

Orismology (the Science of Defining Words) and the Geometrical Foundations of Chemistry. 4. Polycyclic Compounds

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Received August 1, 1995[®]

In trying to clarify the concepts of chemistry, we find that fuzziness sometimes creeps into our thought processes precisely because of our inability to guarantee that the words we (as transmitter of some relevant information) use convey the same denotations and connotations to all receivers of that information. One cannot overlook how orismology—the science of defining words—influences the direction of both laboratory and theoretical research. An 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 also of equal importance in helping us to sort out just what is our perception of these moieties is undertaken. In this fourth article of the sequence, the problems inherent in merely being able to count, let alone assign a canonical nomenclature to multi-ring systems, are examined.

1. INTRODUCTION

In the previous articles of this series, we first noted that one of the primary steps in the process of any type of model building was to replace the elements physically present in the given set with an idealized set of mathematical abstractions that approximates these elements.¹ This was followed by an examination of the inherent topology of the molecules² and the heuristics that are implied in the word “ring”.³ Now we are ready to consider the formulation, description, and naming of multi-ring chemical compounds.

Intuitively, one would anticipate that analysis of a given multi-ring molecule would be undertaken by subdividing it into smaller modules—which we call rings, and then examining the union of the individual rings. Although this is a true statement, one should not overlook the fact that such a process involves at least two *major* heuristic assumptions: (1) The rings that we described in ref 3 are, *in fact*, the individual components that form the building blocks of molecules and (2) we know how to synthesize the molecule from these building blocks.

2. A HISTORICAL ATTEMPT AT ORGANIZATION—SSSR

With the above two assumptions in mind, it has been common for standardization to be sought by introducing a concept called SSSR⁴ (smallest set of smallest rings—where smallest ring size takes priority over smallest number of rings). Such a standardization, however, is equivalent to making the assertions that (1) the graph of a multiple ring system is absolutely isomorphic with the molecule⁵ and (2) that the graph (and consequently the molecule) can be analyzed by first focusing on the smallest rings in the graph and then consider the smallest possible set of these rings that cover all of the edges of the graph. In other words, our goal is to select as the SSSR the smallest set of Eulerian paths⁶ that span the bond set of the molecule. Unfortunately, for selected molecules (as depicted by their graphs), such a goal is unattainable. This was shown in ref 7. Furthermore, in that report, we demonstrated that the underlying foundation

of SSSR is merely a restatement of Euler’s polyhedron equation in topology. Consequently, it is not surprising that problems which are inherent in the blind application of topology to molecular structure have their counterpart in SSSR.

In order to better appreciate a major problem area involved in the use of SSSR, let us examine a figure of speech in the English language that is not often used in scientific writing: The work “metonymy” describes the usage of one word for another closely related to it; e.g., “the kettle is boiling” is understood to mean that water is boiling in the kettle, rather than that molten metal is bubbling on the stove. In other words, an imprecise usage of a word still conveys the desired meaning. Similarly, we note the metonymic usage of the word “ring” as (1) a closed electronic pathway in a molecule and as (2) the boundary of a face of a geometrical model that represents this molecule.

It is here that Fujita’s introduction of ESER (essential set of essential rings)⁸ only serves to exacerbate the problem by formalizing the presence of “rings” throughout the entire sequence of tautomer—conformer—resonance structure—transition state described in ref 1. This is notwithstanding the fact that there does not exist formal covalent bonding in the first and last members of this sequence.

Examining this problem area in more detail before even listing any of the other problems associated with SSSR, we note that seemingly trivial questions, such as

- (1) How many faces does a “simple” geometrical figure, such as a cube, have?
- and
- (2) Do we really want to describe all of the faces of a geometrical model of a chemical molecule?

may not be so trivial, after all.

For the first of these questions, it was shown in ref 9 that a *complete* listing of isolatable faces for even so “simple” a figure as a cube is not the intuitive answer of six. Rather, there are 60 such faces—a fact that any computer not given instructions how to limit its focus will readily confirm. Moreover, the average scientist or mathematician who has not paid attention to some subtle heuristics implied by this question (e.g., until being confronted with this listing) does

[®] Abstract published in *Advance ACS Abstracts*, December 1, 1995.

not appreciate the fact that such a listing obfuscates, rather than clarifies, our perception of a cube. Intuitively, we have a mental picture that focuses only on what we think of as “simple” faces. Furthermore, for that *one specific* geometrical figure the cube, the heuristics of “simple” is easily defined in terms of coplanarity, and the “extraneous” 54 additional faces may be discarded without meaningful loss. In a similar manner, in order to answer the second question, if the molecule under consideration is cubane, we should expect the same set of six faces to be of chemical significance. However, for purposes of nomenclature, and many other descriptions, such a compound is viewed as having only five faces. Such a description arose because of the prevalence of coplanarity in our perception and the consequent use of Schlegel projection.¹⁰

3. CHEMICALLY MORE VIABLE CRITERIA FOR ORGANIZING MOLECULES

From a chemistry bias, we are confronted with the philosophical undesirability of eliminating one face of a “three-dimensional” model for the purpose of “nomenclating”,¹¹ BUT retaining all of the faces for a “two-dimensional” model. Such a world view raises the far more serious pragmatic question: Where is the line of demarcation for the class of molecules between two-dimensional vs three-dimensional?¹⁵ In fact, if we were to carry through the justifications of naming only five of the six faces of cubane, we should find an even smaller set (of only four rectangles), called the “minimum spanning set”, gives all of the same information by covering every edge of the figure.¹⁶ In other words, by recognizing that the chemical properties of cubane are determined by the one-dimensional bond set, rather than either the union of (planar) faces or the solid cube itself, we may shorten the name needed to completely specify every bond in the molecule by using only four rings instead of five.

Determination of how many rings there are in a three-dimensional compound become much more perplexing when the individual faces of the model may no longer be represented by two-dimensional simple figures, such as the squares in cubane. For example, even though the four skew hexagonal faces of adamantane might be approximated by coplanarity, with the resulting final figure being a regular tetrahedron, actual three-dimensional fusion of adamantane modules to form polymantanes is much more complicated. This is seen by using a model of face-fused diamantane and performing standard graph theoretical reduction techniques—namely, replacing each incidence = 2 atom by a single edge. Instead of producing two fused tetrahedra from the two fused adamantane modules—as might have been anticipated by crude analogy—the resultant three-dimensional polyhedron is two disjoint (noninterlacing) regular tetrahedra mated with a skew (chair conformer) hexagon. (See Figure 1). In retrospect, the alternating of vertices forming disjoint tetrahedra should have been anticipated since there does not exist a tessellation of three-dimensional space using regular tetrahedra;¹⁷ thus a geometrically simple picture is not forthcoming. Consequently, continuation of this method to higher face-fused polymantanes results in a model that tends to overwhelm the viewer trying to follow details of structure and connection.

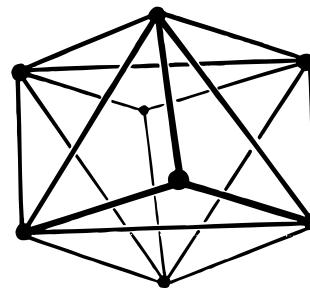


Figure 1. The figure produced by replacing each incidence = 2 atom by a single edge in the three-dimensional fusion of two adamantane modules.

4. MORE PROBLEMS WITH SSSR

A second problem inherent in the perfunctory application of SSSR was summed up by Dyson¹⁸ when he advised “Some skill must be exercised in detecting the smallest rings present”. This is illustrated in ref 19. In other words, despite the fervent wish of many laboratory chemists who feel that nomenclature is an “increasingly irrelevant” subject that now “thankfully” can be handled “blindly” by a computer—and indeed it can, and should be, for the familiar, mundane compounds, the taxonomy schemes that theoretical chemists are constantly trying to perfect in order to better describe and name all kinds of subdivisions of matter (especially newly discovered molecules) are still very much a function of their chemistry.

At this point it should be noted that the main problems associated with SSSR occur for molecules that cannot be represented by a “simple” coplanar graph. This is shown in Figure 2 with the comparison of “prismane” vs “Moebiane” (the mathematical limit of the compound created by Walba²⁰). Note that not only does a “single twist” in one of the “simple faces” greatly change the total number of faces in the model being examined (see Tables 1 and 2 of ref 7), but also in Moebiane we are confronted with a “two-sided” face—a concept that is beyond the capacity of both Euler’s equation and any application derived from Euler’s equation, such as SSSR. In other words, SSSR is a useful tool for that limited set of molecules which are not greatly distorted by projection onto a planar surface; however, as the deviation of the projection from the actual three-dimensional geometry grows, so inversely does the value of the description in terms of SSSR.

5. SOME SELECTED “ESOTERIC” MOLECULES

An additional complication raised by the above paragraph is the following: What meaning is to be assigned to “single twist”? Were the topological domain in which we are working to be that of content-defined figures,¹⁵ there would probably be nearly universal agreement as to what description is applicable to the geometrical model being used; however, the domain used to describe most chemical molecules is that of boundary-definition. At this point it is important to note that in the case of boundary-defined models, there is an odd—even relation between objects and their images, depending on the number of twists. In other words, if a second twist is added to the chain before rejoining, there is a simple topological transformation that reduces the model to simply prismane. Similarly, a third twist becomes isomorphic to Moebiane, etc. This is referred to in topology as “orientable” vs “nonorientable”.²¹

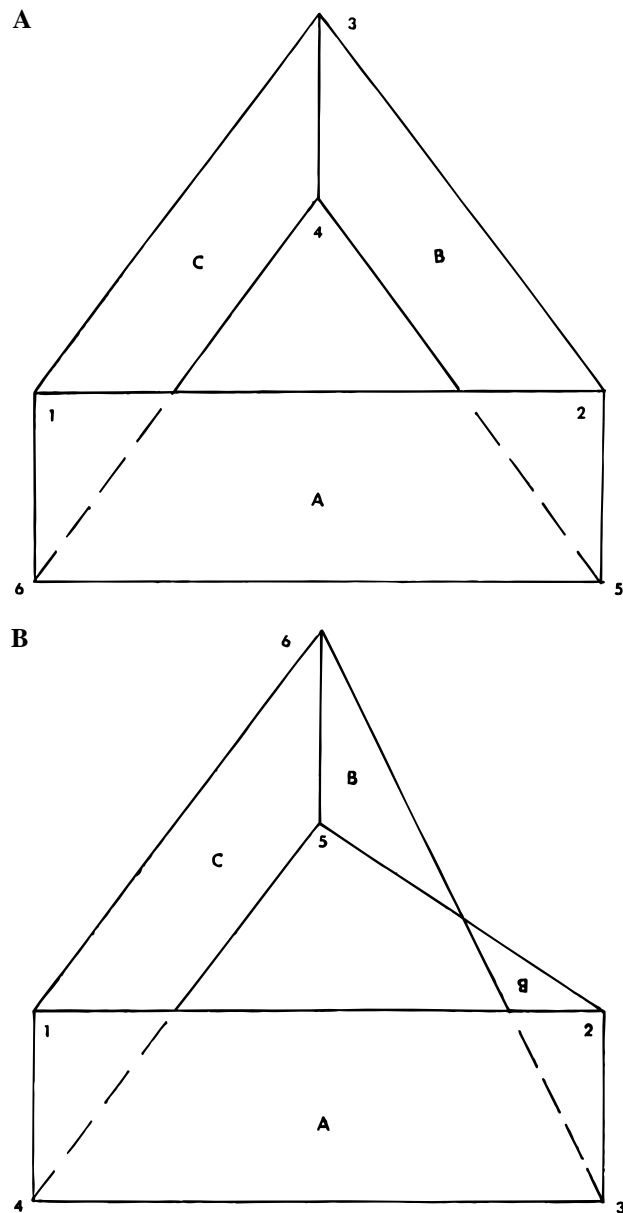


Figure 2. Comparison of "prismane" (A, top) vs "moebiane" (B; bottom).

One additional note of interest is that in exactly the same manner that we could form a molecule whose graph is reducible to $K_{3,3}$, there are molecules whose graphs are reducible to K_5 (part a of Figure 3).²² The "parent"²³ compound for one such set of compounds is the prototypical propellane²⁴ (part b of Figure 3). Part c illustrates three such molecules which have been created in the laboratory.

As mentioned in ref 3, there is an interpretation of the Moebius strip which focus on the content-defined figure. Such a model has no easily recognized correlation to graphs. Instead, its synthesis is easily visualized using planar-defined modules, such as, say, benzene. Although there may be some pragmatic problems in actually synthesizing such a molecule, theoretically, this should not be a problem—so long as the individual modules are not sufficiently distorted that they lose their aromatic character. But such an amount of distortion is now a common property of the helicenes.²⁵ In other words, with impunity, we can allow for a small amount of torsion, say 10 or 15° out of the plane. Consequently, we propose forming such a "planar Moebiane" by breaking

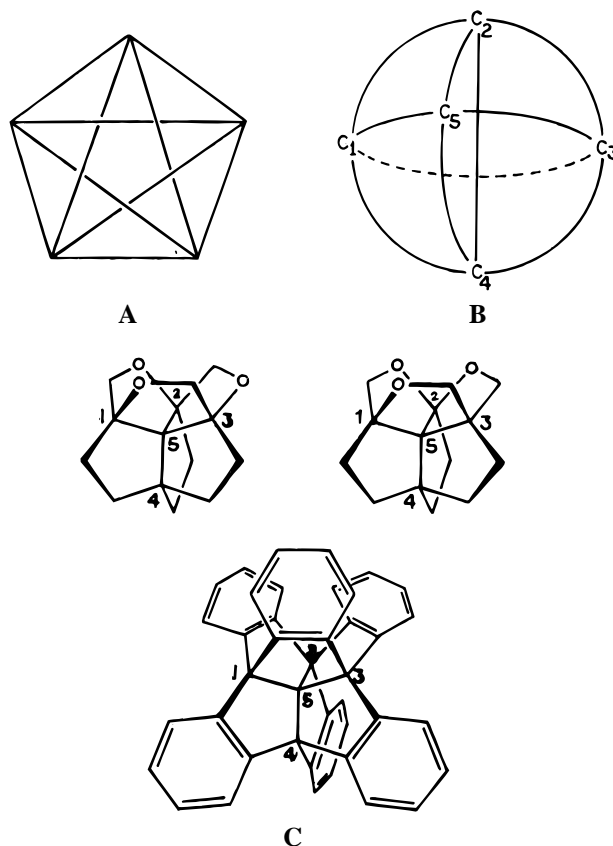


Figure 3. The graph K_5 (A, top left), parent compound for one type of molecule whose graph is K_5 (B, top right), and three actual molecules whose graph is K_5 (C, bottom).

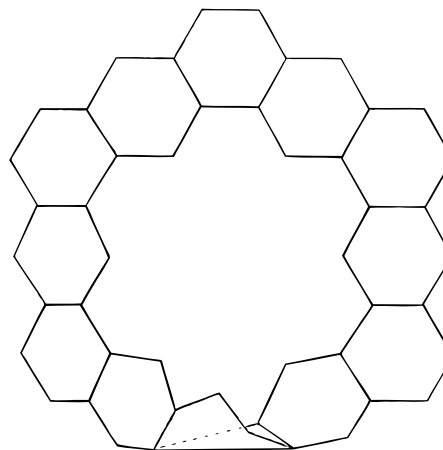


Figure 4. A "content-defined" chemical Moebius strip—the union of 12 benzene modules to form a planar "Moebiane".

a fusion bond between two rings of an "elongated coronene" of, say, 18 or 12 modules, successively twisting each of the rings the above amount and then rejoining the two end rings. This is illustrated for 12 benzene modules in Figure 4.

At this point let us continue to apply our "free-thinking" to even more esoteric figures. For example, ideally, one may envision the Klein bottle as a figure in a Euclidean four-space, which has a three-dimensional representation formed by allowing the figure to intersect itself. This intersection, however, is not represented as a delineated point set but rather as a rotaxane²⁶ with a "movable collar" around the "self-intersecting tube". With this interpretation in mind, and recognizing a chemical model in terms of the union of linear modules in three-space, formulation of a molecular

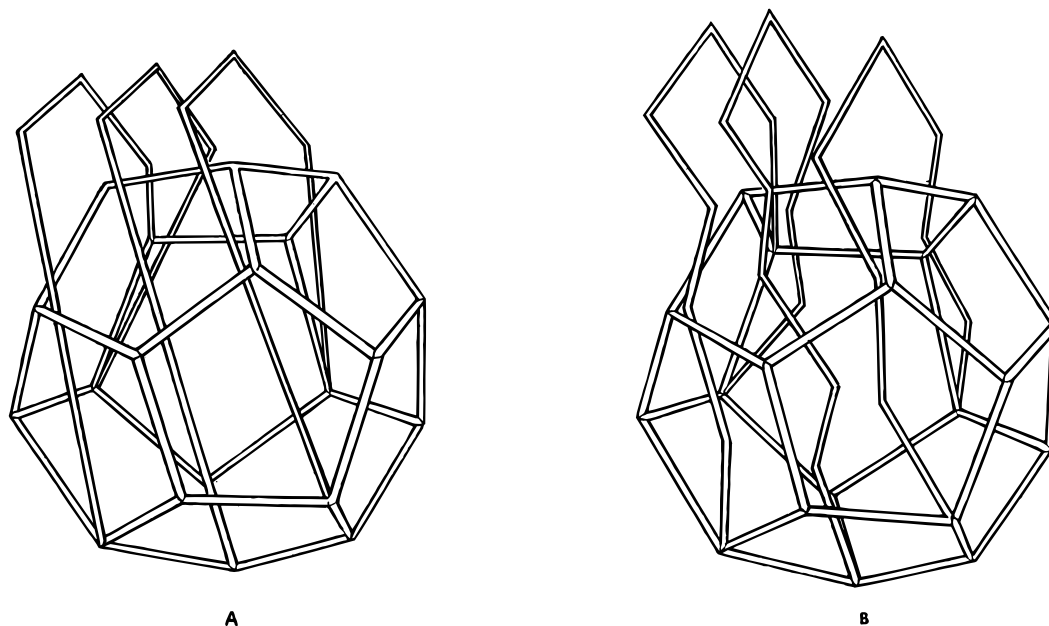


Figure 5. Potential chemical Klein Bottles: (A) Mathematically simplest—using sp hybridized bonds and (B) chemically “more” viable—using sp^2 or sp^3 hybridized bonds.

Klein bottle is a realizable goal.²⁷ Figure 5 shows two “potential” models that would be categorized as “Klein bottles”: In part A of Figure 5, we have created the “interior tubing” using the mathematically simplest combination of atoms that we could find; namely, with sp hybridized bonds we can form geometrically straight lines. This would be accomplished if these “tubes” were polyynes. Part B, on the other hand, illustrates the presence of “more” realistic (if I may use the term loosely) bond angles with either sp^2 or sp^3 hybridization. The price paid for these “easier to formulate” “interior” bond angles is the presence of hydrogen atoms which may be too sterically hindered to be viable.

6. THE CHEMICAL COUNTERPART OF “GEOMETRICALLY SIMPLE”

Returning now to the concept of “simple”, from a geometrical perspective, our intuitive reaction might be to ask what could be conceptually simpler than addition of two figures to form a composite figure, in particular, addition of that simplest of two-dimensional modules that is chemically relevant—benzene rings. Furthermore, let us pick as the addition process the reticular²⁸ fusion at a common edge, and, what seems to be a further simplification, let us be constrained to stay in the plane. A priori, if we have a system of n reticularly fused rings and we fuse one additional ring, we would expect that the final aggregate would have to have $n+1$ fused rings. However, such is not always the case.²⁹ The reason why these “simple” processes sometimes do not work is that, in the geometrical model we have chosen, there have been created polyhedra that are no longer simply-connected.³⁰ The net result of using such a geometrical model is that the concept that “ring” was supposed to describe chemically has suffered the same metonymic confusion noted earlier in this section between a ring and a polyhedral face—irrespective of how such a ring was formed, either conceptually or in the laboratory.

Assuming that we could sweep these “problem areas” away and that we really do have a clear intuitive idea of what is a ring, the next logical question to ask is How may

two distinct rings be related to each other? The answer that is usually given is strictly in terms of the number of common atoms that they share or else in terms of the number of common bonds; i.e., the traditional subdivision of the class of rings is into spiro (one common atom or zero common edges), fused (two common atoms or one common edge), and bridged (three or more common atoms or two or more common edges) compounds. Such a subdivision has been developed over the years and formalized by being listed in the different sections of IUPAC’s³¹ nomenclature rules. At this point it should be noted that the existence of other ring combinations, such as catenanes, rotaxanes, knots,^{32,26} etc. are not included in IUPAC’s rules for nomenclature. This may be attributed to the mission ascribed to IUPAC (although the following statement was given in a different context, it is equally applicable to topological isomerism): “... will not be included in the proposed revised rules because to do so would not conform to the established CNOG (Commission on the Nomenclature of Organic Chemistry of the International Union of Pure and Applied Chemistry) policy to recommending the codified use of existing nomenclature practices”.³³ In other words, only after a number of years has elapsed so that there has been sufficient time for most major innovative methods to be “proof-tested” are changes incorporated into IUPAC’s rules.

A disturbing aspect to the answer given in the beginning of the above paragraph is the inherent heuristic assumption that there is a 1:1 and onto correlation between these two different ways (number of common atoms and number of common bonds) of answering the posed question. In fact, one would not be amiss in asserting that a system containing exactly two rings is a possibility ONLY IF the rings are disjoint (either completely independent or else topologically linked but not geometrically joined, such as links in a chain, i.e., catenanes, etc.). Otherwise, there shall always exist a third ring—even though such a third ring is not counted by traditional methods. For example, in naphthalene, the perimeter 10-membered ring is merely a duplicate of the two six-membered rings and is disregarded in descriptions based

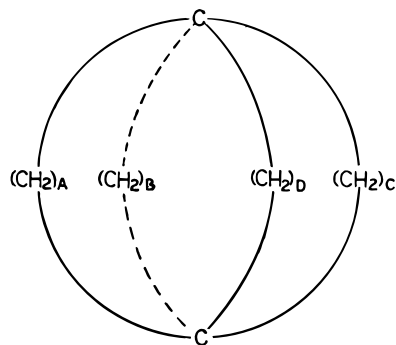


Figure 6. A prototypical paddlane.

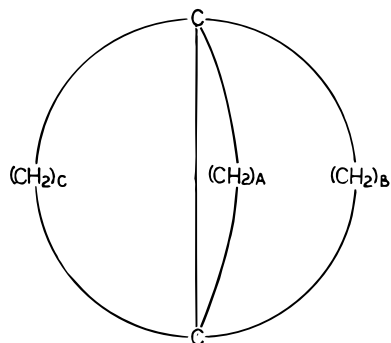


Figure 7. A prototypical propellane.

on SSR⁴ or ESER.⁸ Although this may seem to be trivial for “simple” planar ring systems, *and for simple planar ring systems it is*, this does NOT mean that we may blindly use such a system for noncoplanar ring systems. To the contrary, the correlation between number of common atoms and number of common bonds is valid ONLY when the concept of ring fusion is unambiguously the one applicable to coplanar fusions; namely, every fusion may be considered to be between exactly two rings and forms a connected set starting with a common vertex and then followed by some finite number of common edge/common vertex pairs.

7. MORE “ESOTERIC” MOLECULES

Although the above description seems to be applicable to most classes of chemical compounds, such as all of the categories spelled out by Taylor²⁸ in 1948 and even the larger set Goodson³⁴ described when he recognized the importance of dimension and thus subdivided Taylor’s reticular class into reticular and fusilar in 1980, there exist some compounds for which it is evidently not adequate, in particular, paddlanes (Figure 6) and propellanes (Figure 7).³⁵

Examining Figure 6, one may be tempted to view a paddlane as two intersecting rings with the common set being two nonadjacent atoms only; i.e., there are zero common edges. This is equivalent to considering one ring as C–(CH₂)_A–C–(CH₂)_C and the other ring as C–(CH₂)_B–C–(CH₂)_D. A similar description is generated for a propellane (Figure 7) by considering that one of the methylene chains of a paddlane has been replaced by a single bond. In this latter case, however, there is no intuitive choice as to which of the three chains should be selected to be mated with the C–C bond in forming a “ring”. Instead, it should be noted that the above-described model for both the class of paddlanes and propellanes is substantially better than any which retains the ideas embodied in SSSR; nevertheless, even these pictures are still gross oversimplifications created by an unrealistic reliance on the model chosen.

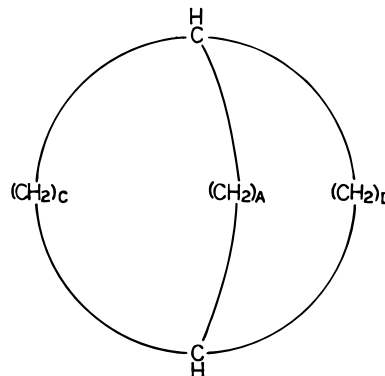


Figure 8. A prototypical ring overlap compound.

A more realistic model of a propellane uses the local geometry at the two incidence equals four carbon atoms: Consider the two tetravalent carbon atoms positioned in a vertical orientation. For a large enough (unstrained) propellane, the four ligands on each of the tetravalent carbon atom have a nearly tetrahedral configuration; consequently, the three chains that emanate from the upper tetravalent carbon atom will be above it, and when reconnected each chain will be below the lower tetravalent carbon. Furthermore, these chains need not be of minimum lengths. Consequently, instead of the rigidity implied in Figure 7, a dynamic equilibrium exists in which the relative positioning of the individual methylene chains is frequently interchanged—much as in the case of two jump ropes of different length held together pairwise at the ends and being twirled in the same or opposite direction. An analogous description of a paddlane applies, so that in both types of molecule, rather than there being a given pairing of “semicircles” (or chord for the propellanes), all permutations of “semicircles” must be examined when trying to designate which pair of “arcs” form a “ring” for these compounds.

In contrast to both the actual physical picture just described and the oversimplified intuitive model given in Figures 6 and 7, tradition and pseudoconsistency with other (unrelated) compounds have produced an interpretation of paddlanes and propellanes in terms of the union of planar segments that is counterproductive.

At this point, it is important to compare a multi-ring system containing “ring overlap” (Figure 8) with propellanes and paddlanes. Notwithstanding that the molecule which Figure 8 is supposed to represent is usually presented as though it had been projected onto a plane, it is more reasonable to consider such a compound as either a propellane with the center bond (between the “tetravalent” carbons) removed (bond saturation is now created by having hydrogen atoms attached to the “free” sites that were created) or alternatively as a paddlane with one of the arcs removed (and similar bond saturation with hydrogen atoms). In other words, in exactly the same manner as it was for the paddlanes and propellanes, the inherent three-dimensional nature of the bonding in a “ring overlap” system makes the use of SSSR as an inferior method of description. In fact, one would not be amiss in asserting that “ring overlap” is merely an inappropriate correction factor to try to force an existing description onto a set of compounds for which it is not applicable.

8. PROBLEMS OF CONSISTENCY

Meanwhile, it should be noted that despite our fundamental inability to even be able to list, no less to describe or to

name, all of the moieties having a given molecular formula, the pragmatic necessity of having a "uniform naming" scheme requires that we formulate a "consistent" system of structure, taxonomy, and nomenclature based on our supposed knowledge. Although we are correct in decrying that the fruits of this pseudoknowledge are the above stated major inconsistencies in every system devised to date, we are now faced with the even more serious problem that advancing knowledge of "ever more curious" molecules has far outstripped our ability to evolve a comprehensive mathematically-consistent system. Some of the problems of merely ordering molecules in an efficient way have deep mathematical roots³⁶ that seem to doom hopes of ever formulating a "desirable", no less an "optimal" descriptive system of organic molecules. In other words, we seem destined to have either an inefficient and inaccurate, although comprehensive, system³⁷ or a collage of disjoint specialty systems that for a very limited class of compounds are more efficient and accurate.

The decision to continue with the presently used, but highly flawed, system has been made by the chemistry community through default; as of necessity it must. Nevertheless, we still decry such a decision, especially when we note the depth of the problem. For example, when using the traditional model, one is saddled with the terms in common usage, namely, "fused" vs "bridged" and "ortho-fused" vs "ortho- and peri-fused". Furthermore, questions of orismology arise because "fused" is an undefined (primitive—see ref 2) word based on the assumption that rings are joined by sharing a common edge, while "bridged" is an undefined (ill-defined; i.e., not mathematically definable in the sense described earlier) word that is being applied to compounds having a "valence bond or an atom or an unbranched chain of atoms connecting two different parts of a molecule",³⁸ where the heuristics of "different parts" is falsely assumed to be unambiguous. The problem is then compounded by the definitions given for "ortho-fused" vs "ortho- and peri-fused", as the model being used for these "definitions" was clearly intended for planar projected molecules only. This is shown by a series of questions relating the propellanes and the paddlanes to the designations of ortho-fused vs ortho- and peri-fused³⁵

- (1) Are the rings in a propellane ortho-fused?
- (2) Are the rings in a propellane ortho- and peri-fused?
- (3) Are the rings in a paddlane ortho-fused?
- (4) Are the rings in a paddlane ortho- and peri-fused?

and the unambiguous answer that contradictions abound and that either description is woefully inadequate.

Ways out of this orismological quagmire have been proposed by many researchers. One that is important is Balaban and Harary's³⁹ division of fused compounds into cata- vs peri-condensed for the limited class of polycyclic aromatic hydrocarbons of ring size six. By this deliberate limitation of focus (to a one parameter system), many of the problems of consistency are avoided. A far more profound subtlety is the use of the neutral word "condensed" in lieu of the related, but somehow different, word "fused". This is an evasion of the problem in that bridged compounds now could be condensed, just as well as could fused compounds.

An interesting orismology objection has been raised by Goodson⁴⁰ to Balaban and Harary's choice of the word "condensed": The word "condensed" is normally used in

chemistry with the denotation of "to undergo condensation"⁴¹ or more precisely "to undergo a condensation reaction"—where a "condensation reaction" is defined⁴² as "A (usually stepwise) reaction in which two or more reactants (or remote reacting sites within the same *molecular entity*) yield a single main product with accompanying formation of water or of some other small molecule, e.g., ammonia, ethanol, acetic acid, hydrogen sulfide". The picture of two geometrical models "reacting at an edge", thereby integrating one copy of this common edge into the product, while throwing out the other one seems to be overusing analogy. Consequently, in retrospect, it would probably have been better had they created an all-together new word which could not convey any irrelevant or misleading connotations.

It should be noted that, despite the potential theoretical virtue of this treatment by Balaban and Harary, from a pragmatic viewpoint, any such limitation of focus is viewed, by the chemistry community at large, as more of a problem than continued usage of the existing nomenclature—withstanding all the faults that the present system may have. Whether Balaban and Harary's scheme is too limited will depend on whether extensions to other parameters, such as different ring sizes and to heteroatoms, can be made at a reasonable price.

Any peruser of the recent literature on theoretical chemistry nomenclature will find that limitations to one-parameter systems abound. For example, for a canonical naming of just the limited class of compounds referred to as either "polybenzenes", or else as "polycyclic aromatic compounds of ring size six", or "PAH6", etc. (to list but a few of the names by which this important class of compounds is known), we alone have formulated systems based on many different mathematical properties. In a similar manner, very many other mathematical chemists have formulated nomenclature systems that either partially work or work for a very limited subset of molecules. Polton,⁴³ for example, has produced a detailed study describing several of these systems in his recent book "Chemical Nomenclature and the Computer".

One of our earliest (1980) treatises that produced a mathematically more logical nomenclature for the class of polybenzenes¹⁷ exploited the idea that such a system tessellated a plane. This tessellating property has been combined with various geometrical and number theory ideas to form other, more sophisticated nomenclature schemes.⁴⁴⁻⁴⁷ Furthermore, the domain of applicability was, subsequently, expanded to a second parameter so as to encompass the class of general arenes.⁴⁸ Although it cannot be ruled out that the tessellation idea might contain the seeds for expansion to the general class of compounds, with many parameters, it does not seem promising at present.

A vastly different, mathematically intriguing, type of system, which, as a curiosity, was shown to be useful for naming the very limited class of acyclic alkanes, was created 28 years ago by Matula.⁴⁹ This system produces a canonical name (number) for a given rooted tree using an algorithm based on prime numbers. However, because the names created are not readily correlated with a structure without the aid of a computer, and, even more damning, expansions to any type of cyclic system was thought to be, at best, too cumbersome to be used by practicing chemists and too limited to be expanded by theoretical chemists when new compositions of matter are formulated or postulated, the

system did not get the attention of the chemistry community until very recently. In 1990, we re-examined the system and were able to apply it to other one-parameter systems, such as the polybenzenes and polymantanes.⁵⁰ Additionally, upon dissecting the principles used, we have discovered that, although the mathematical ideas are valid, the application by Matula to alkanes is slightly flawed⁵¹—with not so coincidentally the same flaw that is endemic throughout the present system of nomenclature. Development involving Matula numbers has been fairly active. In particular, further properties of these “Matula” numbers have been examined by us^{52,53} and by Gutman and Ivic⁵⁴ as well as a comparison of the Matula name with a strictly binary code developed by Trinajstić.⁵⁵ Meanwhile, the limitation of this number theory principle to strictly one parameter systems has been greatly relaxed, so that it may now be applied to ring compounds and to molecules containing heteroatoms.⁵⁶ Nevertheless, the liabilities of unfamiliarity and the need for computer assistance in coding and decoding are still major obstacles to a wider acceptance of this nomenclature scheme, which will not be easily surmounted. Consequently, unless some major further simplifications evolve, it will probably remain an obscure curiosity—known only to a small clique of mathematical chemists.

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CI950083G