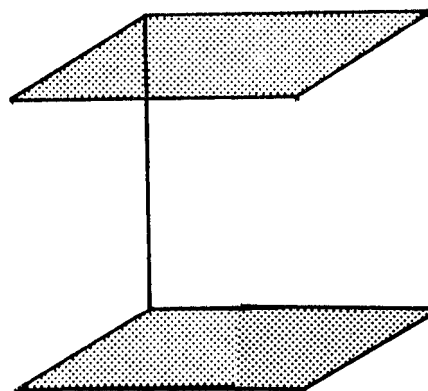


Figure 5. A biphenyl-type union of components in cubane.

a perspective, any graph theoretical “cut edge”, such as the connecting bond in a biphenyl, might be construed as a tricyclic compound. Two “advantages” of this, admittedly unorthodox, “Weltanschauung” are (1) a potentially better, purely mathematical (rather than quantum mechanical) explanation for three-atom, two-electrons bonds as well as (2) a means of including, with four-fold redundancy, three more combinations of “nonsimple” faces that can exist in a cube.<sup>31</sup> (Each of these is analogous to a biphenyl; namely, the nonsimple figure formed from the union of two parallel faces and one connecting edge of a cube, see Figure 5.) In other words, of the  $2^6 = 64$  possible (nonredundant) cases delineating in ref 29, only the null set is now excluded as a potential description of the combination of simple faces that can exist in a chemical moiety.

**4.2. SSSR.** In nomenclature, the idea referred to as the smallest set of smallest rings (abbreviated as SSSR)<sup>32</sup> is used to determine which atoms belong to which rings in formulating the desired name of a multiring compound. The underlying logic of this “simplifying axiom” is a direct application of Euler’s Polyhedron Theorem in topology. In ref 33, we demonstrated that the same inadequacies that exist when the polytope of interest is not simple are equally applicable when the molecule of interest is not adequately described by a simple projection onto a plane. Meanwhile, it should be noted that the philosophy of SSSR served to make the choice as to what was heuristically of greater primacy: namely, smallest ring was chosen over smallest set. In the historical development of chemistry, this made sense so long as the majority of molecules so named were what we have called “essentially planar”.<sup>28</sup> In fact, as our knowledge has expanded, this earlier Weltanschauung has created havoc for selected compounds that once might have been considered as “esoteric”.<sup>34</sup> The reasons why we continue to accept this, admittedly antiquated, system are the lack of consensus as to how best repair a system that many believe is “not too badly” broken as well as in our mandate that any new system have both consistency and generalizability; we have found that all of the alternatives proposed to-date (at least in the minds of those in a position to lead such a change) are worse.

**4.3. Synthetic vs Analytic Nomenclature.** For purposes of completeness, at least up to the present time, the reader is referred to an orismology study that we recently completed: In setting up a system of nomenclature, we noted a fundamental difference that arose when the molecule being named was formed by annexing modules one at a time to a smaller “core” subsystem of atoms (a “synthetic” nomen-

clature) vs when a name was assigned to that molecule by starting from the total fixed aggregation of atoms and breaking the system down into smaller subparts (an "analytic" nomenclature).<sup>35</sup> An interesting geometry-inspired similarity between the comparison of two figures in geometry and our present problem is examined therein.

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$$\begin{array}{c} \text{H} \quad \text{O} \\ | \quad || \\ -\text{N}-\text{C}- \end{array}$$
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