

Figure 1. Tenets of CAS publication policies.

(see Figure 1) of completeness, timeliness, and quality that must be ever so carefully balanced with the economic realities of viable marketing strategies.

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Effect of Taxonomy Class and Spanning Set on Identifying and Counting Rings in a Compound

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Received February 29, 1984

The word "ring" in chemical literature is, at best, ill-defined and, at worst, a constant source of ambiguity. In order to better understand the problem, different meanings for this word in current chemistry usage are examined, as well as a concomitant evaluation of the number of faces that a mathematical model of a chemical molecule will have. Of specific interest is the use (abuse) of projection. Fundamental mathematical differences that arise due to different size embedding spaces are shown to be the cause of an inherent inconsistency in presently used systems of chemical taxonomy generally and in systems of nomenclature, in particular.

WHAT DEFINES A RING?

Ambiguities in the meaning of the word "ring" occur frequently in chemical literature and play a major role in merely counting the number of rings that exist in a compound, let alone determining the composition of individual rings, their dimensionality for taxonomy purposes, or their nomenclature.

For most descriptions, and for every common nomenclature of organic chemistry, an important parameter that must be specified is the number of rings in a compound. Although, in most instances, this is relatively straightforward, such is not always the case. Consequently, before being able to simply count this number, it is necessary to delineate: what defines a ring?

First, it should be noted that the definition of ring is a function of the topology chosen.¹ Next, even in a given taxonomy class, there may exist a great deal of ambiguity; for example, consider the planar taxonomy of a cube: the description of a cube as the union of six faces contains the implicit assumption that the word "face" is limited to a single, simple,

coplanar surface. Not only is this unnecessary; in some instances, it is not even desirable. Consequently, if the term ring is used to denote the boundary of a face, then the number of faces in any given figure, such as the cube, must also be redetermined.

There exist $2^6 (=64)$ combinations of a single faces that must be examined in order to determine the total number of faces and rings in a cube. Of these 64 possible configurations, four combinations (the set of zero simple faces and the three sets of two simple noncontiguous—diametrically opposed—faces) do not fit the extended definition of face. Thus, there exist the following: 6 "simple" faces²—each with 4 edges; 12 "double" faces²—each with 6 edges; 20 "triple" faces²—8 with 6 edges and 12 with 8 edges; 15 "quadruple" faces²—12 with 6 edges and 3 with 8 edges; 6 "quintuple" faces²—each with 4 edges; 1 "sextuple" face²—the entire cube (which is topologically transformable into a sphere and so has zero edges).

In order to now compute the number of rings, note that the sets of single and quintuple faces share a common boundary.

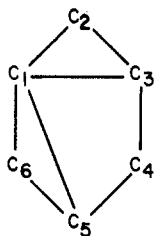


Figure 1.

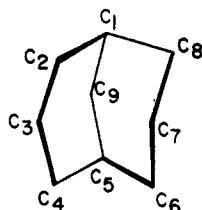


Figure 2.

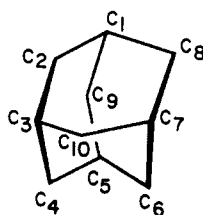


Figure 3.

Similarly, so do double and quadruple faces. Also, half of the set of triple faces shares a common boundary with a member of the other half of this set. Furthermore, each of the three quadruple faces having eight edges has as their boundary the disjoint four-edge rings—which were counted earlier as single rings. Therefore, if one counts each ring only once, the total number of rings in a cube is 28.³

Because the above description of rings would become very unwieldy, especially for indexing and nomenclature, the convention agreed to by chemists is to choose the smallest set of smallest rings (SSSR), where smallest ring takes precedence over smallest set.⁴ In Figure 1 for example, this is considered to be the set of three rings (two triangles and a quadrilateral) rather than the set of only two rings (a hexagon and this same quadrilateral).

Although this simplification usually is satisfactory for essentially planar figures, serious logical inconsistencies arise in the third dimension: In Figure 2 there appears to be universal consensus among both chemists and mathematicians that it would be undesirable to also include the third (eight-membered) ring as a part of the description of this figure. With the addition of a bridge, however, as in Figure 3, the question of whether there is now one or there is now two additional rings depends on the perspective (or bias) of the describer. This depth-implied illustration of adamantane suggests the presence of four hexagonal rings as the SSSR—despite that these rings are not independent. Planar distorted pictures, on the other hand, such as Figures 4 and 5, require only three hexagonal rings. In fact, the fourth of these rings (1-2-3-10-7-8) is often overlooked as not being any more important than the octagonal rings. This perspective has been carried over into IUPAC nomenclature.⁵

HOW MANY FACES DOES A FIGURE HAVE?

The mechanical procedure chosen in order to determine what is the SSSR involves projecting the three-dimensional model onto a plane. Because it is desired that the projection chosen have a minimum number of edges crossing one another

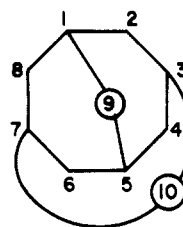


Figure 4.

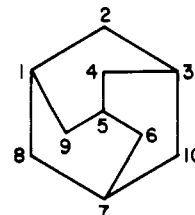


Figure 5.

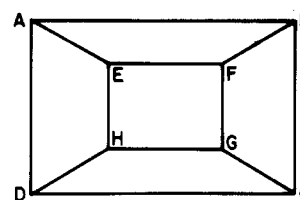


Figure 6.

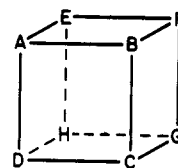


Figure 7.

and because the geometry of projection is an incidence, rather than a metric, geometry, the simplest picture is often the result of distorting lengths and angles. Such a planar projection is called a "Schlegel diagram".⁶ Figures 4 and 5 are different Schlegel diagrams for adamantane. Similarly, Figure 6 is the Schlegel projection of the cube shown in Figure 7.⁷

Although the cube has six distinct simple faces, the Schlegel diagram of this figure appears to have only five faces. There are various ways to describe the sixth face. (1) From the perspective approach, it is the outer perimeter—A-B-C-D; i.e., linear taxonomy is implied even if the rest of the description uses planar taxonomy.¹ (2) From the viewpoint of incidence geometry, it is the figure formed from the set of four edges (A-B, B-C, C-D, and D-A) but not covering any of the other eight edges of the cube. This is possible in two different ways: (a) the boundary-defined quadrilateral, a mathematically valid representation using linear taxonomy; (b) the content-defined quadrilateral—for use with planar taxonomy. Notice, however, that there are two such quadrilaterals—interior and exterior. Of these, the usually implied interior quadrilateral contains the other eight edges of the cube and thus must be discarded. The exterior quadrilateral (defined by the set of four given edges and the rest of the plane) has no such liability. For practical purposes, however, it is usual to consider the Schlegel diagram of the cube as the union of only five faces. Consequently, the common naming schemes for cubane require the specification of only five quadrilaterals in the canonical name.

This raises the philosophical question of the desirability of eliminating one face of a three-dimensional model for the purpose of nomenclature but retaining all parts of a two-di-

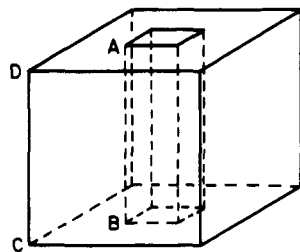


Figure 8.

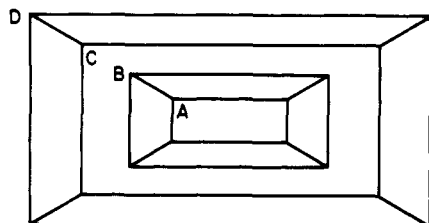


Figure 9.

dimensional model. Although this is usually rationalized by noting that once any five faces of cubane have been given then the sixth face is uniquely determined, there are compelling reasons to be uncomfortable with such a side-stepping of the intrinsic geometry involved. One such reason is that once a subset of only four of the quadrilaterals has been given then the fifth—as well as the sixth—quadrilateral has also been uniquely determined. A nomenclature that requires the description of only four of the six quadrilaterals would be preferable provided it gives a unique name to each compound. In the case of cubane, for example, only the four quadrilaterals A-D-H-E, A-B-F-E, B-C-G-F, and C-D-H-G are required, Figure 6. From these four quadrilaterals the remaining two (A-B-C-D and E-F-G-H) may be formed by using the edges from the given set of four. Such a set is called the "minimum spanning set".

The need for this definition of minimum spanning set raises some fundamental questions about the use of the word ring by much of the chemistry community—especially *Chemical Abstracts*. In footnote 3, for example, Figure 6 was classified as a five ring system, despite acknowledging the existence of a subclass "for which all the atoms and all the edges of the ring system are contained by a subset of the smallest rings". In this context, ring does not mean the one-dimensional boundary of a two-dimensional face; instead, the concept of content-defined simple-connected, planar figure is intended. This is clearly shown by the formula

$$\text{rings} = \text{edges} - \text{nodes} + 1$$

which is comparable to the Euler-Poincare equation for general polytopes

$$\sum_{n=0}^{\infty} (-1)^n S_n = +1$$

where S_n is the number of space segments of dimension n .⁸ The use of such dual meanings for a single word often mires the description of chemical properties of a given compound into an inappropriate taxonomy class.

It should be noted that using the word ring to be synonymous with face in a planar projection is valid if and only if each of the faces is simply connected.⁹ Multiply connected regions such as shown in Figure 8 (and the corresponding Schlegel diagram, Figure 9) complicate the task of defining ring. The equating of number of faces to number of rings now requires adding the topological concept of genus¹⁰ (+1 in this case) in order to preserve the equation. This is comparable to the problem of rings of rings described for polybenzenes in a two-dimensional space.¹¹

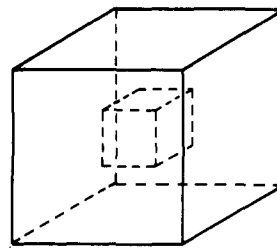


Figure 10.

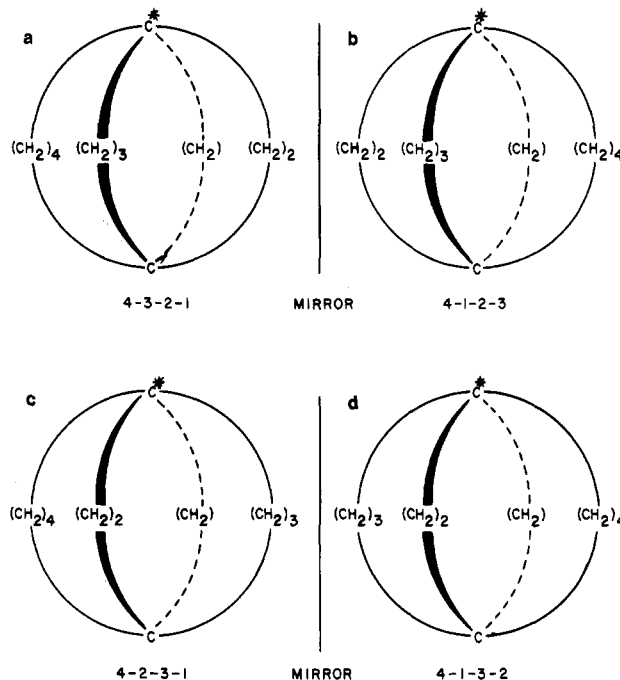


Figure 11.

It is herewith suggested that three-dimensional multiply connected models may be used to describe certain ring compounds. For example, note that in both three-dimensional Figure 8 and its corresponding Schlegel diagram (Figure 9) the set of edges is disjoint. In order for this to correspond to a chemical compound, there would have to be unbonded parts—an idea suggestive of topological isomers.¹²

A different type of multiple connection, corresponding to two-dimensional Betti numbers in topology,¹³ occurs in the case of three-dimensional cages, such as Figure 10. Here the functional relationship between ring and face is even more obscured.

SPANNING SET OF RINGS VS. SCHLEGEL PROJECTION

Because the variety of chemical compounds is rapidly expanding, many of the "ridiculous" mathematical combinations of yesterday are the commonplace of today—such was the fate of the catenanes,¹⁴ dodecahedrane,¹⁵ etc. For this reason, certain mathematically logical extensions of known or suggested compounds will be described in the remaining sections of this paper. For compounds that are intrinsically three dimensional, the indiscriminate use of Schlegel diagrams can lead to major inconsistencies. In fact, the entire concept of projection is, at best, inappropriate for some compounds such as the paddlanes and buttaflanes.¹⁶

Consider (4.3.2.1)-paddlanes. Despite that there exists a unique IUPAC name for such a compound, tricyclo-[4.3.2.1^{1,6}]dodecane, this name does not refer to a unique compound. The presence of two asymmetric carbon atoms has the capability of creating four isomers, Figure 11—two sets of enantiomers, provided the two quaternary atoms are

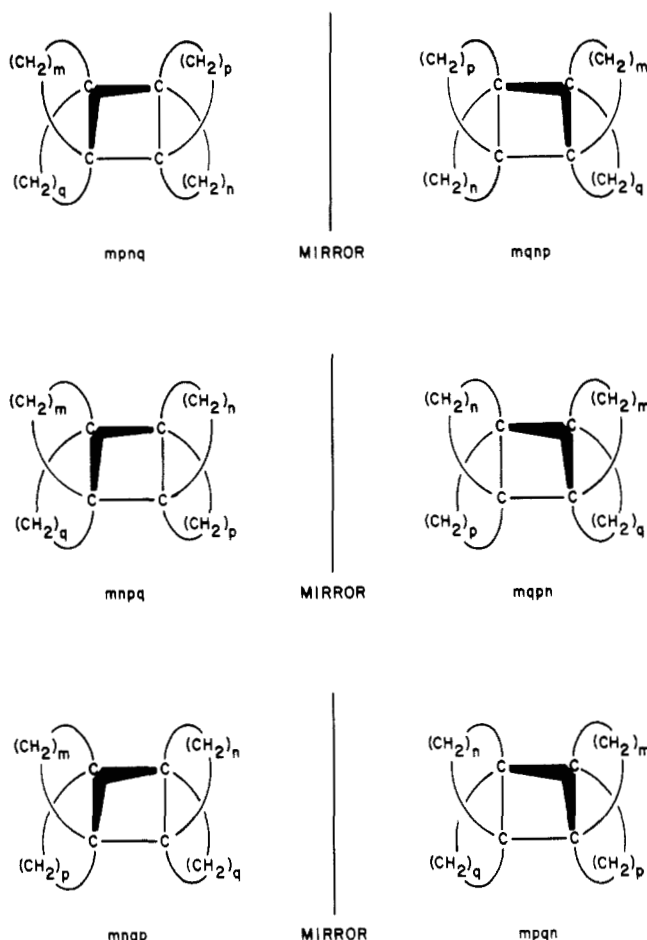


Figure 12.

distinguishable, e.g., one ^{13}C and a normal ^{12}C (or one C and one Si, etc.). For identical carbon atoms, as is the normal situation today, there exists a plane of symmetry and two sets of meso compounds. Despite the limitations of today's isolatable compounds, the perspective of this paper is what is mathematically and chemical possible; therefore, consider the situation in which the quaternary atoms are not identical (i.e., C vs. C*). Now there exists a difference between diastereoisomers. Although this can be easily handled in the paddlane prefix by permuting the second and last digits, this type of option does not carry over to the IUPAC name.¹⁷ IUPAC nomenclature requires that the largest cycle be chosen regardless whether its two-component open paths be adjacent (parts a and b of Figure 11) or opposed (parts c and d of Figure 11) in three-dimensional space.

Despite the geometrical implications that a paddlane is formed by two interdigitating locally planar rings joined at the two quaternary atoms, internal consistency with the techniques used in other bridged compounds has caused the perspective that each bridge must be added one at a time in any synthesis process—such as is used for nomenclature. Thus, either local geometry around the two quaternary atoms shall determine which half-rings comprise the component rings, or else, an arbitrary algorithm must be postulated. Such an algorithm may then have to be corrected and rechecked with each expansion of knowledge.

It should be noted, however, that the use of the local geometry is also not a panacea and that complex questions concerning the applicable topological taxonomy¹ must be answered. Next notice that the different perspectives of the model shown in parts a–d of Figure 11 produce reticularly bridged¹⁸ structures with ring size 9–6–5, 7–6–7, 8–5–6, and 7–5–7 members, respectively. In other words, even as fundamental a property as the number of carbon atoms appearing

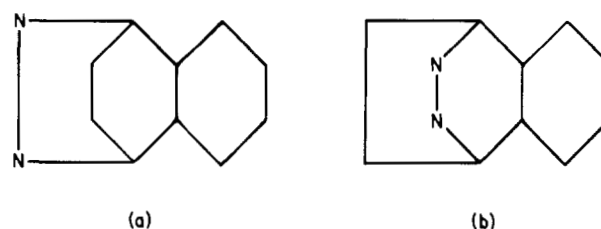


Figure 13.

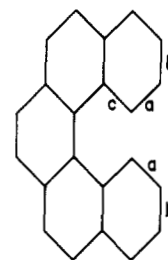


Figure 14.

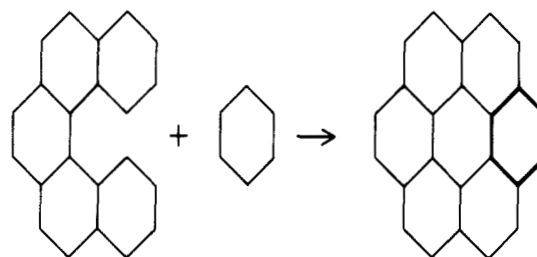


Figure 15.

in the official name is dependent on the projection selected. Such a result is inescapable for three-dimensional models using any Schlegel-based method. This follows directly from not having to name all of the cycles (or even all of the single cycles), inasmuch as the last ring has already been anticipated by the synthesis process. Consequently, any adoption of Eulerian paths,¹⁹ such as the Taylor²⁰–Goodson²¹ nomenclature, will be inadequate for paddlanes.

In a similar manner, if one includes appropriate restrictions on the four quaternary atoms, such as requiring noncoplanarity, (*m,n,p,q*)-buttaflane allows for six different arrangements of the adjoined rings onto the cyclobutane skeleton, Figure 12. Such a structure is of the type postulated for the nonenantiomeric enantiomorphs²² of sulfur.²³ In the event that the cyclobutane skeleton is coplanar, the sets of mirror images coalesce, and only three different isomers must be accounted for in the nomenclature.

The above problem is not restricted to exotic compounds but can arise any time that one or more heteroatoms is contained in a reticularly bridged ring system,⁴ such as shown in Figure 13. For part a of Figure 13, the rings are $\text{C}_4\text{N}_2\text{--C}_6\text{--C}_6$, while in part b there appears to be twice as many nitrogen atoms in this second representation of the same compound. This is because the rings are now designated as $\text{C}_4\text{N}_2\text{--C}_4\text{N}_2\text{--C}_6$. In other words, the simplification created by a decrease in dimension may be an irresolvable source of confusion and ambiguity.

MULTIPLE CONNECTION IN A PLANAR TAXONOMICAL CLASS

Continuing the description of multiply connected figures begun under How Many Faces Does a Figure Have?, there exists a chemical application of this concept that is of more than just theoretical interest. Consider the addition of a benzene ring to the planar five-ring structure shown in Figure 14, with fusion occurring in the plane of the five rings as

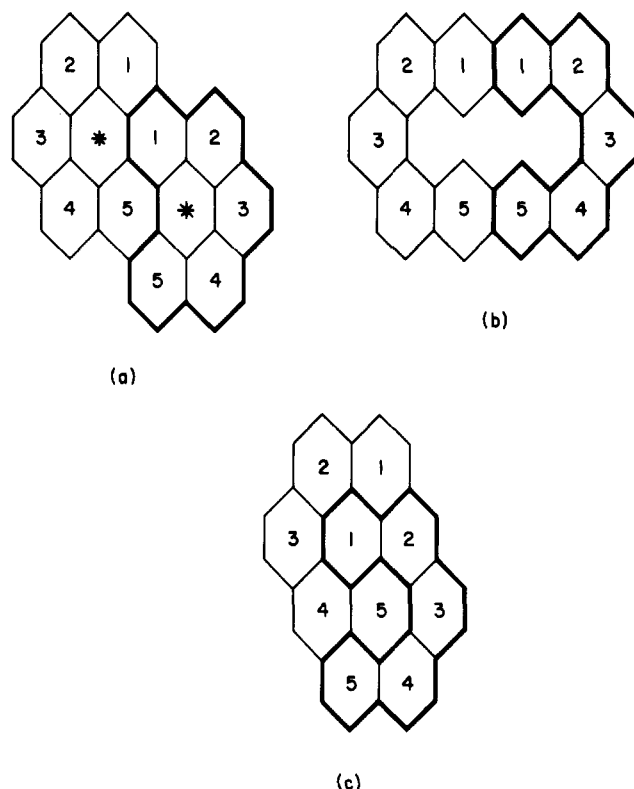


Figure 16.

illustrated by Figure 15, namely, $5 + 1 = 7$. In theory, a six-membered multiply connected ring of rings has been formed; however, there is no difference in the resulting electron path between the six-ring multiply connected system and the corresponding seven-ring simply connected aggregate.²⁴

As a further illustration, consider the fusion of two such five-ring molecules at their end rings. Three of the different coplanar unions that mathematically can be formed are shown in Figure 16. The number of rings in the final configuration depends on whether fusion occurs at edges a, b, or c of Figure 16. These produce ring additions of $5 + 5 = 12$, 11, or 10—due to the formation of 2, 1, or 0 interior rings, respectively. Topologically, these interior rings are equal in number to the genus.

To most chemists, the decision to consider interior rings whether as a part of the figure or as a part of the background is usually made strictly on the basis of whether the interior ring is a benzene ring. In Figure 15 (coronene) and Figure 16a, each such ring is adjudged to be a part of the figure; i.e., there are respectively 7 and 12 rings in the system. In Figure 16b, on the other hand, the 14-membered interior ring is considered to be a part of the background; i.e., this is a 10-ring system.

In a similar manner, none of the circulenes²⁵ (except coronene—which is not classified as a “circulene”) count the interior ring. The reason that coronene is not considered to be a circulene is that the interior ring contributes significantly to the stability of the peripheral aromatic rings. Consequently, from a purely mathematical viewpoint, there is a high degree of subjectivity in merely counting, let alone describing or naming, the rings in this system. Furthermore, the extension of cycloconjugene nomenclature²⁶ to circulenes, although mathematically logical, is chemically counterproductive.

Notice that attention in this section has been limited to the problems associated with counting two-dimensional modules in a two-dimensional embedding space. These problems increase exponentially for three dimensions. Not only does the fusion of adamantane modules have the capability of creating interior (three-dimensional) modules as well as interior

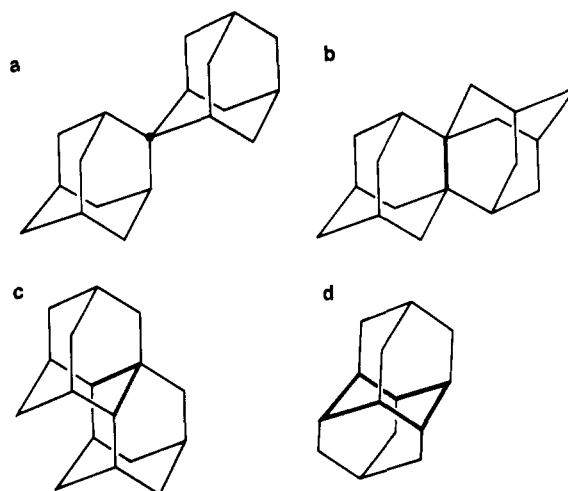


Figure 17.

(two-dimensional) rings, there are four different types of fusion (point, single line, double line—forming an angle, and planar) that can be made between adamantane modules, Figure 17. Combine this with the fact that the number of rings in a single adamantane molecule was a major source of concern and the magnitude of the problem can be seen. Furthermore, in such a study, it would be important to consider problems that arise when counting two-dimensional modules (rings in the *Chemical Abstracts* sense) in a three-dimensional embedding space.

PROBLEMS THAT WOULD ARISE IN A VALENCY EQUAL 4 ENVIRONMENT

The term “valency” in graph theory is used to mean the number of edges emanating from a given node. This differs from the chemical usage in that multigraphs (multiple edges between the same nodes) are not permitted in most graph books. Also, graph theory is normally applied to a chemical skeleton rather than the complete molecule, including the hydrogens. Thus, by use of the term valency in a traditional chemical context and valency with this graph-theoretical connotation, the valency of each carbon in a Kekule form of benzene would be 4, but its valency is 2 (as both the atom of hydrogen and the π -bonds of the multiple bond have been ignored).

In a previous section, the presence of a few atoms in cyclic compounds with a valency = 4 was introduced (paddlanes and buttaflanes). The logical extension mathematically to molecules having quartic graphs has not been produced yet in the laboratory, as the internal strain may be too great for even short-time formulation and isolation of such compounds. The simplest such quartic compound would be octahedrane. This figure has six vertexes—each bonded to four others. If this configuration were to correspond to a chemical compound of carbon and hydrogen, it would have to be an allotropic form of carbon, since there are no additional bonding sites on any of the carbon atoms to accommodate any hydrogen atoms. In addition, such a compound would be highly strained with bond angles of 60° . Consequently, the probability of it being structurally stable is very small. Part of this strain problem, however, might be removed for quartic compound by using a higher coordination number element.

At this point, it is desirable to determine the minimum spanning set of an octahedron. However, it should be noted that the logical extension of the techniques used for a cube produces an inherent ambiguity: Is it desirable to describe the octahedron in terms of its planar faces (as is traditionally done in geometry) or is it better to describe the figure as the union of edges (i.e., an electron pathway)? Note that an octahedron made of planar panels as its means of structural

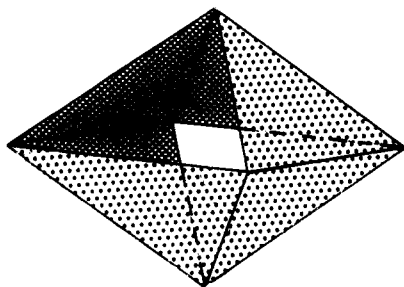


Figure 18.

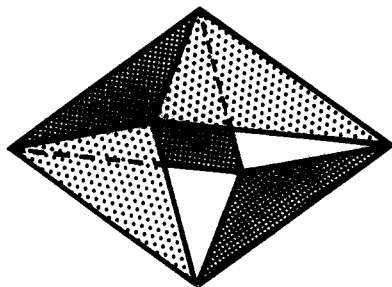


Figure 19.

support (i.e., planar taxonomy) has a minimum spanning set of six such panels, Figure 18. The nomenclature of these six panels would be that of a fused (IUPAC)⁵ or a reticular (Taylor²⁰–Goodson²¹) system. On the other hand, an octahedron formed from “girders” (i.e., linear taxonomy) requires only four planar panels for structural integrity, Figure 19, and uses a nomenclature associated with spiro systems. As far as the relevant physics is concerned, the lack of aromaticity or other planar restraints makes the planar model, Figure 18, of dubious significance. The linear model, on the other hand, may be equally fallacious in the event that there can be formed some type of concatenation of solid octahedral modules, in a manner analogous to the concatenation of modules forming the polymantanes. Nevertheless, since we lack such a solid taxonomy basis, the linear taxonomy nomenclature of Figure 19 with its various spiro connections is the best available choice, at present.

SUMMARY

The purpose of this paper has been to reexamine the mathematical foundations that are supposed to underlie current practices in the taxonomy and nomenclature of chemical compounds. The solution to the ambiguities described herein includes (1) be more precise and consistent in the use of words, but more importantly, (2) know our limitations and do not plow blindly ahead—especially when confronted with an unforeseen extension of a given class or an entirely new class of compounds.

In an attempt to have a single, unified nomenclature, with all the desirable qualities one would like,²⁷ the possibility exists that one will be confronted by an irresolvable source of confusion. Kurt Goedel²⁸ proved that any system of geometry with more than just a few definitions and postulates must be internally contradictory, when the system is carried to its logical conclusion. This same internal contradiction is unavoidable in any logical system, in general, and certainly in one based in geometry. What is important is the recognition of the problem rather than an attempt to “paper over” the inconsistencies. Ad hoc solutions would never have been selected

in the past if a “simple” “obvious” solution existed.

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- The projection in Figure 6 was made from a point above the center of one of the faces onto a parallel planar surface. Because of the projection, the face nearest to the point appears smaller than the congruent farther face.
- In its simplest form for three-dimensional figures, $S_0 = V$ (number of vertices), $S_1 = E$ (number of edges), $S_2 = F$ (number of faces), and $S_3 = 1$. Also, $S_4 = S_5 = \dots = 0$. This thus becomes the usual form of Euler's equation: $V - E + F = 2$. Similarly, for two-dimensional figures, $V = E$.
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