

Graph-Theoretical Algorithm To Canonically Name the Isomers of the Regular Polyhedranes

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The relationship that exists between a central atom with n ligands and a set of molecular cages containing n atoms is recognized as being combinatorially equivalent. This equivalence is then exploited as the framework for establishing the graph-theoretical basis that underlies research we had done earlier concerning the 30 different constitutional isomers possible for hexavalent coordination, as well as its expansion to higher coordination. Based on this, an algorithm that canonically names the different "isomer pairs" formed for each of the five Platonic solids is formulated. The *raison d'être* for such a study at this time is to be able to canonically name the various constitutionally-isomeric substituted cubanes and dodecahedranes that may soon be available. Additionally, the application of this algorithm to other important structures, such as the Archimedean solids, and to nonorientable surfaces is discussed.

INTRODUCTION

In 1968, we described the mathematical possibility of forming 30 different hexasubstituted compounds by having six different ligands on a single central atom (such as sulfur).¹ Also we noted that such a compound would give rise to a "different" type of optical isomerism. The utility of that idea is only now coming to fruition—BUT for a different class of compounds than originally envisioned; namely, for the class of Platonic solids.² We shall see below that these two classes of compounds may, in a very specific way, be viewed as being "mathematically equivalent".

At the time that we suggested the mathematical viability of 30 different isomers for each hexasubstituted sulfur atom in a compound, it was not deemed worthwhile to extend this study to higher coordination than six or to matters of nomenclature inasmuch as no compounds with such high coordination were taken seriously by the chemistry community—let alone actually formed. This was long before the creation of molecules whose *raison d'être* was primarily that of mathematical curiosity, rather than considerations of anticipated chemical importance. Some now familiar examples of such molecules are a "cage"³ of carbon atoms in the shape of a cube,⁴ and in the shape of a regular dodecahedron,⁵ as well as a crown ether in the shape of a Möbius strip,⁶ etc. In fact, not only have such "esoteric" molecules come into the mainstream of chemistry research, also the "tools" of graph theory have become much more familiar to the practicing, as well as the mathematical, chemist. Consequently, a nomenclature for the compounds that we described earlier is now proposed, along with the corresponding names of octasubstituted, dodecasubstituted, and icosasubstituted compounds.

Before progressing further, an important observation that should be noted is that the combinatorics of a single atom having n ligands is identical to that of a molecule possessing the skeleton of a regular n -vertex polyhedron with each vertex having a single additional ligand. In other words, the idea missing in our 1960s study was the viability of the molecular cage. The fallout from this combinatorial equivalence is that the number of possible isomers for a central atom with four different ligands is equal to that of a tetrahedrane containing a different ligand at each carbon of the tetrahedral "cage"; similarly for a central atom with six different ligands and a substituted octahedrane; for a central atom with eight different ligands and a substituted cubane; for a central atom with 12 different ligands and a substituted icosahedrane; and for a central atom with 20 different ligands and a substituted dodecahedrane. This is equivalent to saying that the polyhedral cage may be viewed as a single module—both from an or-

ganizational perspective⁷ and from a basis for nomenclature.⁸

From a chemistry perspective, this is of importance inasmuch as for four-coordination, the central atom with four ligands is ubiquitous in nature while the substituted tetrahedrane is certainly impractical, due to the angle strain required to form the tetrahedrane skeleton. This is not withstanding the fact that substituents on such a cage, such as four *tert*-butyl groups, may stabilize the structure.⁹ In most instances, one or more of the bonds of the tetrahedrane cage would become too labile to remain in this form, and some rearrangement will occur "spontaneously". Also, at the other end of this organizational spectrum, a single atom with 20 ligands is beyond our expectations, but dodecahedrane is known and we expect substituted dodecahedranes to become the subject of intense study.

In order to analyze the relevant molecules, we shall "conveniently label" the graphs produced by a Schlegel projection¹⁰ of each of the five regular polyhedra. (Figure 1 is a representative Schlegel projection; viz., of an icosahedron. Note that one of the 20 triangular face, DJK, has been stretched to form the outer perimeter.) The vertex labeling scheme forms the basis for an algorithm that assigns a canonical name to either each of the permutation of locants on a central atom or to the ligands at the vertices of a polyhedral cage. Additionally this labeling scheme produces a graph-theoretical method for counting the number of possible isomers—without needing to consider symmetry classes. The fruits of the graph-theoretical part of the study is a tabulation, NOT of the desired set, but of half the desired set, with the other half being the mirror image of the tabulated set. In fact, it was exactly this half-set that earlier researchers such as Essen et al.¹² had described for hexacoordination.

At this point it should be observed that had our objective been solely to determine the total number of isomers, we could have noted, using elementary group theory, that the number of isomer pairs is n factorial divided by the number of members of the symmetry group.¹³ Instead, our objective is to obtain a delineation of the different elements so that a canonical ordering of the different combinations is achieved.

TETRACOORDINATION: THE (REGULAR)
TETRAHEDRON

First of all it should be noted that the method being developed for substituted cubanes and dodecahedranes is equally applicable to tetrahedral orientation—with the production of exactly one entity plus its mirror image. This is seen using a Schlegel projection of the tetrahedron onto a plane and the labeling of the "different" vertices according to graph-theo-

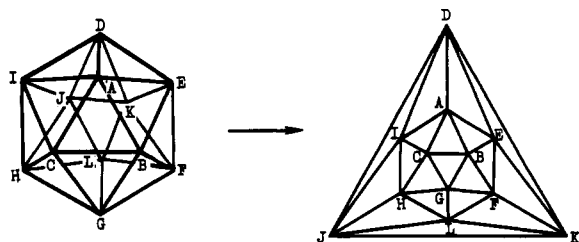


Figure 1.

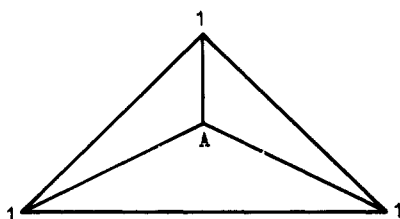


Figure 2.

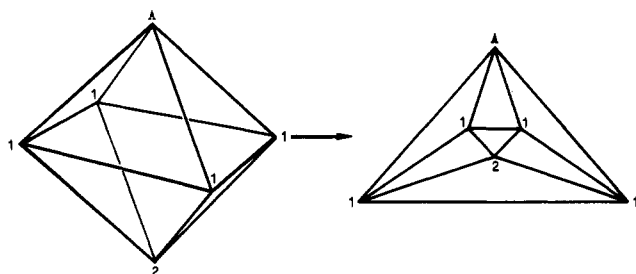


Figure 3.

retical distance (GTD) from an arbitrary vertex, designated as the "root". By such a representation (Figure 2), all three of the remaining vertices are equivalent. Consequently, there is exactly one unique labeling of the vertices and one pair of mirror image isomers—which is the frequently encountered optical isomerism of the tetrasubstituted atom, with four different substituents.

An observation of importance, at this point, is that the tetrahedral cage is intact and that the atoms being replaced are ligands to the cage, rather than members forming the cage, as in the "replacement"-type molecules described by Alkorta et al. in their study of aza analogues of tetrahedrane.¹⁴

HEXACOORDINATION: THE (REGULAR) OCTAHEDRON

Upon examining octahedral vertex orientation (alternately, body-faced cubic orientation), note that, as with all regular polyhedra, each of the graph-theoretical nodes of the system is equivalent; consequently, we may designate any one node as the root "A". In the case of this six-node system, such a procedure produces two distinguishable sets of nodes (with GTD = 1 and 2 from the root) (Figure 3). Since either of these sets of nodes may be designated as "B", we shall analyze both cases.

Standardization is achieved by using a coplanar picture and examining, in increasing sequence, the different possible labelings: namely, first consider as vertex "B" that node which has GTD = 1 from A to B, then GTD = 2. In a similar manner, consider as vertex "C" those nodes having different GTDs from A then from B, etc. Such a procedure conveniently creates a basis for labeling all of the remaining nodes (using GTDs).

The ordinal numbers that first B assumes, then that C assumes, etc. form the foundation for part of the proposed nomenclature algorithm. Before formally describing this algorithm (which, in the Epilogue section, will be shown to

be applicable to a much larger class of figures than just the Platonic solids), note that as well as the first node being arbitrarily chosen and thus not needing to be specified, the last vertex, F, is uniquely determined and similarly needs no sequence number. Consequently, for the six-vertex system, only a four-digit sequence of numbers needs to be specified. Furthermore, because in the case of the octahedron the numbers in the sequence may be only 1, 2, or 3, the "name" may be simplified by the use of ternary numbers. Finally, subtracting one from each number of the sequence produces the more traditional base 3 number. We can use either this ternary number or, more conveniently, the conversion of this number to base 10 as the numerical part of the canonical name. This is supplemented by a *R* vs *S* to designate which one of the enantiomer pair has been specified (in a manner akin to the Cahn-Ingold-Prelog sequencing rules¹⁵). The mechanics of generating the 15 isomer pairs that exist with octahedral orientation is illustrated in Table I.

Remembering that the C-I-P rules for assigning *R* vs *S* are "local" at each stereocenter BUT that we desire to make an assignment on a "global" scale, we may differentiate between the two enantiomers of each pair as follows: Consider the highest priority atom as the "root" of a graph and examine the set of atoms with GTD = 1. (Note that for the regular octahedron, the geometry of the four atoms with GTD = 1 is, in actuality, coplanar; however, even if it were not, we would consider their planar projection for purposes of assigning *R* vs *S*.) Now, we must assign an ordering to these "coplanar" atoms so that if any one of these atoms were absent, the other three would still have the same sequence of atoms according to priority; i.e., the three (or four) atoms would have the sequence of priorities either decreasing clockwise and assigned *S* or decreasing counterclockwise and assigned *R*. This may be accomplished by determining the number of adjacent atom interchanges of the coplanar atoms in order to have the four-atom priority sequence monotonic. If this number of interchanges is even, the configuration is retained; i.e., designated as though there were only three atoms in the circle; however, if the number of interchanges is odd, then the *R* vs *S* is reversed. Note that such an assignment of *R* vs *S* was made so as to reduce to that used for nomenclating tetrahedrally oriented atoms.

A few observations that should be noted are

(1) Each enantiomeric pair is represented by one of 15 numbers between 0 and 30. Because 30 is a relatively small number, we have included a tabulation of all of the numbers from 0 to 30 in Table II—a luxury that shall not be practical for higher coordinations.

(2) In the formulation of Table II those numbers that were not used do not correspond to a viable combination of minimum GTDs.

(3) In the case of the octahedron, there was never a need for more than three cases (see Table I); consequently, we were able to use a base 3 number. In the event that we have four or more different values being assigned to GTD at any step of the synthesis, we shall need to use a base 4 (or higher) numbering in forming the canonical name. This will be the case for the larger polyhedra (see below).

(4) The group theoretical formula of n factorial divided by the size of the symmetry group ($6!/48 = 15$) corroborates the total number of isomer pairs that we found using the procedure chosen.

A theoretical representative example of a hexasubstituted osmium compound is shown in Figure 4. We can determine its proposed name by the following procedure:

(1) Assign letters A through F by decreasing atomic number: iodine = "A", bromine = "B", chlorine = "C",

Table I

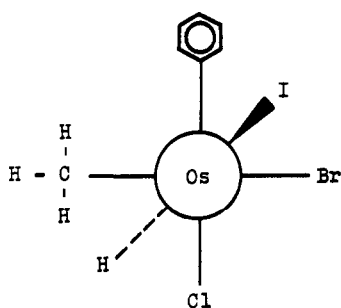
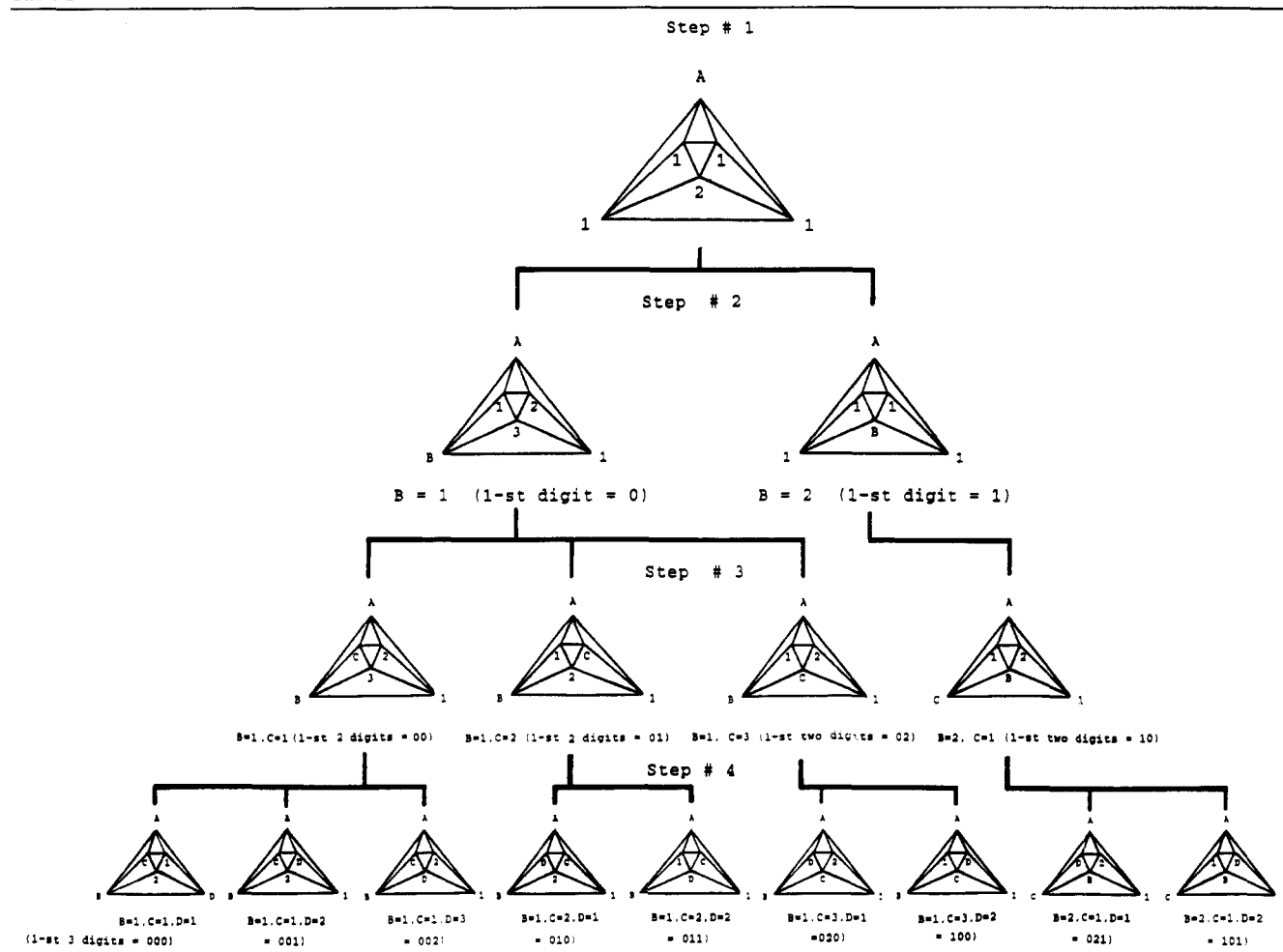


Figure 4.

phenyl = "D", methyl = "E", and hydrogen = "F".

(2) Because the iodine and hydrogen atoms (A and F respectively) are on opposite sides of the osmium atom, using Table I, we note that the only possible names are 0, 3, and 9. Similarly, because the bromine atom and the methyl group are diametrically opposite, B must be opposite E. The possible names for this arrangement are 0, 7, and 19. [Note that the third set of opposing vertices, chlorine atom and phenyl group (C and D), does not give any additional information. The names compatible with C and D being on opposite sides of the central atom are 0, 1, and 30.] In other words, the intersection set of any two of these pairs, as well as of all three of them, is the single name 0. This is equivalent to saying that the locant number part of the desired name is 0.

(3) Working in the reverse direction and putting the first two pieces of the information from the above step onto a graph produces Figure 5. HOWEVER, the two

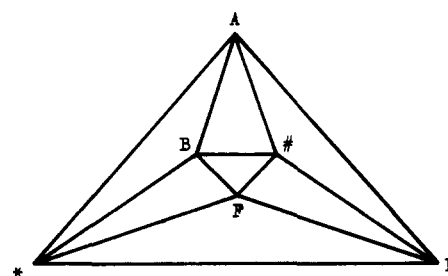


Figure 5.

remaining positions (designated by # and *) are constitutionally equivalent. Consequently, without postulating a priority rule, we cannot use graph theory alone to determine which of these "equivalent" positions should be Cl vs Ph. (A similar result would be produced using any two sets of opposite nodes.)

(4) Using the three-dimensional model (Figure 4), we now examine the set of ligands lying in the plane formed by those atoms which have graph-theoretical distance of one from the highest priority atom, namely iodine. This plane contains the atoms bromine and chlorine and the carbon atoms in the phenyl and methyl groups in the counterclockwise order Br-Ph-Me-Cl (B-D-E-C). In order to place these four letters in a cyclic order, we must make exactly one interchange (D and E). This odd number (one) of interchanges forms a cyclic ordering of the ligands in a monotonically decreasing sequence. Now, since a monotonically decreasing sequence would be designated as *R* and the example sequence underwent an odd number of interchanges, the proposed name is

Table II

	Unreduced #	Reduced #
0	1111	0000
1	1112	0001
2	There are never more than 2 unused vertices from D; thus any number having a 3 in the unreduced units position is meaningless; i.e., in reduced form: 2 (mod 3) is impossible.	
3	1121	0010
4	1122	0011
5	Same reason for non-existence as 2.	
6	1131	0020
7	1132	0021
8	Same reason for non-existence as 2.	
9	1211	0100
10	1212	0101
11	Same reason for non-existence as 2.	
12	1221	0110
13	In this sequence the 2 unused vertices from D are constitutionally equivalent; thus there can not be a 2 or 3 in the unreduced units position.	
14	Same reason for non-existence as 2.	
15	In this sequence there are only 2 constitutionally different nodes from C; thus a 3 in the unreduced "tens" position is impossible.	
16	Same reason for non-existence as 15.	
17	Same reason for non-existence as 2 (or 15).	
18	1311	0200
19	1312	0201
20	Same reason for non-existence as 2.	
21	1321	0210
22	Same reason for non-existence as 13.	
23	Same reason for non-existence as 2.	
24	Same reason for non-existence as 15.	
25	Same reason for non-existence as 15.	
26	Same reason for non-existence as 2.	
27	2111	1000
28	2112	1001
29	Same reason for non-existence as 2.	
30	2121	1010

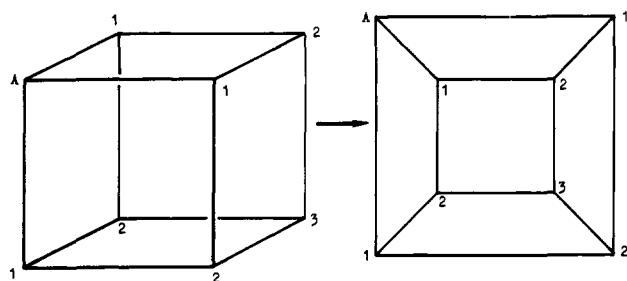


Figure 6.

osmium-0-S-iodide, bromide, chloride, phenyl, methyl, hydride.

OCTACOORDINATION: THE (REGULAR) HEXAHEDRON (CUBE)

The standardized picture for octahedral coordination is seen by considering an atom in the center of a cube and ligands at each of the eight vertices (or alternately in the center of a regular octahedron and ligands in the center of each of the eight faces). As in the previous section, this may be represented by using a Schlegel projection (Figure 6) with any of the equivalent vertices labeled as "A". There are, for this figure, three distinct vertices with GTD from A being 1, 2, and 3, respectively. Similarly, since there are eight vertices, we shall require a sequence of six numbers to name all configuration. Also, since 5 is the maximum number of different locations in any counting sequence, our final name shall be in terms of base 5 numbers. The application of the algorithm produces Tables III-V.

Three observations of importance at this time are

(1) Although it is mathematically possible for a single atom to have eight ligands, the crowding required makes such a configuration very unlikely, instead the substituted cubane is a far more likely prospect.

Table III. Generation of Enantiomer Pairs for the Cubanes: Part 1

	(00)	1 (A=1, B=2, C=2) 2 (A=2, B=1, C=1) 3 (A=2, B=1, C=3) 4 (A=2, B=3, C=1) 5 (A=3, B=2, C=2)
	(01)	1 (A=1, B=2, C=1) 2 (A=1, B=2, C=3) 3 (A=2, B=1, C=2) 4 (A=2, B=3, C=1) 5 (A=3, B=2, C=1)
	(02)	1 (A=1, B=2, C=1) 2 (A=2, B=1, C=2) 3 (A=3, B=2, C=1)
	(03)	1 (A=1, B=2, C=2) 2 (A=2, B=1, C=1) 3 (A=2, B=3, C=1)
	(10)	1 (A=1, B=1, C=2) 2 (A=1, B=3, C=2) 3 (A=2, B=2, C=1) 4 (A=2, B=2, C=3) 5 (A=3, B=1, C=2)
	(11)	1 (A=1, B=1, C=2) 2 (A=2, B=2, C=1) 3 (A=3, B=1, C=2)
	(12)	1 (A=1, B=1, C=1) 2 (A=1, B=1, C=3) 3 (A=1, B=3, C=1) 4 (A=2, B=2, C=2) 5 (A=3, B=1, C=1)
	(13)	1 (A=1, B=1, C=2) 2 (A=1, B=3, C=2) 3 (A=2, B=2, C=1)
	(20)	1 (A=1, B=2, C=2) 2 (A=2, B=1, C=1) 3 (A=2, B=1, C=3)
	(21)	1 (A=1, B=2, C=1) 2 (A=1, B=2, C=3) 3 (A=2, B=1, C=2)

(2) As well as the brute force method of listing all possible combinations of locants and the group theory method of noting symmetry classes, there is also a strictly graph-theory method for determining that the total number of enantiomer pairs is $8!/48 = 840$. This is accomplished by keeping track of when no equivalent vertices exist in a given step. The first occurrence of this is in Table III when the first two digits of the name are 00. Since none of the five remaining vertices are constitutionally equivalent, there will be $5! = 120$ en-

Table IV. Generation of Enantiomer Pairs for the Cubanes: Part 2

000	$\begin{array}{c} A-C \\ B1 \\ 24 \\ D-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-C \\ BE \\ 13 \\ D-2 \\ 0000 \end{array}$	$\begin{array}{c} A-C \\ B1 \\ E3 \\ D-2 \\ 0001 \end{array}$	$\begin{array}{c} A-C \\ B1 \\ 23 \\ D-2 \\ 0002 \end{array}$	$\begin{array}{c} A-C \\ B1 \\ 2E \\ D-3 \\ 0003 \end{array}$	100	$\begin{array}{c} A-D \\ CB \\ 24 \\ 1-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-D \\ CB \\ 13 \\ E-2 \\ 1000 \end{array}$	$\begin{array}{c} A-D \\ CB \\ E3 \\ 1-2 \\ 1001 \end{array}$	$\begin{array}{c} A-D \\ CB \\ 23 \\ 1-E \\ 1002 \end{array}$	$\begin{array}{c} A-D \\ CB \\ 2E \\ 1-3 \\ 1003 \end{array}$
001	$\begin{array}{c} A-C \\ BD \\ 24 \\ 1-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-C \\ BD \\ 13 \\ E-2 \\ 0010 \end{array}$	$\begin{array}{c} A-C \\ BE \\ E3 \\ 1-2 \\ 0011 \end{array}$	$\begin{array}{c} A-C \\ BD \\ 23 \\ 1-E \\ 0012 \end{array}$	$\begin{array}{c} A-C \\ BD \\ 2E \\ 1-3 \\ 0013 \end{array}$	101	$\begin{array}{c} A-1 \\ CB \\ 24 \\ D-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ CB \\ 13 \\ D-2 \\ 1010 \end{array}$	$\begin{array}{c} A-1 \\ CB \\ E3 \\ D-2 \\ 1011 \end{array}$	$\begin{array}{c} A-1 \\ CB \\ 23 \\ D-E \\ 1012 \end{array}$	$\begin{array}{c} A-1 \\ CB \\ 2E \\ D-3 \\ 1013 \end{array}$
002	$\begin{array}{c} A-C \\ B2 \\ D4 \\ 1-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-C \\ B1 \\ D3 \\ E-2 \\ 0020 \end{array}$	$\begin{array}{c} A-C \\ BE \\ D3 \\ 1-2 \\ 0021 \end{array}$	$\begin{array}{c} A-C \\ B2 \\ D3 \\ 1-E \\ 0022 \end{array}$	$\begin{array}{c} A-C \\ B2 \\ DE \\ 1-3 \\ 0023 \end{array}$	102	$\begin{array}{c} A-1 \\ CB \\ D4 \\ 2-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ CB \\ D3 \\ 1-2 \\ 1020 \end{array}$	$\begin{array}{c} A-1 \\ CB \\ D3 \\ E-2 \\ 1021 \end{array}$	$\begin{array}{c} A-1 \\ CB \\ D3 \\ 2-E \\ 1022 \end{array}$	$\begin{array}{c} A-1 \\ CB \\ DE \\ 2-3 \\ 1023 \end{array}$
003	$\begin{array}{c} A-C \\ B2 \\ 34 \\ 1-D \end{array}$	\Rightarrow	$\begin{array}{c} A-C \\ B1 \\ 23 \\ E-D \\ 0030 \end{array}$	$\begin{array}{c} A-C \\ BE \\ 23 \\ 1-D \\ 0031 \end{array}$	$\begin{array}{c} A-C \\ B2 \\ E3 \\ 1-D \\ 0032 \end{array}$	$\begin{array}{c} A-C \\ B2 \\ 3E \\ 1-D \\ 0033 \end{array}$	103	$\begin{array}{c} A-1 \\ CB \\ 34 \\ 2-D \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ CB \\ 23 \\ 1-D \\ 1030 \end{array}$	$\begin{array}{c} A-1 \\ CB \\ 23 \\ E-D \\ 1031 \end{array}$	$\begin{array}{c} A-1 \\ CB \\ E3 \\ 2-D \\ 1032 \end{array}$	$\begin{array}{c} A-1 \\ CB \\ 3E \\ 2-D \\ 1033 \end{array}$
004	$\begin{array}{c} A-C \\ B2 \\ 3D \\ 1-4 \end{array}$	\Rightarrow	$\begin{array}{c} A-C \\ B1 \\ 2D \\ E-3 \\ 0040 \end{array}$	$\begin{array}{c} A-C \\ BE \\ 2D \\ 1-3 \\ 0041 \end{array}$	$\begin{array}{c} A-C \\ B2 \\ ED \\ 1-3 \\ 0042 \end{array}$	$\begin{array}{c} A-C \\ B2 \\ 3D \\ 1-E \\ 0043 \end{array}$	104	$\begin{array}{c} A-1 \\ CB \\ 3D \\ 2-4 \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ CB \\ 2D \\ 1-3 \\ 1040 \end{array}$	$\begin{array}{c} A-1 \\ CB \\ 2D \\ E-3 \\ 1041 \end{array}$	$\begin{array}{c} A-1 \\ CB \\ ED \\ 2-3 \\ 1042 \end{array}$	$\begin{array}{c} A-1 \\ CB \\ 3D \\ 2-E \\ 1043 \end{array}$
010	$\begin{array}{c} A-D \\ BC \\ 24 \\ 1-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-D \\ BC \\ 13 \\ E-2 \\ 0100 \end{array}$	$\begin{array}{c} A-D \\ BC \\ E3 \\ 1-2 \\ 0101 \end{array}$	$\begin{array}{c} A-D \\ BC \\ 23 \\ 1-E \\ 0102 \end{array}$	$\begin{array}{c} A-D \\ BC \\ 2E \\ 1-3 \\ 0103 \end{array}$	110	$\begin{array}{c} A-D \\ 1B \\ 34 \\ C-2 \end{array}$	\Rightarrow	$\begin{array}{c} A-D \\ EB \\ 23 \\ C-1 \\ 1100 \end{array}$	$\begin{array}{c} A-D \\ 1B \\ 23 \\ C-E \\ 1101 \end{array}$	$\begin{array}{c} A-D \\ 1B \\ E3 \\ C-2 \\ 1102 \end{array}$	$\begin{array}{c} A-D \\ 1B \\ 3E \\ C-2 \\ 1103 \end{array}$
011	$\begin{array}{c} A-1 \\ BC \\ 24 \\ D-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ BC \\ 13 \\ D-2 \\ 0110 \end{array}$	$\begin{array}{c} A-1 \\ BC \\ E3 \\ D-2 \\ 0111 \end{array}$	$\begin{array}{c} A-1 \\ BC \\ 23 \\ D-E \\ 0112 \end{array}$	$\begin{array}{c} A-1 \\ BC \\ 2E \\ D-3 \\ 0113 \end{array}$	111	$\begin{array}{c} A-1 \\ 2B \\ 34 \\ C-D \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ 1B \\ 23 \\ C-D \\ 1110 \end{array}$	$\begin{array}{c} A-1 \\ EB \\ 23 \\ C-D \\ 1111 \end{array}$	$\begin{array}{c} A-1 \\ 2B \\ E3 \\ C-D \\ 1112 \end{array}$	$\begin{array}{c} A-1 \\ 2B \\ 3E \\ C-D \\ 1113 \end{array}$
012	$\begin{array}{c} A-1 \\ BC \\ D4 \\ 2-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ BC \\ D3 \\ 1-2 \\ 0120 \end{array}$	$\begin{array}{c} A-1 \\ BC \\ D3 \\ E-2 \\ 0121 \end{array}$	$\begin{array}{c} A-1 \\ BC \\ D3 \\ 2-E \\ 0122 \end{array}$	$\begin{array}{c} A-1 \\ BC \\ DE \\ 2-3 \\ 0123 \end{array}$	112	$\begin{array}{c} A-1 \\ 1B \\ 2D \\ C-2 \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ 1B \\ 3D \\ C-2 \\ 1120 \end{array}$	$\begin{array}{c} A-1 \\ 2B \\ 3D \\ C-E \\ 1121 \end{array}$		
013	$\begin{array}{c} A-1 \\ BC \\ 34 \\ 2-D \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ BC \\ 23 \\ 1-D \\ 0130 \end{array}$	$\begin{array}{c} A-1 \\ BC \\ E3 \\ E-D \\ 0131 \end{array}$	$\begin{array}{c} A-1 \\ BC \\ 23 \\ 2-D \\ 0132 \end{array}$	$\begin{array}{c} A-1 \\ BC \\ 3E \\ 2-D \\ 0133 \end{array}$	120	$\begin{array}{c} A-1 \\ DB \\ 34 \\ 2-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ DB \\ C3 \\ 1-2 \\ 1200 \end{array}$	$\begin{array}{c} A-1 \\ DB \\ C3 \\ E-2 \\ 1201 \end{array}$	$\begin{array}{c} A-1 \\ DB \\ 2E \\ 2-E \\ 1202 \end{array}$	$\begin{array}{c} A-1 \\ DB \\ CE \\ 2-3 \\ 1203 \end{array}$
014	$\begin{array}{c} A-1 \\ BC \\ 3D \\ 2-4 \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ BC \\ 2D \\ 1-3 \\ 0140 \end{array}$	$\begin{array}{c} A-1 \\ BC \\ ED \\ E-3 \\ 0141 \end{array}$	$\begin{array}{c} A-1 \\ BC \\ 3D \\ 2-3 \\ 0142 \end{array}$	$\begin{array}{c} A-1 \\ BC \\ 3D \\ 2-E \\ 0143 \end{array}$	121	$\begin{array}{c} A-D \\ 1B \\ C4 \\ 2-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-D \\ EB \\ C3 \\ 1-2 \\ 1210 \end{array}$	$\begin{array}{c} A-D \\ 1B \\ C3 \\ E-2 \\ 1211 \end{array}$	$\begin{array}{c} A-D \\ 1B \\ 2E \\ 2-E \\ 1212 \end{array}$	$\begin{array}{c} A-D \\ 1B \\ CE \\ 2-3 \\ 1213 \end{array}$
020	$\begin{array}{c} A-D \\ B2 \\ 34 \\ 1-C \end{array}$	\Rightarrow	$\begin{array}{c} A-D \\ B1 \\ 23 \\ E-C \\ 0200 \end{array}$	$\begin{array}{c} A-D \\ BE \\ 23 \\ 1-C \\ 0201 \end{array}$	$\begin{array}{c} A-D \\ B2 \\ E3 \\ 1-C \\ 0202 \end{array}$	$\begin{array}{c} A-D \\ B2 \\ 3E \\ 1-C \\ 0203 \end{array}$	122	$\begin{array}{c} A-2 \\ 1B \\ C4 \\ D-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-1 \\ EB \\ C3 \\ D-2 \\ 1220 \end{array}$	$\begin{array}{c} A-E \\ 1B \\ C3 \\ D-2 \\ 1221 \end{array}$	$\begin{array}{c} A-2 \\ 1B \\ 2E \\ D-E \\ 1222 \end{array}$	$\begin{array}{c} A-2 \\ 1B \\ CE \\ D-3 \\ 1223 \end{array}$
021	$\begin{array}{c} A-1 \\ BD \\ 34 \\ 2-C \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ BD \\ 23 \\ 1-C \\ 0210 \end{array}$	$\begin{array}{c} A-1 \\ BD \\ 23 \\ E-C \\ 0211 \end{array}$	$\begin{array}{c} A-1 \\ BD \\ E3 \\ 2-C \\ 0212 \end{array}$	$\begin{array}{c} A-1 \\ BD \\ 3E \\ 2-C \\ 0213 \end{array}$	123	$\begin{array}{c} A-2 \\ 1B \\ C4 \\ 3-D \end{array}$	\Rightarrow	$\begin{array}{c} A-1 \\ EB \\ C3 \\ 2-D \\ 1230 \end{array}$	$\begin{array}{c} A-E \\ 1B \\ C3 \\ 2-D \\ 1231 \end{array}$	$\begin{array}{c} A-2 \\ 1B \\ 3E \\ E-D \\ 1232 \end{array}$	$\begin{array}{c} A-2 \\ 1B \\ CE \\ 3-D \\ 1233 \end{array}$
022	$\begin{array}{c} A-1 \\ B2 \\ 2D \\ 1-C \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ B2 \\ 3D \\ 1-C \\ 0220 \end{array}$	$\begin{array}{c} A-1 \\ BE \\ 3D \\ 2-C \\ 0221 \end{array}$			124	$\begin{array}{c} A-2 \\ 1B \\ CD \\ 3-4 \end{array}$	\Rightarrow	$\begin{array}{c} A-1 \\ EB \\ CD \\ 2-3 \\ 1240 \end{array}$	$\begin{array}{c} A-E \\ 1B \\ CD \\ 2-3 \\ 1241 \end{array}$	$\begin{array}{c} A-2 \\ 1B \\ 3E \\ E-3 \\ 1242 \end{array}$	$\begin{array}{c} A-2 \\ 1B \\ CD \\ 3-E \\ 1243 \end{array}$
030	$\begin{array}{c} A-D \\ B2 \\ 3C \\ 1-4 \end{array}$	\Rightarrow	$\begin{array}{c} A-D \\ B1 \\ 2C \\ E-3 \\ 0300 \end{array}$	$\begin{array}{c} A-D \\ BE \\ 2C \\ 1-3 \\ 0301 \end{array}$	$\begin{array}{c} A-D \\ B2 \\ EC \\ 1-3 \\ 0302 \end{array}$	$\begin{array}{c} A-D \\ B2 \\ 3C \\ 1-E \\ 0303 \end{array}$	130	$\begin{array}{c} A-D \\ 1B \\ 4C \\ 2-3 \end{array}$	\Rightarrow	$\begin{array}{c} A-D \\ EB \\ 3C \\ 1-2 \\ 1300 \end{array}$	$\begin{array}{c} A-D \\ 1B \\ 3C \\ E-2 \\ 1301 \end{array}$	$\begin{array}{c} A-D \\ 1B \\ 2E \\ 2-E \\ 1302 \end{array}$	$\begin{array}{c} A-D \\ 1B \\ EC \\ 2-3 \\ 1303 \end{array}$
031	$\begin{array}{c} A-1 \\ BD \\ 3C \\ 2-4 \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ BD \\ 2C \\ 1-3 \\ 0310 \end{array}$	$\begin{array}{c} A-1 \\ BD \\ 2C \\ E-3 \\ 0311 \end{array}$	$\begin{array}{c} A-1 \\ BD \\ EC \\ 2-3 \\ 0312 \end{array}$	$\begin{array}{c} A-1 \\ BD \\ 3C \\ 2-E \\ 0313 \end{array}$	131	$\begin{array}{c} A-1 \\ 1B \\ 2C \\ D-2 \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ 1B \\ 3C \\ D-2 \\ 1310 \end{array}$	$\begin{array}{c} A-1 \\ 2B \\ 3C \\ D-E \\ 1311 \end{array}$		
032	$\begin{array}{c} A-1 \\ B2 \\ 2C \\ 1-D \end{array}$	\Rightarrow	$\begin{array}{c} A-E \\ B2 \\ 3C \\ 1-D \\ 0320 \end{array}$	$\begin{array}{c} A-1 \\ BE \\ 3C \\ 2-D \\ 0321 \end{array}$			132	$\begin{array}{c} A-2 \\ 1B \\ DC \\ 3-4 \end{array}$	\Rightarrow	$\begin{array}{c} A-1 \\ EB \\ DC \\ 2-3 \\ 1320 \end{array}$	$\begin{array}{c} A-E \\ 1B \\ DC \\ 2-3 \\ 1321 \end{array}$	$\begin{array}{c} A-2 \\ 1B \\ 3E \\ E-3 \\ 1322 \end{array}$	$\begin{array}{c} A-2 \\ 1B \\ DC \\ 3-E \\ 1323 \end{array}$

antiomer pairs whose name starts with 00. The same will be true for the number of enantiomer pairs whose name starts with 01; however, because of repetition in 02 and 03, there will exist substantially fewer enantiomer pairs whose name begins with these digits. A similar result occurs for all the other possible cubanes whose names begin with a higher first digit (1 or 2).

(3) The hexahedral cage in the envisioned substituted cubane is intact, and the atoms being replaced are ligands to the cage, rather than members forming the cage. Thus it will be seen that the number of isomers achieved for this configuration is much greater than the "replacement"-type molecules described by Alkorta et al. in their study of aza analogues of cubane.¹⁶

Table V. Generation of Enantiomer Pairs for the Cubanes: Part 3^a

200	$\begin{array}{c} A-D \\ \hline \begin{array}{ c } \hline C2 \\ \hline 3B \\ \hline 1-4 \end{array} \end{array} \Rightarrow$	$\begin{array}{c} A-D \\ \hline \begin{array}{ c } \hline C1 \\ \hline 2B \\ \hline E-3 \\ \hline 2000 \end{array} \end{array}$	$\begin{array}{c} A-D \\ \hline \begin{array}{ c } \hline CE \\ \hline 2B \\ \hline 1-3 \\ \hline 2001 \end{array} \end{array}$	$\begin{array}{c} A-D \\ \hline \begin{array}{ c } \hline C2 \\ \hline EB \\ \hline 1-3 \\ \hline 2002 \end{array} \end{array}$	$\begin{array}{c} A-D \\ \hline \begin{array}{ c } \hline C2 \\ \hline 3B \\ \hline 1-E \\ \hline 2003 \end{array} \end{array}$
201	$\begin{array}{c} A-1 \\ \hline \begin{array}{ c } \hline CD \\ \hline 3B \\ \hline 2-4 \end{array} \end{array} \Rightarrow$	$\begin{array}{c} A-E \\ \hline \begin{array}{ c } \hline CD \\ \hline 2B \\ \hline 1-3 \\ \hline 2010 \end{array} \end{array}$	$\begin{array}{c} A-1 \\ \hline \begin{array}{ c } \hline CD \\ \hline 2B \\ \hline E-3 \\ \hline 2011 \end{array} \end{array}$	$\begin{array}{c} A-1 \\ \hline \begin{array}{ c } \hline CD \\ \hline EB \\ \hline 2-3 \\ \hline 2012 \end{array} \end{array}$	$\begin{array}{c} A-1 \\ \hline \begin{array}{ c } \hline CD \\ \hline 3B \\ \hline 2-E \\ \hline 2013 \end{array} \end{array}$
202	$\begin{array}{c} A-1 \\ \hline \begin{array}{ c } \hline C2 \\ \hline 2B \\ \hline 1-D \end{array} \end{array} \Rightarrow$	$\begin{array}{c} A-E \\ \hline \begin{array}{ c } \hline CE \\ \hline 3B \\ \hline 1-D \\ \hline 2020 \end{array} \end{array}$	$\begin{array}{c} A-1 \\ \hline \begin{array}{ c } \hline CE \\ \hline 3B \\ \hline 2-D \\ \hline 2021 \end{array} \end{array}$		
210	$\begin{array}{c} A-D \\ \hline \begin{array}{ c } \hline 1C \\ \hline 4B \\ \hline 2-3 \end{array} \end{array} \Rightarrow$	$\begin{array}{c} A-D \\ \hline \begin{array}{ c } \hline EC \\ \hline 3B \\ \hline 1-2 \\ \hline 2100 \end{array} \end{array}$	$\begin{array}{c} A-D \\ \hline \begin{array}{ c } \hline 1C \\ \hline 3B \\ \hline E-2 \\ \hline 2101 \end{array} \end{array}$	$\begin{array}{c} A-D \\ \hline \begin{array}{ c } \hline 1C \\ \hline 3B \\ \hline 2-E \\ \hline 2102 \end{array} \end{array}$	$\begin{array}{c} A-D \\ \hline \begin{array}{ c } \hline 1C \\ \hline EB \\ \hline 2-3 \\ \hline 2103 \end{array} \end{array}$
211	$\begin{array}{c} A-1 \\ \hline \begin{array}{ c } \hline 1C \\ \hline 2B \\ \hline D-2 \end{array} \end{array} \Rightarrow$	$\begin{array}{c} A-E \\ \hline \begin{array}{ c } \hline 1C \\ \hline 3B \\ \hline D-2 \\ \hline 2110 \end{array} \end{array}$	$\begin{array}{c} A-1 \\ \hline \begin{array}{ c } \hline 2C \\ \hline 3B \\ \hline D-E \\ \hline 2112 \end{array} \end{array}$		
212	$\begin{array}{c} A-1 \\ \hline \begin{array}{ c } \hline 2C \\ \hline 3B \\ \hline 4-D \end{array} \end{array} \Rightarrow$	$\begin{array}{c} A-E \\ \hline \begin{array}{ c } \hline 1C \\ \hline 2B \\ \hline 3-D \\ \hline 2120 \end{array} \end{array}$	$\begin{array}{c} A-1 \\ \hline \begin{array}{ c } \hline EC \\ \hline 2B \\ \hline 3-D \\ \hline 2121 \end{array} \end{array}$	$\begin{array}{c} A-1 \\ \hline \begin{array}{ c } \hline 2C \\ \hline EB \\ \hline 3-D \\ \hline 2122 \end{array} \end{array}$	$\begin{array}{c} A-1 \\ \hline \begin{array}{ c } \hline 2C \\ \hline 3B \\ \hline E-D \\ \hline 2123 \end{array} \end{array}$

^a For each of the 140 structures shown in part 2 (Table IV), there are three different positions possible for F. Next for each of these there are two different positions for G (and then only one position for H). This yields a grand total of 840 isomer pairs or 1680 total isomers—in the event that all eight ligands are different.

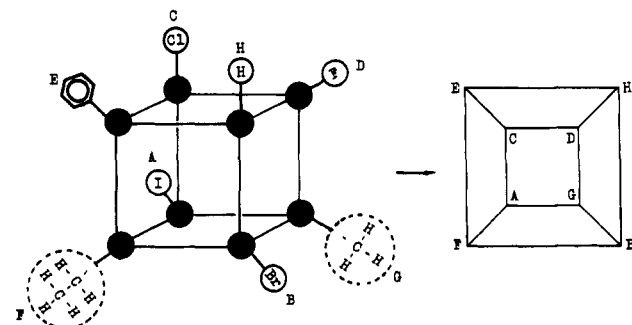


Figure 7.

Figure 7 is a representative hypothetical octasubstituted cubane. Using the same techniques as above for coordination 6, from Table IV, we see that this compound would be designated as

$$(1 \times 5)^5 + (1 \times 5)^4 + (1 \times 5)^3 + (2 \times 5)^2 + (1 \times 5)^1 + 0$$

which equals 3930. This number, however, is only the partial name. It is the name for both the given compound and for the mirror image compound; consequently, we must supplement it with an *R* or *S* designator. Applying the criteria described in the previous section to Figure 7a, the proposed name is 3930 - *R* - iodo-,bromo-,chloro-,fluoro-,phenyl-,ethyl-,methyl-,hydrocubane. (Although the hydro does not have to be named, the inclusion of all eight ligands is recommended for clarity.)

DODECACoordination: THE (REGULAR) ICOSAHEDRON

For the fourth of the regular polyhedra, the icosahedron, it should be noted that a coordination of 12 is normally far too large to be viable for a single central atom surrounded by ligands (i.e., the first of the two sources of such coordination). Similarly, it makes a very unlikely source of isomers for carbon cages. Nevertheless, we note that such a geometry is of more than just mathematical interest, as it shall have relevance in

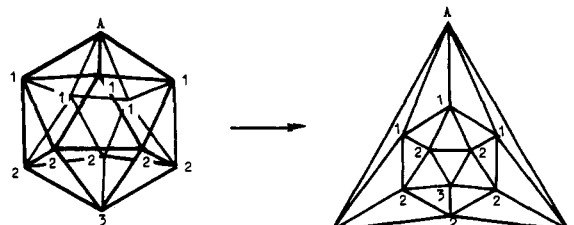


Figure 8.

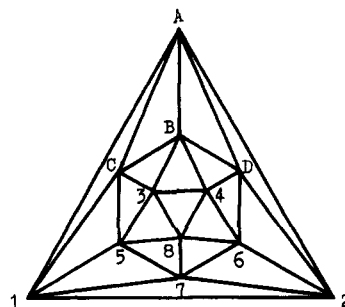


Figure 9.

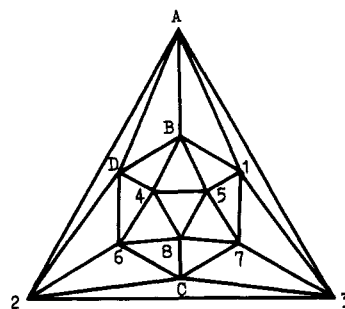


Figure 10.

the domain of inorganic, especially boron, chemistry. We may readily generate the mathematically possible isomers for icosahedral coordination by following the identical procedure used above. Figure 8 illustrates formation of the Schlegel projection for a regular icosahedron, as well as the first step of the corresponding table for the generation of enantiomer pairs. Table VI is the complete computation of the first three steps. In all, a total of 11 steps, each more tedious than the previous one, would be required in order to complete this process by brute force and to determine the total number of isomers.

In exactly the same number as for cubane, this number can be computed by group theory as $12!/60$ or by the strictly graph-theoretical method of noting the above-stated factorial relation whenever there are no constitutionally equivalent vertices,¹⁷ i.e., whenever no two vertices in a step have the same set of GTDs. For example, note that of the 14 different configurations obtained in Table VI, step 3, eight have no constitutionally equivalent vertices; i.e., no repeated set of GTDs, or equivalently, no symmetry. Consequently, configurations whose names begin with 00, 01, 02, 03, 10, 11, 13, and 14 will each contribute $9! = 362880$ enantiomer pairs, or a subtotal of 5 806 080 enantiomers. A representative example is given in Figure 9 for the class of enantiomer pairs that begin with the designation 000₉. Similarly, of the remaining six configurations, these can be further subdivided into those without additional symmetry and those with. The first of these classes is illustrated in Figure 10 with the class of enantiomer pairs that begin with the designation 040₉. For this subclass there will be $6 \times 4 \times 8! = 967680$ enantiomer pairs or 1 935 360 enantiomers. The subclass with additional symmetry is shown in Figure 11 and contributes $6 \times 4 \times 7! = 120960$ enantiomer pairs. Thus there will be a grand total

Table VII. Generation of Enantiomer Pairs for the Dodecahedron

Step # 1					
Step # 2					
1-st digit = 0	1-st digit = 1	1-st digit = 2	1-st digit = 3	1-st digit = 4	
1 (A=1, B=2) 6 (A=3, B=3) 2 (A=2, B=1) 7 (A=3, B=4) * 3 (A=2, B=2) 8 (A=4, B=3) 4 (A=2, B=3) 9 (A=4, B=5) 5 (A=3, B=2) a (A=5, B=4) *	1 (A=1, B=1) 9 (A=3, B=2) * 2 (A=1, B=2) a (A=3, B=3) 3 (A=1, B=3) b (A=3, B=4) 4 (A=2, B=1) c (A=3, B=5) 5 (A=2, B=2) d (A=4, B=2) * 6 (A=2, B=3) e (A=4, B=3) 7 (A=2, B=4) f (A=4, B=4) 8 (A=3, B=1) g (A=5, B=3)	1 (A=1, B=2) 9 (A=3, B=1) 2 (A=1, B=3) a (A=3, B=2) 3 (A=1, B=4) b (A=3, B=3) * 4 (A=2, B=1) c (A=3, B=4) * 5 (A=2, B=2) d (A=4, B=1) 6 (A=2, B=3) e (A=4, B=2) 7 (A=2, B=4) f (A=4, B=3) 8 (A=2, B=5) g (A=5, B=2)	1 (A=1, B=3) 6 (A=3, B=1) * 2 (A=1, B=5) 7 (A=3, B=2) 3 (A=2, B=2) 8 (A=3, B=3) 4 (A=2, B=3) 9 (A=4, B=2) 5 (A=2, B=4) a (A=5, B=1) *	1 (A=1, B=4) 2 (A=2, B=3) 3 (A=3, B=2) 4 (A=4, B=1)	
Representative examples of Step # 3 (lowest combination having this graph theoretical configuration)			Representative examples of Step # 4		of Step # 5
1-st 2 digits = 00	1-st 2 digits = 40	1-st 2 digits = 41	1-st 3 digits = 400	1-st 3 digits = 408	1-st 4 digits = 4080
1 (A=1, B=2, C=2) 2 (A=2, B=1, C=2) 3 (A=2, B=1, C=3) 4 (A=2, B=2, C=1) 5 (A=2, B=2, C=3) 6 (A=2, B=3, C=1) 7 (A=2, B=3, C=2) 8 (A=3, B=2, C=3) 9 (A=3, B=2, C=4) a (A=3, B=3, C=2) b (A=3, B=3, C=4) c (A=3, B=4, C=2) d (A=4, B=3, C=3) e (A=4, B=3, C=5) f (A=4, B=5, C=3) g (A=4, B=4, C=4) h (A=5, B=4, C=4)	1 (A=1, B=4, C=2) 2 (A=2, B=3, C=1) 3 (A=2, B=3, C=3) 4 (A=2, B=3, C=5) 5 (A=3, B=2, C=2) 6 (A=2, B=3, C=3) 7 (A=3, B=2, C=4) 8 (A=4, B=1, C=3) * 9 (A=4, B=1, C=5) *	1 (A=1, B=4, C=1) 2 (A=1, B=4, C=2) 3 (A=1, B=4, C=3) 4 (A=2, B=3, C=1) 5 (A=2, B=3, C=2) * 6 (A=2, B=3, C=3) * 7 (A=2, B=3, C=4) 8 (A=3, B=2, C=1) 9 (A=3, B=2, C=2) a (A=3, B=2, C=3) b (A=3, B=2, C=4) c (A=3, B=2, C=5) * d (A=4, B=1, C=2) e (A=4, B=1, C=3) f (A=4, B=1, C=4)	1 (A=1, B=4, C=2, D=2) 2 (A=2, B=3, C=1, D=2) 3 (A=2, B=3, C=1, D=3) 4 (A=2, B=3, C=2, D=1) 5 (A=2, B=3, C=2, D=3) 6 (A=2, B=3, C=3, D=1) 7 (A=2, B=3, C=3, D=2) 8 (A=3, B=2, C=2, D=1) 9 (A=3, B=2, C=2, D=2) a (A=3, B=2, C=3, D=2) b (A=3, B=2, C=3, D=4) c (A=3, B=2, C=4, D=2) d (A=3, B=2, C=4, D=3) e (A=4, B=1, C=3, D=3) f (A=4, B=1, C=3, D=5) g (A=4, B=1, C=5, D=3)	1 (A=1, B=4, C=2, D=3) 2 (A=2, B=3, C=1, D=4) 3 (A=2, B=3, C=1, D=5) 4 (A=2, B=3, C=2, D=1) 5 (A=3, B=2, C=2, D=3) 6 (A=3, B=2, C=3, D=2) 7 (A=3, B=2, C=3, D=4) 8 (A=4, B=1, C=3, D=2)	1 (A=1, B=4, C=2, D=3, E=2) 2 (A=2, B=3, C=1, D=4, E=2) 3 (A=2, B=3, C=1, D=4, E=3) 4 (A=2, B=3, C=2, D=3, E=1) 5 (A=2, B=3, C=2, D=3, E=3) 6 (A=2, B=3, C=3, D=2, E=1) 7 (A=2, B=3, C=3, D=2, E=2) 8 (A=3, B=2, C=2, D=3, E=2) 9 (A=3, B=2, C=2, D=3, E=4) a (A=3, B=2, C=3, D=2, E=2) b (A=3, B=2, C=3, D=2, E=4) c (A=3, B=2, C=4, D=1, E=2) d (A=3, B=2, C=4, D=1, E=3) e (A=4, B=1, C=3, D=2, E=3) f (A=4, B=1, C=3, D=2, E=5)

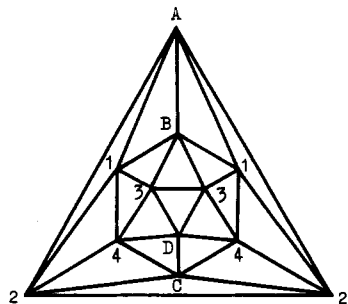


Figure 11.

ICOSACOORDINATION: THE REGULAR DODECAHEDRON

The last of the regular polyhedra, the dodecahedron, has 20 vertices, and thus the possibility of a different ligand at each of these locations. Figure 12 illustrates formation of the

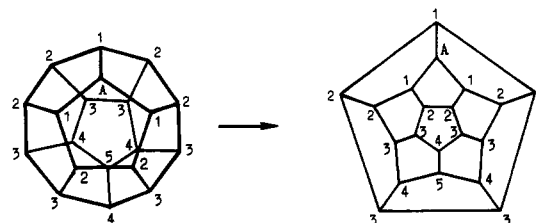


Figure 12.

Schlegel projection of the regular dodecahedron, while Table VII illustrates how the same procedure used for the smaller regular polyhedra may be applied, with the formulation of the associated nomenclature that would be applicable. Note that in step 1 there are five different graph theoretical distances from a selected "root" vertex—giving rise to a first digit of from 0 through 4 in the name. Each of these, in turn, is examined. The maximum number of different locants is achieved in step 3. Because this maximum number is 17, we

shall use heptadecimal digits (0–9, followed by *a–h*—where lower case rather than capital letters were selected inasmuch as the capital letters had already been used to label vertices of the graph). Similarly, because the first vertex was arbitrarily selected and the last is uniquely determined, the proposed name of such a compound will be an 18-digit-long heptadecimal number (or its decimal equivalent), followed by a *R* or *S*, and then the sequence of 20 decreasing atomic number ligands, followed by the word “dodecahedrane”.

Working out the combinatorics, assuming that all the ligands are different (either by group theory = $20!/120$), or by the above-described techniques used for cubane and icosahedrane, there would be 20 274 183 401 472 000 enantiomer pairs, or slightly more than 4×10^{16} different enantiomers of such a dodecahedrane. Naturally, this number will be much smaller as the number of identical ligands increases. For example, there are only 1 unsubstituted dodecahedrane, 1 monosubstituted dodecahedrane, 5 disubstituted dodecahedrane “pairs” (see step 1 of Table VII)—which, when the ligands are alike, is exactly 5, but for unlike ligands can give rise to 5–10 different enantiomers depending on symmetry, etc. Similarly, continuing to the number of trisubstituted dodecahedralanes, we note, from step 2 of Table VII, that provided the three ligands are all different, there are 56 different graphs. Consequently, there shall be between 56 and 112 different enantiomers—depending on whether the mirror images are superimposable. Furthermore, we note that this number will be substantially less if two or more ligands are alike. A group theoretical analysis of substituted dodecahedralanes has been supplied by Fujita.¹⁸

EPILOGUE

Some of the logical extensions of this work that may result in actual chemical molecules or others which might produce interesting results just from the perspective of mathematical completeness are

(1) The algorithm procedure developed for Platonic solids is applicable to other important geometric configurations, in particular the 13 (or 15—depending on one’s perspective) Archimedean solids, as well as all figures in which the all of the vertices are initially equivalent. Furthermore, it is adaptable to a wider class of figures (some of which are important in chemistry) such as the trigonal and pentagonal bipyramids, etc. For this extended class the choice for *A* is not completely arbitrary, rather two or more values for *A* must be followed through. Consequently, the canonical name for such a figure will require $n - 1$ (rather than just $n - 2$) locants, and it is suggested that we use just the appropriate different base number, rather than converting this number into base 10, as well as the choice of *R* vs *S*, and the word describing the geometric shape and the names for the locants. The additions to the nomenclature algorithm to account for such figures are straight-forward.

(2) Although the appropriate geometry for most molecules is the embedding of the union of one-dimensional bonds in a three-dimensional space,⁷ the presence of a nonorientable surface, such as a Möbius strip, is

readily denominated using the given algorithm. For such a configuration, there will be only 10 enantiomer pairs for the six-vertex surface (represented in graph theory as $K_{3,3}$) vs 15 for the octahedron and only 750 enantiomer pairs for the twisted eight-vertex surface vs 840 for the cube.

(3) In line with the recent studies of the fullerenes,¹⁹ the admittedly remote possibility of “internal”, as well as “external”, ligands for the larger Platonic solids, such as dodecahedrane, must not be overlooked. In fact, with appropriate distortions, even a cubane might allow for one, or maybe two, small ligands to be internal. If such a scenario were viable, the number of “topological” isomers that such figures could have would be significantly larger than the 1680 cubanes or the 4×10^{16} dodecahedralanes suggested in the previous sections.

REFERENCES AND NOTES

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- (2) A “Platonic solid” is one of the five polyhedra that can be formed in a three-dimensional space so that each face is a “regular” (i.e., equilateral, equiangular, convex) polygon and each polyhedral angle has the same number of edges. These five are tetrahedron, octahedron, cube, dodecahedron, and icosahedron.
- (3) The word “cage” in this context is that of a three-dimensional module (the older definition before there were known molecules in which a smaller entity was topologically enclosed, but not chemically bound).
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- (10) “When a model is seen in perspective from a position just outside the center of one face, this face appears as a large polygon with all the remaining faces filling its interior.”¹¹
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