Orismology (The Science of Defining Words) and the Geometrical Foundations of Chemistry. 2. Inherent Topology

Seymour B. Elk

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

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 also carry, often influences the direction in which both laboratory and theoretical research progresses. Examination of the role that synthetic geometry (including topology, graph theory, etc.) plays not only in describing the physical foundations that underlie the organization and description of chemical moieties but, of equal importance, in helping us to sort out just what is our perception of these moieties is undertaken, with particular emphasis on what may be called the "inherent topology" that molecules seem to possess.

1. INTRODUCTION TO "TOPOLOGY" FROM A CHEMISTRY PERSPECTIVE

One of the first steps in the process of any type of model building is to replace the elements physically present in the given set with an idealized set of mathematical abstractions that approximates these elements.[1] A second important step, which is particularly relevant to the model building of chemical molecules, is to determine exactly what is the inherent topology of the molecules under consideration—an orismological problem that, when carried to its extreme, would necessitate an examination of all of the connotations and denotations in the word "topology". This is especially true since there has evolved an aura about ideas "topological" so that the use for this word has been distended to include all kinds of things that are better described using other more appropriate words. Two examples that come to mind immediately are "topological indices"[2]—which are much more in the domain of graph theory than in topology—and "orbital topology"[3]—which is more appropriately subsumed by considerations of "orbital symmetry".

Although many formal definitions of the word topology abound, especially in the theoretical mathematics literature, for the purpose of chemistry, some less formal definitions, such as

> "a branch of mathematics that investigates the properties of a geometric configuration that are unaltered if the configuration is subjected to any one-to-one continuous transformation"[4]

and

> "... a development in geometry that ... has as its object the study of the properties of geometrical figures that persist even when the figures are subjected to deformations so drastic that all their metric and projective properties are lost"[5]

are better suited to our purposes. In other words, we wish to emphasize the ideas inherent in the early development of what was then called "analysis situs",[6] while evading the rigorous formalism that would be daunting to the practicing chemist.

Because the importance of any mathematical concepts in a burgeoning science is one of pragmaticism, the task which we have undertaken in this report is to stay within the

limitations imposed by this simplification of the word "topology" without oversimplifying. With such an objective, let us now turn to an examination of some important lines of demarcation in chemistry that have long been recognized as existent—but never clarified. In doing so, however, it is important to remember that, although the immediate focus might be on the selection of geometrical models, the real requirement is that the model selected has the greatest chemical relevance. The most obvious example of this is that Dewar benzene is not a "benzene" of any sort, being, instead, an aliphatic bicyclic compound. Toward this goal of chemical relevance, we focus in this report on two questions that are central to an understanding of the relation of geometrical models to chemistry:

(1) What is the appropriate "embedding space"?[7]
(2) What meaning is to be assigned to "homaloidal"?[8]

2. "APPROPRIATE" EMBEDDING SPACE

Turning our attention to the first of these questions, we note that one of the most important parameters in the geometrical description of any mathematical figure (and consequently of any physical object that such a figure is supposed to model) is its dimension. However, a formal definition of the word "dimension" is predicated, to a large extent, on whether the perspective of the user is that of pure vs applied mathematics. Limiting attention to applied mathematics, a definition of convenience is given in Van Nostrand's *International Dictionary of Applied Mathematics* as

> "The dimension of a set of elements is most conveniently defined as the number of parameters necessary to give an analytic description of the set."[9]

Note that this dictionary gives a definition of the word "dimension" in terms of "analytic"; however, it does not give a definition of "analytic". In other words, to the editors of this dictionary, the word analytic is more primitive,[10] and so needs no definition. Were it not for the perspective chosen below, we would believe this to be a spurious conclusion!

Rather than pursuing the denotations and connotations that are inherent in the definition of "analytic", with its more theoretical mathematical implications, we, instead, recognize that a formal definition of the word "dimension" that would be satisfactory to a mathematician would seem pedantic to a practicing chemist; consequently, we assume that the

definition of dimension is intuitively unambiguous. With such a heuristic in mind, it is important to review two important related concepts that apply to a chemical model: (1) dimensionality and (2) minimum embedding space.

2.1. Dimensionality. In the process of formulating a definition for the word "dimensionality" in ref 1, we first asked: "what is the dimension of the various modules being used in order to construct the model of the named structure?" We then assigned the term "dimensionality" to the dimension of a module in a molecular model, PROVIDED all of the modules were of the same dimension. Furthermore, we editorialized, that this was the norm—rather than the exception. The examples given were that the skeleton of cyclohexane is formed by the union of line segments and thus has dimensionality = 1, while benzene has both its carbon skeleton and its hydrogen atoms coplanar and thus has dimensionality = 2. We further deduced that it would be convenient to assign a dimensionality = 1 to the fusion of all acyclic and most alicyclic compounds and a dimensionality = 2 to all compounds whose graphs can be pruned (of side chains) to form a kernel of fused benzenoid rings. The alicyclic compounds not included in this set would be those which Goodson designated as "fisular".[11] Furthermore, by such a definition, we have excluded assigning a dimensionality to biphenyl and polyphenyl type molecules since one of the modules (the connecting "bridge") is linear, while the rings are planar, as well as to those "Tinkertoy" molecules developed by Michl,[12] etc.

It should be noted that at the time ref 1 was written, we further buttressed this idea with the observation that the fusion of any number of unstrained benzene rings also produced a coplanar orientation that was breached only when these rings sterically interfered with each other, as in the case of the helicenes.[13] Now, however, with the flood of new chemistry that has emanated from the discovery of the fullerenes,[14] etc., redefinition of the term "dimensionality" to reflect aspects of local, in contradistinction to the more familiar global, cohomaloidality is necessary.

What we missed in ref 1 and are proposing as a subject of study is that, for purposes of taxonomy and consequently for nomenclature, etc., rather than continuing the traditional ideas of "strained"[15] and "constrained" molecules being included with unstrained molecules in common taxonomy classes across the entire spectrum of molecules, let us have a larger number of smaller taxonomy classes—so that the "common" properties within a class be more distinctive. In other words, chemistry has matured from the binary division into aliphatic and aromatic. (See development of this idea below.) Instead it is time to recognize that as one particular constraint becomes the dominant feature of a molecule's reactivity and its otherwise salient parameter is subordinated, this is sufficient justification for segregating it from its former taxonomy class and treating it separately. For example, cyclopropane's formation and its reactivity are much more related to its ring strain than to it being an alkane. In many respects, one would not be amiss in correlating cyclopropane with "cycloethane", i.e., ethene—a fact that we recognize, but for which we use different terms, when we discuss the ideas that are inherent in "geometrical isomerism". That this is a taxonomy, as well as an orismology, problem can be readily deduced from the difference between Harary's[16] and Nash-William's[17] concepts of "what is a graph?" and our consequent pseudoconversion of polybenzenes into acyclic polyenynes.[18] Similarly, many of the "compact" polycyclic aliphatic compounds are more influenced by potential three-dimensional interactions than by the fact that

they are aliphatic. For example, the skeleton of a dimethyl *cis*-decalin (*cis*-2,7-dimethylbicyclo[4,4,0]decane) would have a geometrical configuration that is almost the prototype of a polymantane, whereas the skeleton of the corresponding *trans*-decalin (without the methyl groups) is "reasonably" approximated and thus "adequately" described by a coplanar geometry. Even the presence of the two methyl groups, which are axial to each other, does not significantly influence the "essentially coplanar" properties of the trans isomer. It is only when we use the traditional unrealistic coplanar picture[19] that these two disubstituted decalin molecules fall into a common taxonomy class.

At this point in the study, some may be disappointed that we do not delve more deeply into the question of the "dimension of a graph"; however, to do so would make the evasion in section 1 of the formal definition of the dimension of a space, or of an object in that space (i.e., a "space segment"), seem that much more arbitrary. Consequently, in this report, we have avoided formal use of "abstract graphs", preferring to retain the geometrical representation that such a graph implies; i.e., we eschew the perspective that a graph is merely "a point set, along with the set of binary relations between members of that point set".

Three further comments on "dimensionality" are in order at this time:

(1) We have the ability to assign a dimensionality of 1 to all alicyclic compounds if we are using a positive definition of the word "aliphatic" but not if that term has been negatively defined. This is true since we have not made provisions to exclude the class of polymantanes[20] (and also the trivial class of a single atom, to which we assign dimensionality = 0).

(2) Although the definition of "dimensionality" given in ref 1 superficially appears to be adequate, it fails to address a second important question: "What is a description of the fusion set?" or, at an even more fundamental level, what do we want the word "fusion" to denote and connote? In other words, in retrospect, we had intuitively assumed that only one type of fusion set was of importance; namely, fusion would always take place at a covalent bond chemically, which is mathematically equivalent to at a single line segment—even though we know that this is not the case for spiro ring compounds in "two dimensions" and various linear and point connections in irregular polymantanes. Turning to the dictionary definition of "fusion", "a merging of diverse elements into a unified whole",[21] we note that neither the method of merging nor the final form of the diverse whole has been clarified. In fact, because of this built-in ambiguity, in ref 22, we showed how the "fusion" of modules can be used in many ways to convey differing ideas. This is to say nothing of the familiar use of this same word for chemical processes entirely unrelated to model building.

(3) Even without the new problems raised by the fullerenes, we were still confronted by not inconsequential problems in trying to describe dimensionality for the cyclophanes. Such problems arise because "pruning" the side chains of a cyclophane does not produce a single benzenoid kernel, rather it creates more than one such kernel. In other words, for compounds having mixed taxonomies, the concept that "dimensionality" was intended to describe is neither unique, nor evident to "all reasonable persons"; consequently, we must tread carefully when trying to expand the concept, lest we create internal contradictions.

2.2. Minimum Embedding Space. We turn now to "the minimum embedding space"—a term that we had defined in 1, namely, the smallest (homaloidal) space in which the

skeleton of that molecule is able to exist. For example, the skeleton of cyclohexane has a dimensionality of 1, a minimum embedding space of 2, and normally occupies a portion of three-dimensional space, whereas a fusion of benzene rings, such as coronene, has dimensionality = 2, a minimum embedding space of 2, and normally occupies a portion of a two-dimensional space.

From a chemistry perspective, because there is only one highly unstable conformer of cyclohexane that has a planar skeleton and because there are no important chemical properties of this molecule that take place in the plane, there is negligible chemical benefit in describing cyclohexane either (a) in terms of a single planar segment—even though this gives the traditional picture of this molecule, i.e., as the same coplanar hexagon that we had used for benzene, but with each carbon atom having two hydrogen ligands in addition to the bonds to other carbons of the cycle—or (b) as the union of planar segments bounded by smaller polygons, such as four triangles, a quadrilateral and two triangles, etc. Instead, cyclohexane is best viewed as either the union of line segments (i.e., one-dimensional) or as a skewed hexagon (a one-dimensional figure in a three-dimensional embedding space), in which the concept of area is ill-defined. This is in contradistinction to benzene which should be described only in terms of planar taxonomy.

3. HOMALOIDALITY

Now, in order to answer the question, what meaning is to be assigned to "homaloidal", let us return our attention to "dimension"—in its simplest practical case: linearity.

The ordinary (Euclidean) geometry used in describing the models of chemical moieties (molecules, polymers, crystals, etc.) has as its main mathematical construct the concept of figure—where "figure" is predicated on connecting entities called "points" by means of other entities called "lines" and then connecting parts of these lines (called "line segments") to create "planar" constructs, etc. In this process there has been created the heuristic elements of "straight", "connecting", "interior", etc., as well as a class of words that have been designated as "primitive".[10]

If we wish to develop any internally consistent system, some starting ("primitive") words must be accepted as understood—an important fact recognized by Euclid.[23] This is equivalent to saying that it is *not* possible to define everything. In particular, words can only be defined in terms of other words—whose meanings are accepted as being known. Knowledge of what a specific word is supposed to both denote and connote is dependent on the user. Whether a particular word is to be denoted as being primitive depends on the user's perceptions and biases. It is not unusual to find instances where a word which was considered primitive to one person has a precise definition in another person's frame of reference. For example, the concept of a line might be considered as primitive (as was assumed by Euclid) or else it may be defined in terms of more sophisticated concepts. One such definition—which uses a much larger knowledge base—is a one-dimensional homaloidal manifold, where the terms "dimension", homaloidal", and "manifold" are assumed to be understood by the reader, and each of these terms is judged to be more primitive than "line". Which words you denote as primitive depends on your individual bias. It is a strictly heuristic decision on what is the base of knowledge and thus of reference.

This creates a somewhat undesirable situation: So long as we are merely formulating a system, it is usually possible to

effectively mask nearly all problems of consistency by making the appropriate intuitive assumptions. Subtle difficulties arise only when an attempt is made to close the system and then analyze any given figure within the system.[24]

In the formulation of an efficient model for chemical moieties it is important to distinguish between a "discrete" and a "continuous" geometry[10] and to recognize that it is a heuristic element of most continuous geometries that the entities designated as figures have the same dimension as that of the embedding space. In chemistry, on the other hand, this geometrical generalization of thinking in terms of entire spaces is a poor one. To the contrary, the geometry that is most relevant is one in which chemical action takes place primarily between pairs of atoms. Consequently, in order to try to introduce order, the focus must be on the union of these linear pairs. For example, in cyclobutane, which is frequently modeled as a skew quadrilateral, the tetrahedral superstructure of the skew quadrilateral is of negligible (some may say zero) significance. Similarly, no chemical significance is given to an imagined pathway connecting non-adjacent carbon atoms—even though in some conformers such a metric distance would be less than the equilibrium value of 154 pm between graph theoretically adjacent atoms. This is equivalent to saying that the chemical concept usually described by localized bonding has been represented in the model by a geometrical one.

Furthermore, we note that, as a general rule, the one-dimensional orientation of chemical bonds is adequate for most molecules that had, up to this time, been catagorized as "aliphatic"; that is, the model being used does not take into consideration either two-dimensional or three-dimensional modules. In this model there is no chemical relevance to either the solid cube or to the interior of the six planar faces in, say, cubane; rather the set of twelve edges between pairs of adjacent carbon atoms, as well as the eight line segments between carbon and hydrogen atoms, serve as the locus of *all* chemical properties—with the space between being considered as "empty". More succinctly, one could say that for most compounds, such as both cyclobutane and cubane, despite the specification of a three-dimensional embedding space, a local linear geometry, rather than either the planar (boundary-defined) or solid (content-defined) geometries, is the most desirable one to use in describing such chemical compounds. This is in contradistinction to the relevant solid geometry that is a characteristic of adamantane[1] and its higher analogs[20] (the polymantanes) and also to the use of a solid topology in describing the intramolecular hydrogen bonding of various macromolecules, such as DNA.

4. COMBINED QUESTIONS OF MINIMUM EMBEDDING SPACE AND HOMALOIDALITY

At this point in the study it is desirable to consider the history of the distinction being made between compounds that are classified as "aromatic" vs "aliphatic": First of all, we note that, in accordance with the Kekule–Couper–Butlerov theories of valence developed in 1858–1861—which laid the foundations for modern structural formulas—all known organic compounds were placed into one of two broad catagories: aliphatic (derived from "FAT") or aromatic (having a characteristic odor).[25] As more knowledge was achieved during the subsequent years, the original binary relationship was seen to be inadequate. In fact, both of these words have undergone major changes in connotation and denotation, so that today there are two concurrent BUT UNEQUAL ways of "defining" these "terms":

Figure 1.

In a superficial survey made by examining all of the *beginning* texts and general condensed chemical dictionaries that happened to be on the shelves of various local university and public libraries at the time (approximately 30 total), we found that each such reference book tried to either define or adequately describe "aromatic"; however, they seem to be split into three disjoint classes with respect to how they wish to define "aliphatic"—with the apparently deciding factor being the author's (probably subconscious) attitude with respect to a positive vs negative definition of a word. (Note that a term is "positively-defined" if it belongs to a set that has some single characteristic or set of characteristics that can be used to test for inclusion in that set. Similarly, a term is "negatively-defined" if it belongs to the complement of that set. The terms "positively-defined" and "negatively-defined" can be grouped together in the single term "mathematically-defined", and one can assert that if there does not exist such a binary test, then as the field of allowable members is expanded, finer distinctions as to what constitutes set membership come to the fore, until ultimately the determination of set membership becomes a heuristic decision. Of even greater significance to a burgeoning science is the observation that, unlike in a mathematics wherein the boundaries of discussion are fixed by the definer, as more scientific knowledge is gained, the original line of demarcation that formed the basis for defining some specific word often gets further removed from the observed phenomenon that led to the defining of the word in the first place. This results in the need for a balance to be struck between the goal of using only mathematically-definable terms and the use of "more fuzzy" words that connote physically observable and measurable concepts.[26]

Applying the distinction of postively- and negatively-defined to the word aliphatic in freshman-level college texts produces the following:

(1) The majority just use the word aliphatic without ever attempting to give a formal definition *of any sort.*[27]

(2) The next largest group negatively-define the word. For example, Streitweiser and Heathcock advise "compounds with no aromatic rings are known as aliphatic compounds".[28]

(3) A minority of texts and dictionaries that try to be more precise, and thus do give a positive definition, include some specific properties of straight or branched chain arrangements of constituent carbon atoms which are sufficient for the vast majority of molecules. Nevertheless, it should be noted that, even in this limited set, such a "definition", while seeming to be permissible for most "familiar" compounds, will turn out to be inadequate for "selected" molecules.

In a similar manner, we note that the connotation "aromatic" is supposed to carry today has gone through very many revisions and nowadays presupposes the entire Huckel theory, as well as some other ideas that extends the idea far beyond the benzenoid type compounds[29] for which this word was originally intended. Despite the importance of some of these other extensions, we believe that there is still a rich lode to be mined from one such particular geometrically-biased concept of aromaticity—that is, still focused directly on the class of benzenoid compounds:

In ref 1, we described four "simple" topologically distinct taxonomy classes that can exist for a cube—with the implicit assumption that the delineation of what is "simple" is a function of what is the base of knowledge of the user of that word. In some instances, such as a "simple" figure, we know of no satisfactory definition that partitions the set of all figures into "simple" and "not simple", even though some desired properties
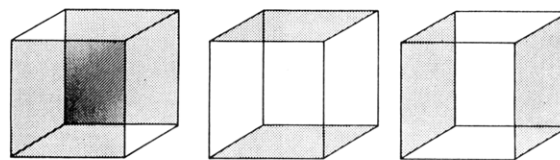
of "simple" figures, such as "simple-closure", "simply-connected", etc., are mathematically-definable.

To re-iterate, the four distinct taxonomy classes described for the cube are (1) the set of vertices—a set containing 8 zero-dimensional elements; (2) the set of edges—a set containing 12 one-dimensional elements; (3) the set of faces—a set containing 6 two-dimensional elements; and (4) the set of cells—the set containing 1 three-dimensional element—the cube itself.

The importance of these dimensionally segregated classes arises because a unique, mathematically consistent set of definitions can be formulated ONLY within a given taxonomy class. Mixed taxonomy classes, such as the set of two diametrically opposed faces and four edges for a cube, are NOT unique. In this case, any one of three such sets may be selected (Figure 1). Consequently, whenever possible, it is desirable that the choice of taxonomy class be the same for all components in the model to be used in the description of chemical compounds.

Although the above paragraph describes the mathematical ideal, none of these math models may be adequate for certain molecules. For example, in the case of the cyclophanes,[30] it is pragmatic for there to exist concurrent, but unequal, taxonomies. For these compounds the ability to formulate a comprehensive (expandable, but still simple and internally consistent) nomenclature may be beyond our capabilities—either mathematically or simply from a practical perspective. This is not to say that when attention is limited only to that class of compounds, better (more efficient) nomenclatures are unattainable; rather that the mathematical virtues of, say, a nodal nomenclature[31] may be more than counterbalanced by a chemically illogical taxonomy. The historical development of chemical nomenclature, for example, contains frequent intuitive subdivisions that could not be logically justified—even in the formulator's mind. Austin Patterson, for example, advised in his "Proposed International Rules for Numbering Organic Ring Systems" that "any distinction between classes B and C must be more or less arbitrary, but the line drawn in these rules conforms fairly closely to actual usage."[32] Whatever that is supposed to mean!

A note of extreme importance at this point is that the picture which Patterson had formulated in his mind was based on the then-known organic compounds of interest. This was expressed using terminology that is unacceptable by today's standards, not the least of which is the use of intuitive terms—such as "above and to the right" in his rule 7.[33] In other words, contrary to the present trend in geometry that recognizes the increased probability of introducing error by reliance on any pictorial representation,[34] Patterson based his terminolgy on simplistic pictures that could be easily drawn on a plane surface—inasmuch as such a representation was likely to be used by practicing chemists, who, as a general rule, were not interested in the mathematical subtleties that might be desired. With such a background, it is not surprising that there are many flaws in the system.

Returning to our examination of the concept of homaloidal—in particular to our concept of "straight" with respect to the "quote" straight-chain "unquote" alkanes—we
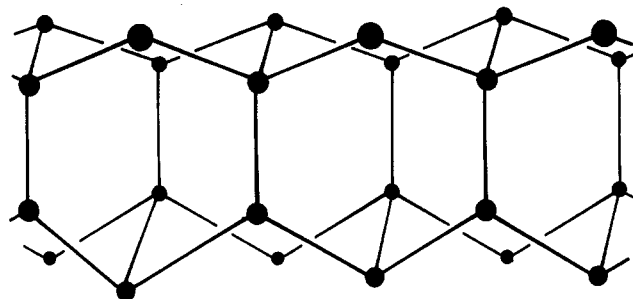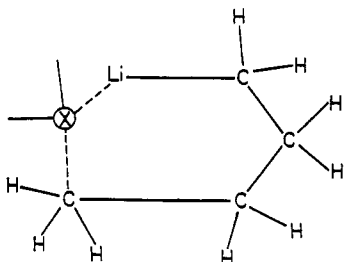
Figure 2.

Figure 3.

note an unusual description, which is contrary to our intuition, has been created as a consequence of the process of forming figures by annellating line segments, in contradistinction to the more familiar (and elementary) process of intersecting entire lines. Namely, all annellations must occur at an angle prescribed by the type of orbital being used: tetrahedral for sp^3, trigonal for sp^2. It is only for an sp orbital that the intuitive idea of straight is in evidence. This is equivalent to saying that "straight" has lost its intuitive meaning in either an sp^2 or sp^3 environment. In the absence of straight in the truly geometrical sense, there is, however, the related concept of shortest graph theoretical path. The foundations for this are developed in ref 10. The results of such a development is that, at the atomic level, in an sp^2 environment, a conjugated system of double and single bonds approximates our intuitive concept of straight by means of an all-*trans* conformation. Similarly, in an sp^3 environment, the configuration that is the nearest to this intuitive concept has a bipartite system of alternating bonds that are setwise parallel (Figure 2).

At this point it is important to reiterate the conclusion reached in ref 10: Unlike the sp^2 environment, all of the C–C bonds in an sp^3 environment are single bonds, which, were it not for the formation of rings, would offer no restriction to the free rotation about this bond. Because of this, we may envision segments of the skeleton of an *n*-alkane as being either "straight"—as exemplified by analogy to *trans*—or "circular"—by analogy to *cis*. In other words, from the limited perspective of only the geometry, an active element, such as lithium, on one end of an *n*-alkyl chain can be involved in a reaction occurring at either one or both ends of the chain simultaneously—depending on whether the reacting conformer is straight or circular. For example, the circular conformer of say *n*-butyllithium would have the requisite geometry to form a six-membered intramolecular ring by acting as a "pincer" on a single atom (Figure 3).

Additionally, as well as the usage of "straight" with respect to the bonding of atoms, there is also the concept of "straight" with respect to modules (composed of more than a single atom). In an sp^2 environment, there is the class of polycyclic aromatic hydrocarbons referred to as "acenes",[35] and, for sp^3 orbitals, there exists face-fusion of adamantane modules to form "straight polymantanes". (This may be seen in Figure 2 by

focusing attention on the modules, rather than the individual bonds.) Furthermore, so long as these (congruent) modules tessellate the embedding space (i.e., regular hexagons in the plane and adamantane modules in three dimensions), the intuitive concept designated by the word "straight" remains unambiguous.

The importance of the fusion of modules being able to tessellate the embedding space is seen by examining a situation where such a tessellation is not attainable, namely, for condensed five-membered ring systems. Such systems, because of the proximity of the pentagonal angle of 108° to the tetrahedral angle, *seem* to form straight molecules. Nevertheless, in such a system, even at the modular level, in order to approximate straight, the alternation of pentagonal rings in an up vs down orientation is required.[36] The logical conclusion of such a requirement of alternation of "up" vs "down" is that, using the Patterson convention for drawing rings with an odd number of sides,[32] we produce a circular fusion of pentagons—rather than a straight one. Similarly, all attempts at fusing together "straight" chains of pentagonal modules, with the objective of tessellating the plane with pentagons, produces skew hexagons, instead of the desired coplanar (even if not regular) pentagons. Furthermore, the surface thought to be a plane was, in actuality, a pleated fusion of individual adamantane "faces". Such a surface is the nearest construct that the word "plane" could mean in a polymantane.[20]

The allowed linear fusion of cyclopentane modules, on the other hand, does produce some interesting geometrical chemistry, including an algebra describing the fusion of an additional ring to a set of already fused rings.[37] When carried to its logical conclusion, the annellation of cyclopentane modules in the plane creates the need for an analog to the helicenes,[38] which may be called "helicanes".

5. CONCLUSION

As a final remark in this study, we note that the rapid advances that are taking place in the laboratory necessitate the reexamination of many aspects of the inherent topology that had, up to this time, been assumed to be based on immutable models that were infinite, binary, etc. Instead of this "comfortable" model which has hitherto been used (or maybe I should say "misused"), an accounting of some of these unanticipated manifestations will lead to a vastly different, hopefully more realistic, and maybe even a more aesthetically-pleasing, taxonomy scheme.

ACKNOWLEDGMENT

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(7) The term "embedding space" refers here to the mathematical space in which the physical molecule may be idealized without sacrificing its important chemical properties. For example, a plane is adequate when the system being examined is a benzene molecule (either in isolation or in combination with other benzene modules). In a similar manner a "three-dimensional" space is more appropriate in the description of even a single molecule of cyclohexane. On the other hand, if our focus is on explaining the effect of benzene on living tissue (i.e., the benzene molecule intercalating in the DNA helix), the coplanarity of the benzene, while important, is only a part of the description and thus the appropriate embedding space is three-dimensional.

(8) A word that is independent of the size of the embedding space and is the generic word meaning straight in one dimension, flat in two dimensions, etc.)?[9]

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