

THE INFLUENCE OF DIMENSION ACROSS **ALL** OF CHEMISTRY  
WITH SPECIAL EMPHASIS ON THE GEOMETRY AND  
NOMENCLATURE OF TETRAHEDRAL MOIETIES

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**ABSTRACT:** The lines of demarcation that historically separated the various subdivision of chemistry (especially the view that inorganic chemistry was characterized mainly by ionic bonding in contradistinction to almost exclusively covalent bonding in organic chemistry) are long passe. What is important, and what characterizes modern chemistry, is the geometrical ubiquity that spans all of the historical “fiefdoms” of classical chemistry. This report focuses on the three-dimensional commonality of molecules that were frequently pigeon-holed in one of these fiefdoms instead of describing them in terms of their common geometry. Special emphasis is directed to modeling several, previously regarded as unrelated, molecules using the components of a “3-simplex” (i.e., a tetrahedron) and to the formulation of a common nomenclature that spans all of chemistry.

## 1. INTRODUCTION

This study of the influence of dimension across the entire spectrum of chemistry begins with an examination of the role played by the simplest

“homaloidal” figure\* that exists in a given space. Such a figure is referred to as a “simplex”, or more precisely an “n-simplex”, where the n denotes the dimension of the figure†. For example:

- (1) All single atom molecules, such as the inert gases, as well as single atom ions, are represented as 0-simplexes;
- (2) All diatomic molecules (O<sub>2</sub>, F<sub>2</sub>, CO, etc.) are 1-simplexes;
- (3) The core of a three member ring, such as the three carbon atoms in cyclopropane (or the two carbon and one oxygen atom in an epoxide) in the “organic” domain, as well as the recently created three gallium atom ring core in the “inorganic” domain, which, with appropriate stabilizing ligands, displays aromatic character in a manner analogous to the cyclopropenyl cation [1] are examples of 2-simplexes [‡2];
- (4) Examples of molecules that are geometrically modeled as a 3-simplex (Figure 1) include:

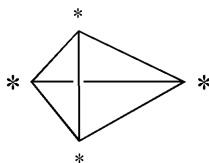


Figure 1: Mathematical model of a 3-simplex

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\* The term “homaloidal” denotes that the curvature of the respective segments of the figure are all zero; that is, the edges are all straight in a one-dimensional space, the faces are all flat in a two-dimensional space, etc.

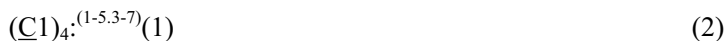
† Namely, a tetrahedron is a 3-simplex, a triangle a 2-simplex, a line segment a 1-simplex and a point a 0-simplex.

‡ Although it may appear to many (especially in the graph theoretical community) to be semantically undesirable to consider the entire molecule, rather than just the core, as the “simplex”, it is common practice (in graph theory) to focus attention on the “block” (defined as a “maximally non-separable subgraph” [2]) that is formed by removing all acyclic subgraphs which are attached to this block by single edges. Consequently, when the “would be pruned” subgraphs are congruent and attached to a common atom, one often regards a node of a ring together with its acyclic subgraphs as a module. In other words, cyclopropane may be viewed as an example of a 2-simplex of the C module, where each underscore line denotes a hydrogen atom in an internal chain; i.e., C is an abbreviation for CH<sub>2</sub>. By the convention of Reference 3, one does not include a terminal hydrogen atom; instead the methyl group CH<sub>3</sub> is denoted by CH, which is attached to an aliphatic (R) or aromatic (Ar) group by a single bond; namely, RCH.

- (a) In the “inorganic” domain, that allotropic form of the element phosphorus known by the common name “white phosphorus”. This allotrope occurs in nature as an aggregation of four atoms per molecule, with each of the phosphorus atoms situated at the vertices of a regular\* tetrahedron and connected by a single bond to the other three phosphorus atoms of that molecule. Using the nomenclature described in [3] the canonical name for this molecule is:



- (b) In the “organic” domain, there exist two important theoretical possibilities of creating a molecule containing a carbon atom at each of the vertices of a tetrahedron. In the more viable, but still highly unlikely, of these scenarios one would have a hydrogen atom singly-bonded to that carbon and directed outward to form a molecule known by the common name “tetrahedrane”. Using the nomenclature of Reference [3], such a molecule would have as its systemic name:



It should be noted, however, that internal forces between the atoms in such an eight atom aggregation has, so far, precluded the formation of a stable molecule having this geometry. Greenberg and Liebman [4] describe some of the earlier studies that attempted to form such a molecule.

- (c) An even more unlikely candidate for a tetrahedral carbon molecule would have no hydrogen (or other ligand) atoms attached to the four carbon atoms, which would now be joined by bonds with bond order 1.5 (denoted as  $\beta$  bonds in [3]) whose canonical name would be:



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\* The term “regular”, when applied to polytopes of any dimension, denotes all segments (sides, faces, etc.) and all angles (planar, polyhedral, etc.) of a given dimension that comprise the polytope are congruent (when shape is defined) or equal (when shape is not a criterion). Note that no mention has been made of either convexity or simplicity.

To-date, formation and isolation of tetrahedrane (2) remains high on the wish list of potential molecules yet to be created in the laboratory, while “tetrahedrene” (3) is considered so esoteric as to be beyond any *reasonable* hope of creating.\*

As well as these latter categories, it should be observed that all acyclic compounds *may* be viewed as the union of 1-simplexes, while monocyclic compounds *may* be viewed as topologically partitioned to be modeled by a 2-simplex. Such modeling, although possible, is rare inasmuch as most three member rings are highly strained. Consequently, instead of following such a development, attention is directed not so much to the possible, but rather to the ubiquitous:

One model in two dimensional space that is serendipitously important is formed by considering the three vertices and the three midpoints of the edges of a regular 2-simplex (the equilateral triangle) as the set of vertices of a reference figure. Next, project each of these midpoint along the line passing through the opposite vertex, first inward so that the three lines intersect at a common point which is the circumcenter of the simplex and then an equal distance outward so that the set of vertices lie on the circumcircle. Note that this set of six points, which are the vertices of a regular hexagon, may now be viewed as an “extension of the 2-simplex”. This is in addition to its other more familiar roles in especially “organic” chemistry, including especially it being the largest regular polygon that tessellates 2-space [5].

We now turn to a similar extension of the regular 3-simplex; namely, let us insert auxiliary vertices bisecting each of the edges. Note the concurrence of the inward projections perpendicular to the edge of these new auxiliary vertices at the center of the sphere that circumscribes this regular tetrahedron, as well as that an equal outer projection from these added vertices produces a prototypical module (Figure 2) that has tetrahedral angles ( $109^{\circ}28'$ ) at each of the vertices and which tessellates 3-dimensional Euclidean space. This particular geometrical model, which has ten vertices, twelve edges and four skew hexagonal faces, has its chemical counterparts in most of the historical “fiefdoms” of classical chemistry. The next six sections describe important examples of such chemical moieties in their respective traditional subdivisions of chemistry.

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\* Remember that nomenclature must be capable of assigning a canonical name to any mathematically viable combination of atoms and bonds. Chemical stability, while highly desirable pragmatically, is **not** a consideration in the formulation of nomenclature.

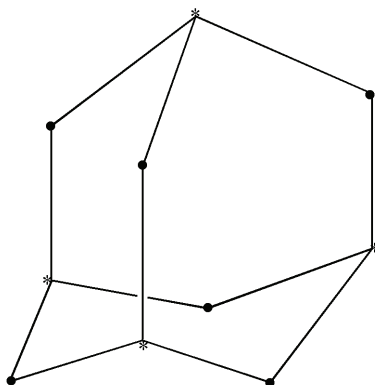
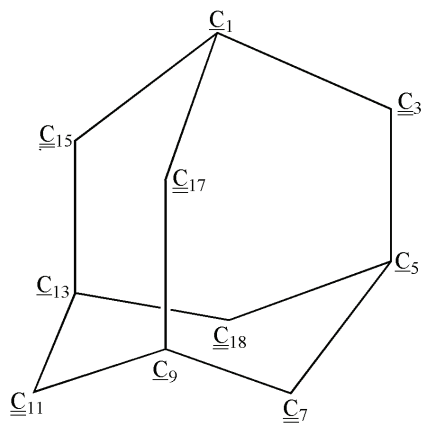


Figure 2: The prototypical model formed by insertion of atoms bisecting each edge of the 3-simplex.

## 2. "ORGANIC CHEMISTRY"

Insert a methylene module (a carbon atom and two hydrogen atoms) at the midpoint of each of the six edges of the tetrahedron. The generic



Adamantane

Figure 3: The three dimensional module of adamantane with its two different submodules emphasized

symbol of an asterisk (\*), which represented a vertex of the simplex in Figure 1 has now been replaced by a  $\underline{C}$  module in Figure 3; also, the symbol ( $\bullet$ ), which denotes an edge extender, has been replaced by a  $\underline{C}$  module. In other words, this molecule may be viewed as having two distinct sets of modules (V and E). Consequently, rather than the traditional empirical formula being  $C_{10}H_{16}$ , a more descriptive empirical formula is:  $\underline{C}_4\underline{C}_6$ , which is a special case of the generic empirical formula  $V_4E_6$ . This particular molecule, which is known by the common name adamantane\*, is the prototype of many similar molecules having "extended tetrahedral" geometry.

Before examining this larger class of extended tetrahedron molecules, the IUPAC name for adamantane: Tricyclo[3.3.1.1<sup>3,7</sup>]decane bears some critical examination. This name, especially the "tricyclo" part, is, at best, confusing inasmuch as (see [6]) there are four, rather than three, important "hexagons" in this molecule. Moreover, were it not for IUPAC fiat, a mathematically more consistent point of focus would have been on either this larger set of hexagons, or, better, on one of the larger (eight member) rings. By IUPAC's biasing its system of nomenclature on SSSR (smallest set of smallest rings), all of the octagonal rings in adamantane have been relegated to a status of insignificance. To the contrary, in determining what we deemed to be important in establishing the proposed system of nomenclature of [3], cognizance was taken of the fact that for aliphatic compounds all of the "hexagonal" faces are not only skew hexagons, but also that there is no planar subset that contains four of these six  $\underline{C}$  vertices. For this reason a greater consistency is achieved by placing emphasis on the largest (in this case octagonal) ring for all such molecules, rather than on any set of less significant hexagonal ones. Consequently, the systemic name† for adamantane is:



Note this discarding of the "simplistic empirical formula"  $C_{10}H_{16}$ , which disregarded modularization, and replacing it with the more "meaningful empirical formula":  $\underline{C}_4\underline{C}_6$ , leads directly to the common binary

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\* The name "adamantane" (as well variations containing heteroatoms, such as nitrogen and thus the name "adamanzane", etc.), like the name "cumulene", has been used as both an entire class of compounds and as the smallest (prototype) member of that class.

† Observe that by eliminating all of the "extender modules" (i.e.,  $\underline{C1}$ 's) from this name (and thus having to adjust the locant numbers for the two bridges), one obtains the systemic Cartesian name for tetrahedrane given above as (2).

formula  $V_aE_b$  which can be ascribed to the five Platonic solids: having  $a$  vertices and  $b$  edges; e.g., the canonical name for the tetrahedron with 4 vertices and 6 edges is:

$$(V1E1)_4^{(1-9,5-13)}(1E1) \quad (5)$$

It is precisely this modularization that reinforces the desirability of having a common nomenclature that spans all of chemistry.

Continuing in the traditional “organic” fiefdom, one can now replace either the  $\underline{C}$ s or the  $\underline{C}$ s (or both) with a common module, such as nitrogen

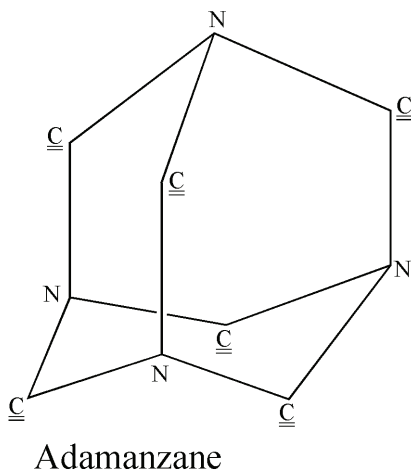


Figure 4: Replacing the  $\underline{C}$  modules in adamantane with N atoms produces adamanzane

atoms for the  $\underline{C}$ s\* or the edge (methylene) groups with longer chains, such as ethylene, propylene, etc. For the case that nitrogen atoms replace the  $\underline{C}$

\* Because the name “adamanzane”, where the z is from the prefix “aza” associated with nitrogen, has crept into the common nomenclature and is now generally recognized, substitution of “hydrogen-suppressed ‘3-coordinated’” carbon atoms ( $\underline{C}$ ) by other elements, such as silicon, phosphorus, sulfur, etc. atoms suggests that common, as well as IUPAC, names for such compounds might be: adamansilanes, adamanphosphoranes or simply adamanphanes, adamanthianes or adamanthanes, etc. Unfortunately, consistency is not in evidence in the literature. To the contrary, in the “hits” that one gets by a Google search of “adamanthane”, two potentially conflicting uses of this word are encountered (one in the traditional organic domain and a second that would be more accurately classified as “inorganic” — see section 3 below). With regard to the

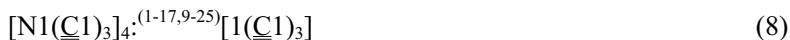
modules, i.e., when  $V = N$  and  $E = \underline{C}$ , (Figure 4), common name = adamantane or, using the extended nomenclature created by Springborg described in the next paragraph: [ $1^6$ ] adamantane), the systemic name\* [7] becomes:



In extensive studies by Springborg et al [8] on molecules in which six propylene chains connect the four vertices, (common names [ $3^6$ ] adamantane and [ $3^6$ ] adamantane,  $V$  represents either  $\underline{C}$  or  $N$  and, in both instances,  $E = 1(\underline{C}1)_3$ . Consequently, these molecules have systemic names:



and



Additionally, this team has produced a large number of variations of what are called “bowl” vs. “cage” adamantanes. The relevant terminology here is that cages have bridges between all six pairs of “3-coordinated ( $\bullet$ ) atoms” vs. bowls which have bridges between only five such pairs. Note that unlike the ambiguity that arises for various combinations of chain length, such as  $[(2.3)^2.2^1]adz$  vs.  $[2^2.3^2.2^1]adz$ , each of the various structural isomers are distinguishable in the proposed systemic nomenclature in much the same manner as with the compounds nomenclated in the tables of Chapter 2 of Reference [3].

traditional “organic chemistry” usage of this name, this author, upon following up on the listing on their web site ([www.mt.com](http://www.mt.com)) of some important properties of “adamantane” [7], was advised by Mettler-Toledo that their use of this name **may** originally have been a misspelling, but that now it has become an accepted (European) variation for the name of that hydrocarbon compound more commonly known in the United States as “adamantane”. Sci-Finder similarly lists several additional foreign studies that have used the name in this way.

\* Observe that when the replacement module is the same length as the original module, all of the locant numbers remain unchanged. Compare formulas (1) with (2) and also (4) with (6), (7) and (8) in the “organic domain”. Additionally, as is the main premise of this section, (5) is the generic model for several molecules in other historically segregated domains.



### 3. "INORGANIC CHEMISTRY"

In the domain of "inorganic" chemistry, one encounters three distinct molecular sets whose geometry is based on the tetrahedron. The first of these has empirical formula  $V_4E_6$  and is nomenclated exactly as in the above section, while a second set of molecules having empirical formula  $V_4F_4$  is also of importance. A third set  $V_4E_6F_4$  which presents many more permutations as to what is the best ordering of components is encountered less frequently. Additionally, from a strictly mathematical completeness perspective, one might consider the set  $E_4F_6$  to be of interest ; however, without the inclusion of atoms (represented by V), this set will **not** be of **any** chemical significance.

#### 3.1. $V_4E_6$

3.1.1. Just as one of the allotrope of phosphorus has tetrahedral geometry, similarly one encounters the same extension of tetrahedral geometry (as described for "organic" molecules) in modules formed from phosphorus and oxygen atoms. In particular, one notes that the two common oxides of phosphorus are **not** the lowest combination of atoms ( $P_2O_3$  and  $P_2O_5$ ) traditionally taught in beginning chemistry courses. Instead, these molecules occur as dimers ( $P_4O_6$  and  $P_4O_{10}$ ), rather than as monomers, with each dimer having tetrahedral shape: namely,  $E = O$  and  $V =$  either P (Figure 5a) or P2O (Figure 5b). This produces as the respective systemic canonical names:

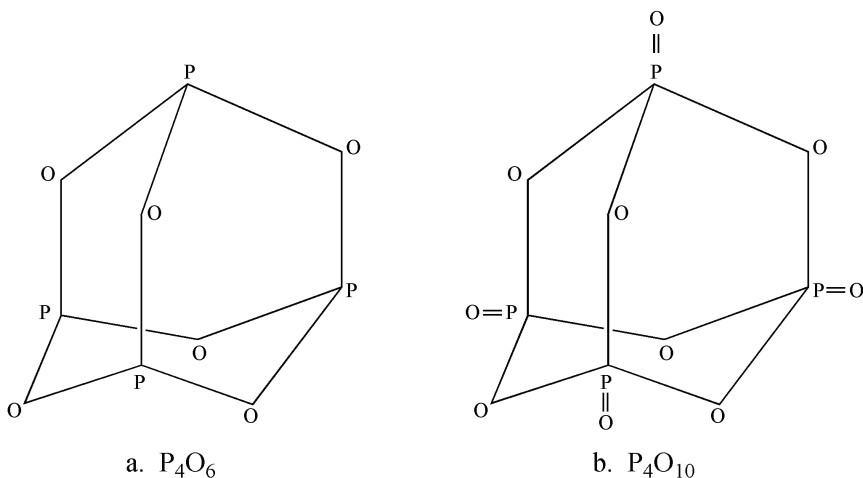
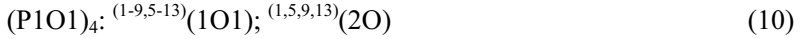


Figure 5: Phosphorus oxide dimers which have adamantyl (extended tetrahedral) geometry



and



where the “trioxide” (9) differs ONLY by the atom designation; i.e., all of the respective locant numbers are identical. The “pentoxide” (10), as well as duplicating the “trioxide” in locant designation, introduces two distinct types of oxygen modules: doubly bonded to a single phosphorus atom as part of the vertex module, and singly bonded to each of two phosphorus atoms as the edge module.

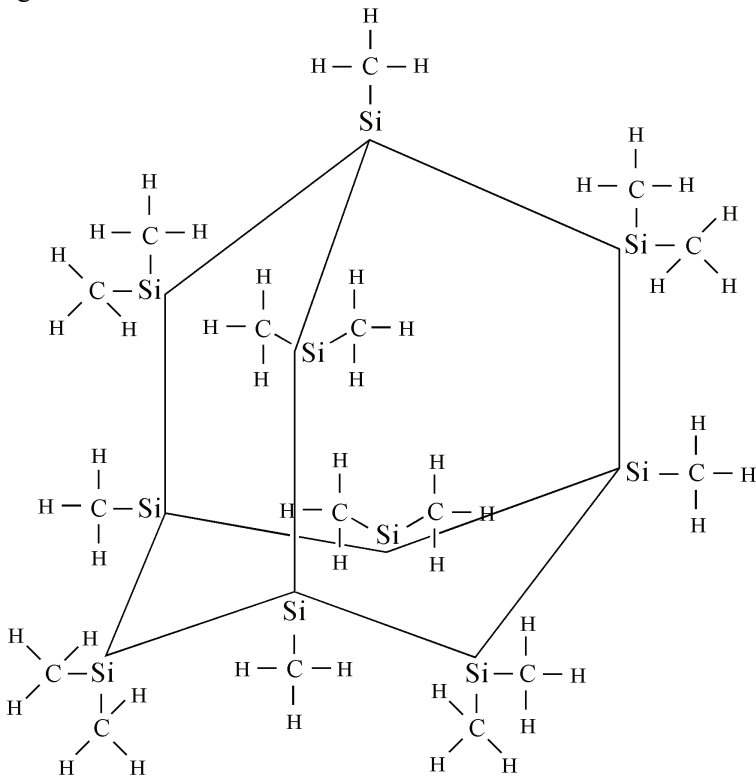
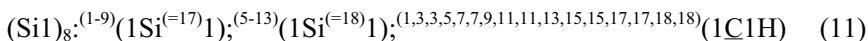


Figure 6: A silicon module which has adamantyl (extended tetrahedral) geometry

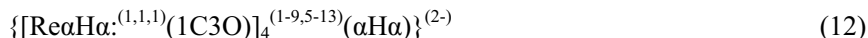
3.1.2. Attention is now directed to a silicon analog of adamantane with 10 silicon atoms at the ten vertices. However, unlike the simpler “adamansilane” (Si<sub>10</sub>H<sub>16</sub>) which would have hydrogen atoms attached to the silicon atoms, this molecule, referred to as “sila-adamantane” has replaced those hydrogen atoms with methyl groups [9] (Figure 6). The systemic name for this molecule:



seems more complicated than all of the other examples given so far for which (5) is the prototype ONLY because of the underscoring convention. If one were to create a corresponding convention for attached methyl groups (rather than hydrogen atoms or, as described in the footnote in Chapter 1 of [3] to denote a singly bonded fluorine atom in highly fluorinated compounds), an identical V<sub>4</sub>E<sub>6</sub> empirical formula exists along with the systemic name: (V1E1)<sub>4</sub>^{:(1-9,5-13)}(1E1), where V = Si1C1H and E = 1Si1^{:(3,3)}(1C1H). It is only when the actual atoms, rather than the modules are incorporated into the canonical name that formula (11) is produced.

3.1.3. An Israeli-German team described selected cadmium selenide clusters having the extended tetrahedral structure associated with adamantane as “adamanthanes” [10]. Whether this was just an extension of the European usage of the “th” for an “admantane-like” molecule, or whether it was a deliberate “misspelling” to indicate the Column 16 similarity (selenium is directly below sulfur in the periodic table)\* is speculation that only the author or editor of that journal could resolve, if they wanted to.

3.1.4. For the rhenium carbonyl hydride ion [11], [H<sub>6</sub>Re<sub>4</sub>(CO)<sub>12</sub>]<sup>2-</sup>, V = Re(CO)<sub>3</sub> and E = H. Each of the carbon atoms in the three CO modules is attached to a vertex rhenium atom, which has a hydrogen atom along each of the edges joining it to the other three Re atoms. This is a straight-forward extension of Figure 2 above and may be nomenclated as:



where, as developed in [3], the symbol  $\alpha$  denotes a bond with bond order greater than 0 and less than 1; in particular, in this case a traditional hydrogen bond, which is deemed to have bond order 1/2.

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\* IUPAC uses the prefix *thia* to designate a sulfur substitution.

3.1.5. Some compounds that have  $V_4E_6$  tetrahedral geometry but which do not fit neatly into the various historical fiefdoms include:

3.1.5.1. As well as the simplest phosphorus oxide ( $P_4O_6$ ) described above with its tetrahedral geometry, one also encounters the corresponding phosphorus nitride [12]. Here, however, the line between what has traditionally been designated as an “organic” (vs. an “inorganic”) compound is further blurred because nitrogen has three bonds, rather than the two normally associated with oxygen. When this third bond is to a methyl group one forms the phosphorus methyl nitride with empirical formula  $P_4(NCH_3)_6$  and systemic name:



3.1.5.2. We next focus on a basic beryllium acetate in which four beryllium atoms are located at the vertices of a tetrahedron; however, unlike previous examples, these four atoms are also attached to a central oxygen atom [13]. (Note that these four atoms are NOT graph theoretically adjacent

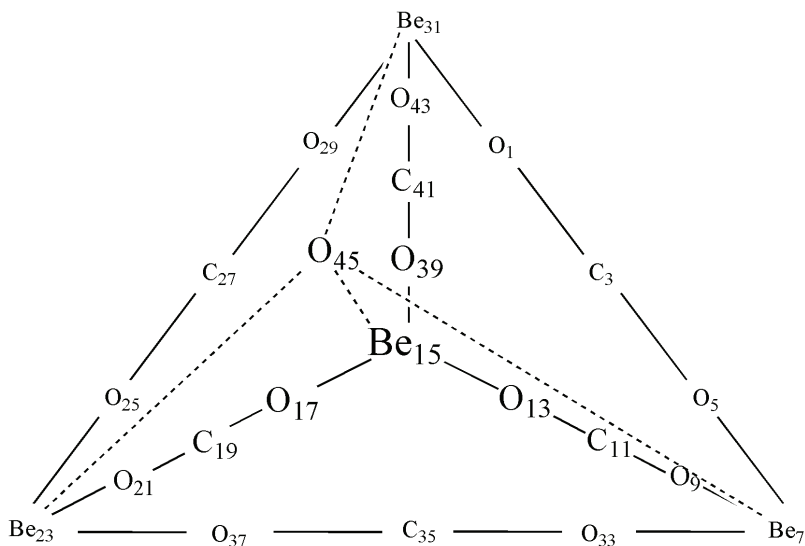
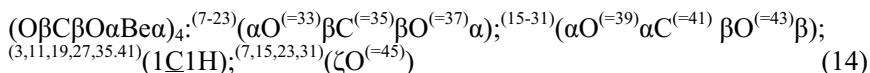


Figure 7: A basic beryllium acetate

to one another. Instead this much of the molecule forms a star.) In order to describe this molecule using the  $V_4E_6$  empirical formula, one views the V component as being in the traditional “inorganic domain” with each beryllium atom covalently bonded to one-quarter of the central oxygen atom, while the E component is in the traditional “organic domain” with all six of the acetate modules ( $CH_3CO_2$ ) being hydrogen bonded at each end to a beryllium atom. The canonical name, using the standardized bond orders introduced in [3]\* for this  $OBe_4(CH_3CO_2)_6$  molecule (Figure 7) is:



Further examples of this particular class of molecules having tetrahedral geometry in the classical inorganic domain are frequently being discovered, meanwhile, we turn to a second variation of the place of the tetrahedron in chemical structure and examine traditional “inorganic” molecules with a different empirical formula:

### 3.2. $V_4F_4$

3.2.1. Starting from the above rhenium ion in paragraph 3.1.4. above and removing two hydrogen atoms [14], one forms the neutral molecule  $H_4Re_4(CO)_{12}$ . Like the above ion, this molecule can similarly be modeled using a tetrahedron; however, with a different perspective: Instead of the bipartite division as a Vertex – Edge model, one now encounters the bipartite division of a Vertex – Face model. This, in turn, leads to a different standardized geometry and nomenclature. In particular, rather than the hydrogen atoms being situated along an edge of the tetrahedron, they are positioned at the center of the faces, which may be geometrically modeled as a stella octangula; i.e., two interpenetrating tetrahedra [15]. In order to translate this solid into a model that is described using graph theory, one views the face-centered (hydrogen) atoms as alpha bonded to each of its three rhenium neighbors and replaces the traditional Schlegel projection [16] with a net [17]† (Figure 8). By this perspective, each of the hydrogen atoms

\*  $\alpha = 0.5$ ;  $\beta = 1.5$ ;  $\zeta = 0.25$

† Note that in the net of Figure 9 the single ruthenium atom with locant #3 has three images. Similarly, the three edges emanating from  $Re_3$  are each repeated twice; while the remaining three vertices and three edges have a single representation. In this manner, the four vertices of the tetrahedron are represented by six points in the net and the six edges in that polyhedron appears as nine line segments. By this technique, one is able to situate the four hydrogen atoms as bonded to neighboring atoms and thereby to apply graph theory in order to nomenclature this molecule.

is viewed as being alpha bonded to each of its three facial vertices, with the systemic canonical name for this molecule becoming:

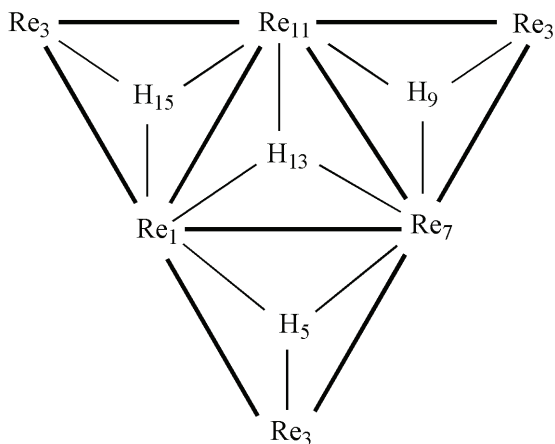
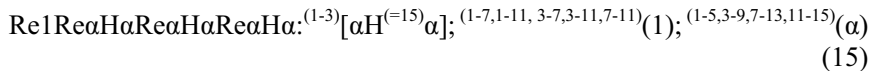


Figure 8: The net used to nomenclature  $\text{H}_4\text{Re}_4(\text{CO})_{12}$

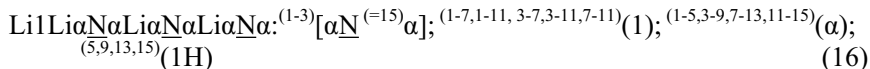
Before progressing further, one observes that this vertex-face tetrahedral model bears an intriguing relationship to the lutetium compound illustrated in Chapter 2 (Item 26, Figure 24, Formulae 35 and 36) of [3]; namely, in place of there being two interpenetrating 3-simplexes [(tetrahedra), one formed by the four rhenium atoms and the other by four hydrogen atoms] which then form the stella octangula, the lutetium compound introduced an element of degeneracy by having the second interpenetrating simplex be a triangle. This has been reflected in the nomenclature by the alpha\* bonding being of bond order lower than one-half, namely one-third, in only one of the four hydrogen bonds in the lutetium compound, but in all of the face bonds in the rhenium compound described above.

3.2.2. Lithium forms a sequence of Vertex-Face tetrahedral molecules with lithium atoms at the vertices and the four rightmost (non-inert) row 2

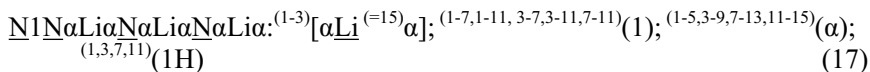
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\* Using the nomenclature system of [3], an alpha bond has bond order between 0.2 and 0.8 and occurs in many scenarios such as the two sets of hydrogen bonds between the two boron atoms in diborane-6, etc.

atoms with a charge = -1 (F, OH, NH<sub>2</sub> and CH<sub>3</sub>) emanating from the circumcenter of each face [18]. Although one might expect the canonical names of a representative molecule to be:



the lower atomic number of lithium vs. that of the N is contrary to the Cartesian naming algorithm developed in [3]; consequently, although this “name” is a valid one, it is not the desired canonical name. Instead, one notes that the vertices of one tetrahedron of a stella octangula are the circumcenters of the opposite faces of the other tetrahedron; consequently, the canonical name is:



### 3.3. V<sub>4</sub>E<sub>6</sub>F<sub>4</sub>

3.3.1. As well as the above described “binary” compounds, one occasionally also encounters “trinary” compounds. One such example of this formulation is a germanium sulfide halide, such as Ge<sub>4</sub>S<sub>6</sub>Br<sub>4</sub>. Here the vertex module is a germanium atom and a radially extending halide atom while the edge module is a single sulfur atom diradical [19]. The systemic canonical name for this molecule is thus:



## 4. “NATURAL PRODUCTS CHEMISTRY”

Directing our focus next to the domain referred to as “natural product chemistry”, we note that tetrodotoxin, C<sub>11</sub>H<sub>17</sub>N<sub>3</sub>O<sub>8</sub>, (Figure 9), which was recently in the news as a neurotoxin [20], is a modified adamantane module which no longer maintains the tetrahedral distinction between vertex and edge modules implied by the formula (5). Instead, using the numbering system introduced in [3] wherein the four “vertex” module carbon atoms are C<sub>1</sub>, C<sub>5</sub>, C<sub>9</sub> and C<sub>13</sub>, only C<sub>5</sub> and C<sub>9</sub> remain as in adamantane. C<sub>1</sub> has as its fourth ligand a negatively charged oxygen atom, while C<sub>13</sub> is the start of a six member ring containing two nitrogen atoms which ends at the “edge” module C<sub>18</sub>. Similarly, of the remaining five “edge” modules two (C<sub>3</sub> and C<sub>17</sub>) are oxygen atoms, two (C<sub>11</sub> and C<sub>15</sub>) are COH groups and the fifth (C<sub>7</sub>) has a COH and a hydroxyl group as ligands. In other words, one might have

anticipated that, disregarding the stereochemistry [21], one would follow the protocol used to name adamantane and assign as its partial canonical name:

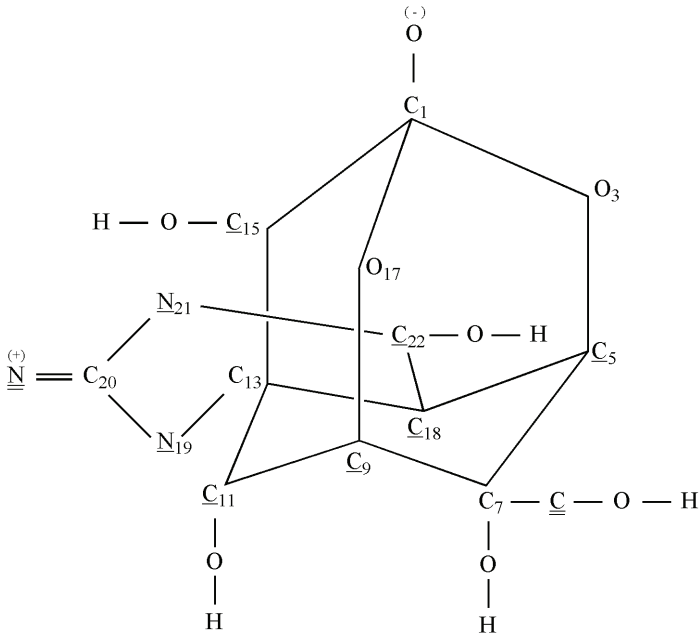
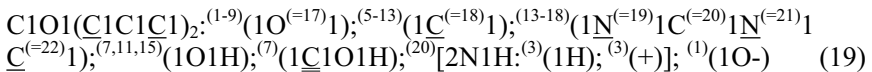
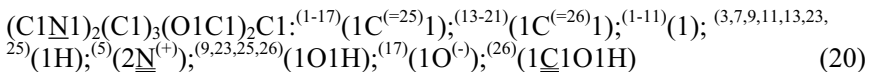


Figure 9: Tetrodotoxin - named non-canonically as derivative of adamantane



However, upon examining Figure 9, one notes that there exists a longer primary cycle, as illustrated in Figure 10. Consequently the canonical name (without indicating the stereochemistry) for tetrodotoxin becomes:





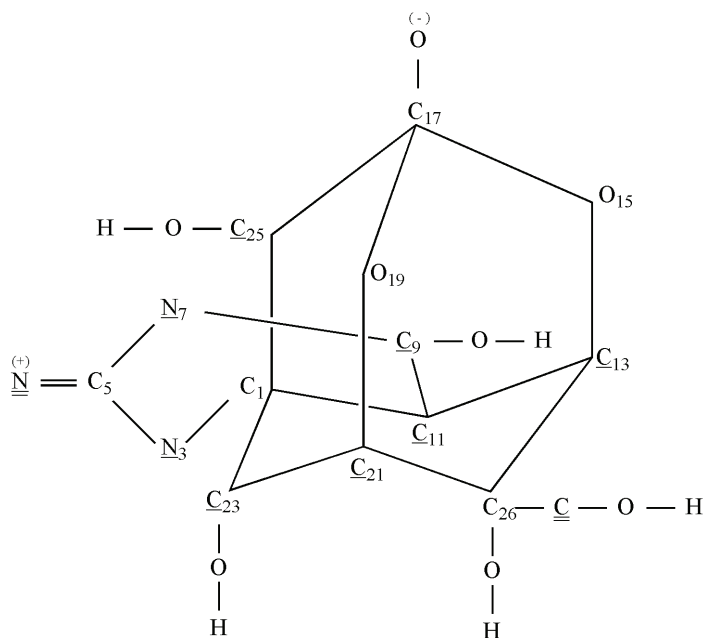


Figure 10: Tetrodotoxin - named canonically

## 5. “BORON CHEMISTRY”

In the domain of boron chemistry, which, until recently, was viewed as being a part of “inorganic chemistry” (but now is often viewed as having more in common with the chemistry traditionally associated with the “organic” domain), one encounters further examples involving tetrahedral shape. In [22], as well as p. 186 of [3], we viewed the molecule with molecular formula  $B_4H_{10}$ , not as the traditional ACS Council’s representation [23], but rather as having a tetrahedral geometry with  $V = \underline{B}$  and  $E = \alpha H\alpha..$  This produces as the uncorrected systemic canonical name introduced in [3]:



which is character by character equivalent to (5) above, and the corrected version in which fluxions are incorporated:

$$(\underline{B}\alpha H\alpha)_4^{(1-9,5-13)}(\alpha H\alpha)^{(1-5,9-13)}(\alpha) \quad (22)$$

At this point, one notes that every  $V_4E_6$  modularization need not produce a viable molecule. In particular, consider the known boron hydride with formula  $B_6H_{10}$ . Mathematically, one could make the tetrahedral assignment of  $V = H = 4$  and  $E = \underline{B} = 6$ . However, the affixing of hydrogen atoms at the vertices of a tetrahedron, while relegating to the edge modules boron-hydrogen pairs is based on a geometry that is highly unlikely. In other words, despite that the algebra works, based on an extrapolation of all of the molecules we presently know, such a geometry is **most probably** not viable.

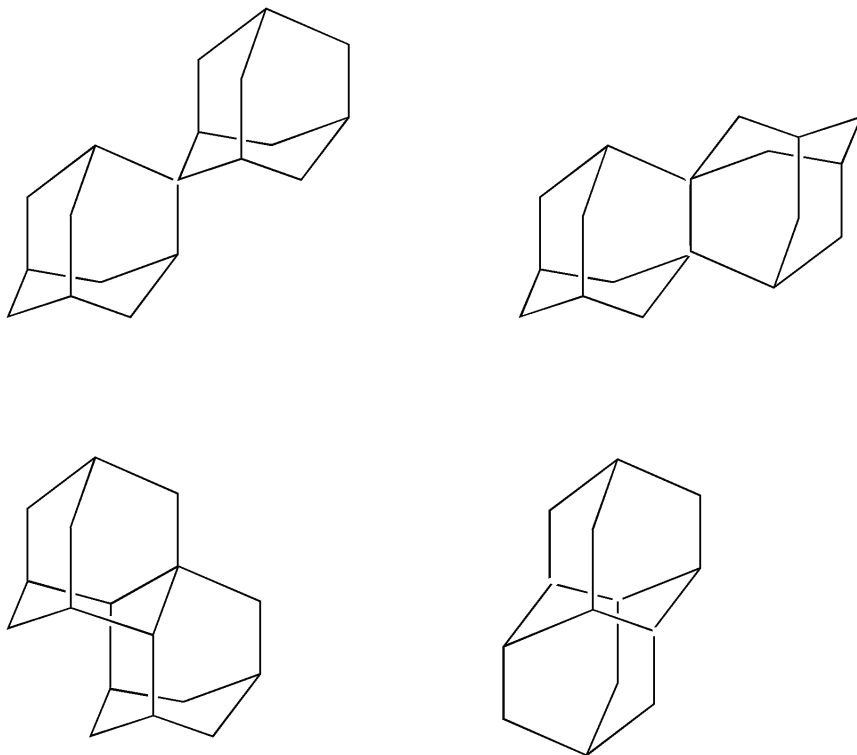
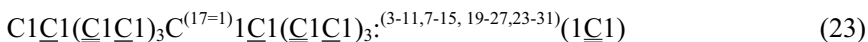


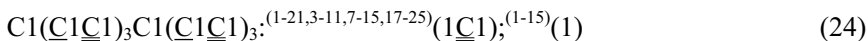
Figure 11: The four combinations of 4 adamantane modules to produce diamantane

## 6. "POLYMER CHEMISTRY"

When multiple copies of the adamantane module are combined so that each hydrogen atom is replaced by a carbon of another adamantane module, the diamond crystal is formed. This important form of carbon is described and nomenclated in detail in Chapter 8 of [3]. Note that the price paid for such an "across the field" standardization is the ability to readily compare molecular structures. Such a price is paid by every analytic, versus synthetic, nomenclature [24]. For example, of the four mathematically possible diamantanes, the point fusion of two adamantane modules (part a of Figure 11), would be nomenclated as:



Upon comparing this name to the name assigned to adamantane [see (3)], one notes that there is insufficient overlap in the two names for the proposed nomenclature to be useful in QSAR (quantitative structure activity relationships) studies. Without translating the name into a structural formula and then making the comparison of connectivities, none of the systematic nomenclatures (IUPAC, nodal, or the proposed one) alone allow for determining how close two structure really are to each other. Moreover, the degree of similarity gets progressively less as one examines the canonical names of edge fused adamantane modules (part b of Figure 11):



This name, while still bearing some resemblance to (4) in that certain combinations of atom-bond sequences and of locant sequences are repeated, has a familial relation that is nowhere near as clear. By the time that one reaches the face fusion (part d of Figure 11), nearly all of the "local" similarity in the canonical name

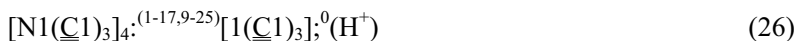


has been obscured.

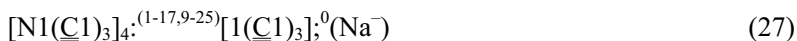
## 7. "TOPOLOGICAL CAGES"

As well as the creation of "endothelial compounds", such as atoms constrained to stay inside a fullerene [25], molecular "cages" associated with adamantane in Section 2 above have been created. One of special interest has as its cage the molecule nomenclated as (7) above. Now,

however, interior to this cage one has  $H^+$  and  $Na^-$  ions, rather than, if one were to expect ions, the anticipated  $Na^+$  and  $H^-$  ions. This aggregation [26], which has as its common name “hydrogen sodide” is the first known example of such an ion separation in a metal hydride. In all other known cases, the electron transfer in a binary compound containing sodium and hydrogen had produced the more familiar ions of  $Na^+$  and  $H^-$ , which was designated by the name *sodium hydride*. As indicated in Chapter 7 of [3], the systemic canonical name for the cage is augmented by the respective ion contained in an individual cage; viz:



and



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