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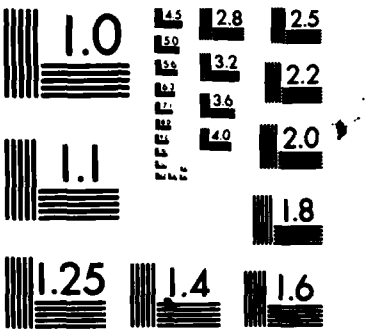

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The lowest degree chirality polynomials for the regular octahedron, cube, and regular icosahedron are discussed. All three of these regular polyhedra are chirally degenerate since they have more than one lowest degree chiral ligand partition by the Ruch-Schönhofer scheme. The two lowest degree chirality polynomials for the octahedron have degree 6 and can be formed from three degree 3 generating polynomials f, g, and h through the relationships f(g+h) and f(g-h) where f, g, and h measure the effects of the three separating reflections planes (σ_h), (continued)

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the four threefold rotation axes, and the three fourfold rotation axes, respectively. The permutation groups of the vertices of the cube and icosahedron contain only even permutations which leads to a natural pairing of their chiral ligand partitions according to equivalence of the corresponding Young diagrams upon reflection through their diagonals. The two lowest degree chirality polynomials for the cube have degree 4 and can be formed from two degree 4 generating polynomials f and g through the relationships -2g and f-2g where f and g measure the effects of the S_6 improper rotation and C_4 proper rotation axes, respectively. The four lowest degree chiral ligand partitions for the icosahedron have degree 4 and lead naturally to a single degree 4 chirality polynomial with 120 terms of the general type $(x-y)^2(z-w)^2$. This chirality polynomial for the icosahedron cannot be broken down into simpler generating polynomials in contrast to the lowest degree chirality polynomials for the octahedron and cube. This appears to relate to the origin of the icosahedral group from the simple alternating group A_5. The full icosahedral chirality polynomial can be simplified to give a chirality polynomial for the chiral boron-monosubstituted ortho and meta carboranes of the general formula $B_2C_{10}H_{11}X$.

Abstract

The lowest degree chirality polynomials for the regular octahedron, cube, and regular icosahedron are discussed. All three of these regular polyhedra are chirally degenerate since they have more than one lowest degree chiral ligand partition by the Ruch-Schönhofer scheme. The two lowest degree chirality polynomials for the octahedron have degree 6 and can be formed from three degree 3 generating polynomials f, g, and h through the relationships f(g+h) and f(g-h) where f, g, and h measure the effects of the three separating reflection planes (ϕ_h), the four threefold rotation axes, and the three fourfold rotation axes, respectively. The permutation groups of the vertices of the cube and icosahedron contain only even permutations which leads to a natural pairing of their chiral ligand partitions according to equivalence of the corresponding Young diagrams upon reflection through their diagonals. The two lowest degree chirality polynomials for the cube have degree 4 and can be formed from two degree 4 generating polynomials f and g through the relationships -2g and f-2g where f and g measure the effects of the S_6 improper rotation and C_4 proper rotation axes, respectively. The four lowest degree chiral ligand partitions for the icosahedron have degree 4 and lead naturally to a single degree 4 chirality polynomial with 120 terms of the general type $(x-y)^2(z-w)^2$. This chirality polynomial for the icosahedron cannot be broken down into simpler generating polynomials in contrast to the lowest degree chirality polynomials for the octahedron and cube. This appears to relate to the origin of the icosahedral group from the simple alternating group A_5. The full icosahedral chirality polynomial can be simplified to give a chirality polynomial for the chiral boron-monosubstituted ortho and meta carboranes of the general formula $B_2C_{10}H_{11}X$.

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TECHNICAL REPORT NO. 27

Chemical Applications of Topology and Group Theory. 22. Lowest Degree Chirality Polynomials for Regular Polyhedra

by

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1. Introduction

The geometrical and algebraic theories of chirality[1,2,3,4,5,6,7,8] are important for the understanding of chemically significant pseudoscalar measurements such as optical rotation and circular dichroism. Such theories have the following objectives:

(1) Determination of the ligand partitions for a given achiral molecular skeleton which lead to chiral systems, namely how unsymmetrical must a ligand partition be before all improper rotation symmetry elements S_n (including reflection planes $S_1 \equiv \sigma$ and inversion centers $S_2 \equiv i$) of an achiral skeleton are destroyed. This leads naturally to the idea of chiral dimensionality,[1] $X_d = n!/|G|$, for an achiral skeleton having n sites and point group G; the chiral dimensionality corresponds to the number of enantiomer pairs when each site of the skeleton has a different ligand or substituent.

(2) Determination of mathematical functions (chirality functions) by which the magnitude and sign of a given pseudoscalar property (the dependent variable) can be calculated for a given skeleton using parameters which depend only upon the ligands located at specific sites on the skeleton (the independent variables). The chirality polynomial of lowest degree in the Ruch-Schönhofer scheme[4,5] is particularly significant since by using algebraic invariant theory Meinköhn[9,10] has shown that only the lowest degree chirality polynomials for a given skeleton are required to have the desirable property of depending only upon the differences between the ligand parameters. For this reason this paper will be concerned only with the chirality polynomials of the lowest degree.

An essential feature of chirality algebra is the dissection of a molecule into a collection of ligands and an underlying skeleton. This terminology refers to a coordination compound of the generic type ML_n (M = central atom, generally

a metal; L_n = n ligands not necessarily equivalent). However, with no essential changes in the mathematics the theory can also consider organic skeletons, polyhedral boranes, or metal cluster compounds having n substituents or ligands. As in my previous papers[1,8] ligand partitions are represented by symbols of the type $(a_1^{b1}, a_2^{b2},\ldots,a_k^{bk})$ where a_k and b_k are small positive integers indicating b_k sets of a_k identical ligands and $a_m \geq a_{m+1}$ $(1 \leq m \leq k)$.

The essential ideas of chirality algebra were first presented by Ruch and Schönhofer[3,4] and have been reviewed by Ruch[2] at an elementary level and by Mead[5] at a more advanced mathematical level. Chirality functions have been tested experimentally for the methane,[11,12] allene,[13] polarized rectangle[8] (e.g., [2,2]-metacyclophane[14,15] and 2,2'-spirobiindane[16,17] skeletons), cyclopentane,[18] and ferrocene[19] skeletons with varying degrees of success. My own papers relate chirality algebra to the framework groups[8] of Pople[20] and use concepts from permutation group theory and Meinköhn's[9,10] development of algebraic invariant theory to study of chirality in transitive skeletons[1] with particular emphasis on a group theoretical basis for the extensively discussed[4,5,7,21] idea of qualitative completeness. This paper extends the ideas of the previous paper[1] to those necessary for the study of the lowest degree chirality polynomials of three of the four regular polyhedra with non-trivial chirality functions, namely the octahedron, cube, and icosahedron. In this connection the structures of the previously reported lowest degree chirality polynomials of the octahedron[1,3,4] and the cube[3] are discussed and that of the icosahedron is presented for the first time. The octahedral skeleton is important in six-coordinate complexes ML_6, the cubic skeleton is important in cubane and inorganic analogues, and the icosahedral skeleton is important in icosahedral boranes and carboranes such as substitution products of the three isomers of $C_2B_{10}H_{12}$.

2. Background

The determination of the lowest degree chirality polynomial for a given skeleton having n sites involves the following two steps which are discussed in detail elsewhere[5,6,8]:

(1) The chiral ligand partitions are determined by considering the point group G as a subgroup of the symmetric group P_n and calculating by standard group theoretical procedures[22,23,24,25] the number of times that the chiral representation $\Gamma*$ of G appears when each irreducible representation of P_n is restricted to elements of G. In this connection the chiral representation $\Gamma*$ has +1 characters for proper rotations and -1 characters for improper rotations. Character tables for the symmetric groups P_n are required for this step.[26,27,28]

(2) The chirality polynomial X for a given chiral ligand partition $(a_1^{b1}, a_2^{b2}, \ldots, a_k^{bk})$ found in the above step has a term of degree g for each element of G corresponding to its effect in permuting the sites represented by an appropriately selected monomial M of degree g. These terms have positive signs for proper rotations and negative signs for improper rotations. The chirality polynomial can thus be represented schematically as

$$X(a_1^{b1}, a_2^{b2}, \ldots, a_k^{bk}) = G*M \qquad (1)$$

The "star" operation "*" in equation 1 refers to a sum of all of the permutations of the sites represented by M by all of the elements in G with positive signs for proper rotations and negative signs for improper rotations.[6]

The set of elements in the point group G are conveniently described by its cycle index Z(G) which is defined as follows[1,8,29]:

$$Z(G) = \frac{1}{|G|} \sum_{i=1}^{i=c} a_i x_1^{c_{i1}} x_2^{c_{i2}} \ldots x_n^{c_{in}} \qquad (2)$$

The variables in equation 2 are defined as follows:

$|G|$ = number of elements in G

n = number of sites in the skeleton

c = number of terms in the cycle index

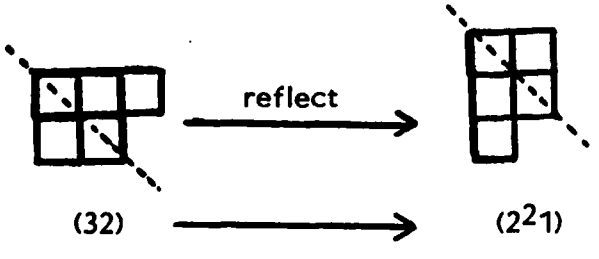
a_i = number of elements in the permutation group having the indicated cycle structure

x_k = dummy variable referring to cycles of length k

c_{ik} = exponent indicating the number of cycles of length k in term i

The parity of a permutation is odd or even depending upon whether the total number of cycles of <u>even</u> length in the permutation is odd or even, respectively. A group containing only even permutations may be called an <u>even permutation group</u>; important examples of even permutation groups encountered in this paper are the groups of the cube and the icosahedron.

Another fundamental idea of chirality algebra is that of depicting ligand partitions as a collection of boxes called Young diagrams.[30] A Young diagram for a ligand partition $(a_i^{b1}, a_2^{b2}, \ldots, a_k^{bk})$ has $\sum_i b_i$ rows where the first b_1 rows have a_1 boxes, the next b_2 rows have a_2 boxes, etc. Reflection of a Young diagram through its diagonal gives its <u>dual</u> Young diagram, e.g.



(3)

A pair of Young diagrams consisting of a Young diagram and its dual is called a dual pair. A Young diagram which is identical to its dual is called self-dual, e.g.

(31^2) (31^2) (4)

A balanced set of Young diagrams or corresponding ligand partitions contains only dual pairs and self-dual Young diagrams.

Important properties of ligand partitions and their Young diagrams are their degrees and their dimensions. The degree g of a ligand partition can be determined from the corresponding Young diagram by the following sum over all of its columns:

$$g = \frac{1}{2} \sum_{k=1}^{m} c_k(c_k-1) \tag{5}$$

where c_k is the length of column k and m is the number of columns. The degree g as determined by equation 5 corresponds to the degree of the lowest degree chirality polynomial. The dimension of a partition of n ligands is the dimension of the corresponding irreducible representation of the symmetric[30] group P_n. The sum of the dimensions of the chiral ligand partitions for a given skeleton with n sites is its chiral dimensionality, X_d, which may be calculated by the following equation:

$$X_d = n!/|G| \tag{6}$$

This equation is useful for checking the calculations of the ligand partitions and

indicating the size of the total set of chiral ligand partitions. The chiral dimensionalities of the regular polyhedra of interest in this paper, namely the tetrahedron, octahedron, cube, icosahedron, and dodecahedron are 1, 15, 840, 3991680, and approximately 2.0274183×10^{16}, respectively. The regular dodecahedron is excluded from detailed consideration in this paper not only by its unmanageably large chiral dimensionality but by the intractably large size and complexity of the required character table for the symmetric group P_{20} of order $20! \approx 2.432902 \times 10^{18}$. Study of the regular dodecahedron is only feasible by using computers with the prior need for development of software to handle character tables for groups as large as P_{20}. Such efforts do not yet appear warranted since the first regular dodecahedral skeletons, namely dodecahedrane derivatives,[31,32] have only recently been prepared and still are only available in very limited quantities.

Study of the chirality polynomials of the cube and icosahedron is facilitated by the even permutation groups of these skeletons. In this case the following theorem is used:

Theorem: The chiral ligand partitions of a skeleton having an even permutation group form a balanced set.

The proof of this theorem depends upon the observation that irreducible representations of the symmetric group P_n which correspond to ligand partitions having dual Young diagrams have the same characters for all even permutations.[26,30] Therefore, if the permutation group is an even permutation group with no odd permutations, both members of a dual pair must appear equally in the representation of P_n subduced by G.

In this paper the sites of the regular polyhedra are labelled by capital letters as indicated in Figure 1. For clarity the same letters will also be used to represent the parameters for the ligands located at these sites.

The chirality polynomial for the tetrahedron is well known[2,3,4,5,6] and using

the notation in this paper can be written as follows:

$$X(1^4)(T_d) = (A\text{-}B)(A\text{-}C)(A\text{-}D)(B\text{-}C)(B\text{-}D)(C\text{-}D) \qquad (7)$$

In the context of this paper this chirality polynomial may be regarded as trivial, and therefore is not discussed further. Also the lowest degree chirality polynomial for the trigonal antiprism (framework group $D_{3d}[3\sigma_d(L_2)]$),[8] although not that of a regular polyhedron, is significant in this paper for indicating the effect of an S_6 axis, such as in a cube. This degree 2 polynomial corresponds to a chiral ligand partition (42) and can be written as follows:

$$X(42)(D_{3d}) = (A\text{-}B)(D\text{-}F) - (A\text{-}C)(D\text{-}E) \qquad (8)$$

3. The Octahedron

The chiral dimensionality of the octahedron is $6!/|O_h| = 720/48 = 15$ and the octahedron has two chiral ligand partitions, namely (31^3) and (2^3) of dimensions 10 and 5, respectively. Both of these chiral ligand partitions are of degree 6 indicating that the lowest degree chirality polynomial contains terms corresponding to both chiral ligand partitions. A polyhedron, such as the octahedron, having more than one lowest degree chiral ligand partition may be called chirally degenerate.

In order to construct the lowest degree chirality polynomial for the regular octahedron consider the following three degree 3 polynomials:

$$f(A...F) = (A\text{-}F)(B\text{-}E)(C\text{-}D) \qquad (9a)$$

$$g(A...F) = (A-B)(B-C)(C-A) + (C-F)(F-E)(E-C) + (A-E)(E-D)(D-A) + (B-D)(D-F)(F-B) \quad (9b)$$

$$h(A...F) = (A-B+F-E)(A-D+F-C)(B-D+E-C) \quad (9c)$$

The polynomial f measures the effects of the three orthogonal separating[8] reflection planes (σ_h) of the octahedron. The polynomial g measures the effects of the four threefold rotation axes (C_3) of the octahedron noting the following degree 3 chirality polynomial for the the polarized triangle representing the prototypical C_3 axis[3,4]:

$$t(A,B,C) = (A-C)(B-A)(C-B) \quad (10)$$

Similarly the polynomial h measures the effects of the three orthogonal C_4 axes of the octahedron noting the following degree 3 chirality polynomial for the polarized square[8] representing the prototypical C_4 axis:

$$q(A...D) = (B-A)(D-C)(A-C+B-D) \quad (11)$$

The three linear factors in h (equation 9c) correspond to the (A-C+B-D) factor in q (equation 11) with the B-A and D-C factors in q corresponding to the factors in f (equation 9a). The degree 3 polynomials f, g, and h may be called <u>generating polynomials</u> for the lowest degree chirality polynomials of the regular octahedron since arithmetic functions of f, g, and h generate these chirality polynomials.

The degree 6 chirality polynomials corresponding to the two chiral ligand partitions of the octahedron can be constructed from the degree 3 generating polynomials f, g, and h as follows:

$$X(2^3)(O_h) = f(g+h) = (2)O_h*(a^2b^2cd) \qquad (12a)$$

$$X(31^3)(O_h) = f(g-h) = (2)O_h*(a^3b^2c) \qquad (12b)$$

In equations 12a and 12b the designations $O_h*(a^2b^2cd)$ and $O_h*(a^3b^2c)$ refer to the construction of these chirality polynomials by application of the 48 permutations of O_h to monomials of the forms a^2b^2cd and a^3b^2c, respectively, as outlined generically in equation 1 where G is O_h and M is a monomial of the prescribed forms.

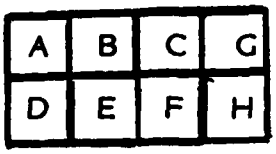
4. The Cube

The (vertex) cycle index of the cube has the following form:

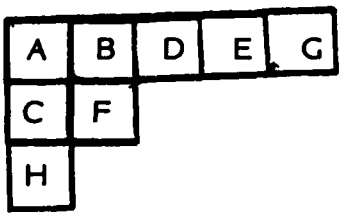
$$Z(\text{cube}) = x_1^8 + 8x_1^2x_3^2 + 13x_2^4 + 12x_4^2 + 8x_2x_6 + 6x_1^4x_2^2 \qquad (13)$$

The parities of all of these permutations are even indicating that the permutation group of the cube is even. Therefore, the chiral ligand partitions of the cube form a balanced set having total dimension 840 corresponding to the chiral dimensionality of the cube ($8!/|O_h| = 40320/48 = 840$). These chiral ligand partitions are listed in Table 1 as dual pairs with minimum degree corresponding to the lower degree of the two chiral ligand partitions forming a dual pair. The self-dual chiral ligand partition (421^2) is starred.

Table 1 indicates that the cube, like the octahedron, is chirally degenerate with the two degree 4 lowest degree chiral ligand partitions (4^2) and (521) corresponding to the following Young tableaux for the labelling in Figure 1:



(4^2)



(521)

(14)

The degree 4 chirality polynomials for these chiral ligand partitions can be obtained from the following two degree 4 generating polynomials:

$$f(A...H) = (A\text{-}G)^2[(B\text{-}E)(C\text{-}F) - (D\text{-}E)(C\text{-}H)] - (B\text{-}H)^2[(A\text{-}C)(D\text{-}E) - (C\text{-}F)(E\text{-}G)] - (C\text{-}E)^2[(A\text{-}F)(B\text{-}D) - (F\text{-}H)(D\text{-}G)] + (D\text{-}F)^2[(A\text{-}H)(B\text{-}E) - (C\text{-}H)(B\text{-}G)] \quad (15a)$$

$$g(A...H) = (A\text{-}C)(B\text{-}G)(F\text{-}H)(E\text{-}D) - (A\text{-}H)(B\text{-}D)(F\text{-}C)(E\text{-}G) \quad (15b)$$

Each term of the generating polynomial f consists of a degree 2 factor (e.g., [(B-E)(C-F) - (D-E)(C-H)] for six vertices related by an S_6 axis resembling the degree 2 chirality polynomial for a trigonal prism or antiprism (see equation 8) and a second degree 2 factor (e.g., $(A\text{-}G)^2$) corresponding to the two vertices on this S_6 axis. The four terms in the generating polynomial f relate to the four S_6 axes in the cube. Each term of the generating polynomial g consists of a product of four differences involving diagonals of four (square) faces of the cube related by the C_4 axis. Thus the generating polynomial f reflects the three-fold and six-fold symmetries of the cube and the generating polynomial g reflects the four-fold symmetry of the cube.

The degree 4 chirality polynomials corresponding to the two chiral ligand partitions of the cube can be constructed from the generating polynomials f and g as follows:

$$X(4^2) = -2g = (2)O_h^*(abcd) \tag{16a}$$

$$X(521) = f\text{-}2g = (2)O_h^*(a^2bc) \tag{16b}$$

The chirality polynomial for the cube given by Ruch and Schönhofer[3] can be expressed in terms of the generating functions f and g as

$$X(\text{cube}) = af - bg \tag{17}$$

This chirality polynomial appears qualitatively complete as long as $a \neq 0$ and $b \neq 2a$; if these inequalities are not satisfied, equation 17 reduces to equation 16a (for $a = 0$) or equation 16b (for $b = 2a$).

5. The Icosahedron

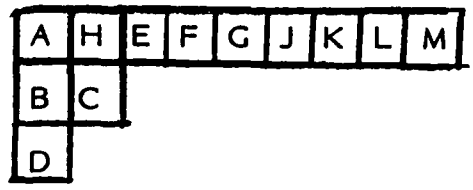
The vertex cycle index of the icosahedron has the following form:

$$Z(\text{icosahedron}) = x_1^{12} + 24x_1^2x_5^2 + 20x_3^4 + 16x_2^6 + 24x_2x_{10} + 20x_6^2 + 15x_1^4x_2^4 \tag{18}$$

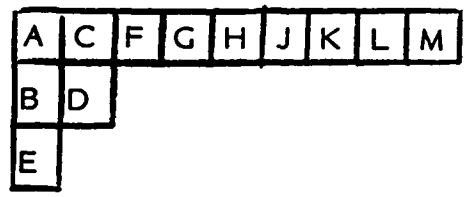
The parities of all of these permutations are even indicating that the permutation group of the icosahedron is even. Therefore the chiral ligand partitions of the icosahedron form a balanced set having total dimension $12!/|I_h| = 479{,}001{,}600/120 = 3{,}991{,}680$. These chiral ligand partitions (Table 2) were determined by the standard group theoretical procedure[5,8] using the character tables for the symmetric group P_{12} given by Zia-ud-Din.[28]

Table 2 indicates that the icosahedron is chirally degenerate like the octahedron

and cube. The icosahedron thus has four degree 4 lowest degree chiral ligand partitions, two of the type (921) and two of the type (84). The Young tableaux for the two (921) chiral ligand partitions are listed below using the labelling in Figure 1:

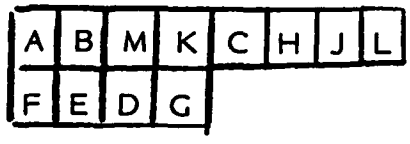


$(921)_o$

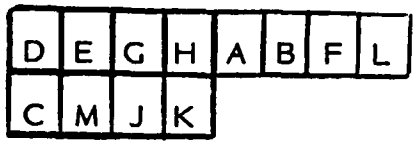


$(921)_m$

The chiral ligand partitions $(921)_o$ and $(921)_m$ correspond to the chiral isomers of the ortho and meta icosahedral carboranes $C_2B_{10}H_{11}X$ (Figure 2). The Young tableaux for the chiral ligand partitions $(84)_i$ and $(84)_o$ are listed below



$(84)_i$



$(84)_o$

In order to obtain these chiral ligand partitions construct the icosahedron from two nested D_{3d} trigonal antiprisms sharing the C_3 axis. Combine the lowest degree chiral (42) ligand partitions of these trigonal antiprisms in two ways to give (84) ligand partitions preserving the chirality by not introducing any improper rotation axes in the combination process. One of these chiral (84) ligand partitions, namely $(84)_i$, has the four equivalent ligands at vertices of the inner trigonal antiprism whereas the other chiral (84) ligand partition, namely $(84)_o$, has the four equivalent ligands at vertices of the outer trigonal antiprism.

These four chiral ligand partitions can be used to construct the lowest degree

chirality polynomial for the icosahedron by the standard group-theoretical procedure[6,8] which can be represented schematically as follows:

$$X(\text{icosahedron}) = I_h*[a^2bc(921)_o] + I_h*[a^2bc(921)_m] + I_h*[abcd(84)_i] + I_h*[abcd(84)_o] \quad (19)$$

Since the icosahedral group I_h has 120 elements, the procedure represented by equation 19 generates 480 terms. Because of the high symmetry of the icosahedron this is not as forbidding as it might seem and the procedure indicated in equation 19 using monomials derived from the Young tableaux $(921)_o$, $(921)_m$, $(84)_i$, and $(84)_o$ generates the equation listed in Table 3 for the lowest degree chirality polynomial of the icosahedron. This equation has 120 terms of the general type $(x-y)^2(z-w)^2$. These 120 terms can be grouped into six sets of 20 terms each. Each of the six sets is characterized by a common $(x-y)^2$ factor where x and y are parameters for ligands at the antipodal vertices related by the inversion operation ("para" vertices in icosahedral carborane nomenclature[33]). The six sets of 20 terms arise from the six such pairs of antipodal vertices in the regular icosahedron. The other factor, $(z-w)^2$, corresponds to the ligand parameters for a pair of non-adjacent, non-antipodal vertices ("meta" vertices in icosahedral carborane nomenclature[33]). The alternation of signs in the equation in Table 3 causes the 240 pairs of terms of the type x^2z^2 to cancel out completely in accord with the fact that the expansion indicated in equation 19 does not use the impossible a^2b^2 monomial for a lowest degree chirality function. In the equation in Table 3 the 480 terms of the type x^2wz arise from the (921) chiral ligand partitions and the 120 terms of the type xywz arise from the (84) chiral ligand partitions as indicated in equation 19.

It is instructive to compare the general form of the lowest degree chirality polynomial of the icosahedron (Table 3) with those of the octahedron (equations

9 and 12) and the cube (equations 15 and 16). The polynomial f(A...H) for the cube (equation 15a) and the chirality polynomial for the icosahedron both have factors of the type $(x-y)^2$ in which x and y are a pair of antipodal vertices. The remaining factor of a term of the generating polynomial f(A...H) (equation 15a) resembles the chirality polynomial of the trigonal antiprism (equation 8) which is the symmetry of the set of six vertices of a cube remaining after removing a pair of antipodal vertices. However, the same is not true for the icosahedron chirality polynomial in Table 3. Thus the 20 terms remaining after factoring $(A-M)^2$ from the first 20 terms of the icosahedron chirality polynomial do not resemble the chirality polynomial for the pentagonal antiprism determined by Ruch and Schönhofer.[3] This as well as the inability to decompose the icosahedral chirality polynomial in Table 3 into a simpler set of generating polynomials similar to f, g, and h (equation 9) for the octahedron or f and g (equation 15) for the cube may relate to the fact that the icosahedral group is isomorphic[34] to the direct product[35] of C_2 with the simple[36] group A_5. The simplicity of A_5 appears to have the effect of mixing up the portions of the lowest degree chirality polynomial of the icosahedron so that it cannot be decomposed into generating functions reflecting its different symmetries in contrast to the chirality functions of the octahedron and cube discussed above.

The lowest degree chirality polynomial in Table 3 is rather forbidding for actual chemical applications although it would be required in the unlikely case of an icosahedral borane or carborane having a different substituent in each of its twelve positions. More realistic cases of possible chemical interest are the chiral monosubstituted carboranes $C_2B_{10}H_{11}X$ in Figure 2. Thus among the four possible ortho carboranes monosubstituted on boron only one (Figure 2a) is chiral corresponding to the ligand partition $(921)_o$ above. Similarly among the four possible meta carboranes monosubstituted on boron only one (Figure 2b) is chiral corresponding to the

ligand partition $(921)_m$. The single para carborane isomer is not chiral. For both of the chiral boron monsubsituted carboranes $C_2B_{10}H_{11}X$ in Figure 2 the chirality polynomial in Table 3 reduces to

$$X(921)(C_2B_{10}H_{11}X) = (c-b)^2[(x-c)^2 + (x-b)^2 - (c-b)^2] \qquad (20)$$

In equation 20 x is the parameter for the substituent X, b is the parameter for a BH vertex, and c is the parameter for a CH vertex.

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TABLE 1

THE CHIRAL LIGAND PARTITIONS OF THE CUBE

LISTED AS DUAL PAIRS

Dual Pair	Minimum Degree	Multiplicity	Dimension
$(521) + (321^3)$	4	1	64
$(4^2) + (2^4)$	4	1	14
$(431) + (32^21)$	5	1	70
$(51^3) + (41^4)$	6	2	35
$(42^2) + (3^21^2)$	6	2	56
$(421^2)^*$	7	2	90

TABLE 2

THE CHIRAL LIGAND PARTITIONS OF THE ICOSAHEDRON

LISTED AS DUAL PAIRS

Dual Pair	Minimum Degree	Multiplicity	Dimension
$(921) + (321^7)$	4	2	320
$(84) + (2^4 1^4)$	4	2	275
$(831) + (32^2 1^5)$	5	6	891
$(91^3) + (41^8)$	6	4	165
$(82^2) + (3^2 1^6)$	6	8	616
$(741) + (32^3 1^3)$	6	12	1408
$(6^2) + (2^6)$	6	4	132
$(821^2) + (421^6)$	7	8	945
$(732) + (3^2 21^4)$	7	12	1925
$(651) + (32^4 1)$	7	8	1155
$(731^2) + (42^2 1^4)$	8	26	2376
$(642) + (3^2 2^2 1^2)$	8	26	2673
$(72^2 1) + (431^5)$	9	14	2079
$(641^2) + (42^3 1^2)$	9	24	3080
$(63^2) + (3^3 1^3)$	9	12	1650
$(5^2 2) + (3^2 2^3)$	9	6	1320
$(81^4) + (51^7)$	10	4	330
$(6321) + (4321^3)$	10	46	5632
$(5^2 1^2) + (42^4)$	10	18	1485
$(543) + (3^3 21)$	10	16	2112

TABLE 2 (Continued)

Dual Pair	Minimum Degree	Multiplicity	Dimension
$(721^3) + (521^5)$	11	14	1728
$(5421) + (432^21)$	11	48	5775
$(631^3) + (52^21^3)$	12	36	3696
$(62^3) + (4^21^4)$	12	20	1925
$(53^21) + (43^21^2)$	12	40	4158
$(4^3) + (3^4)$	12	10	462
$(62^21^2) + (531^4)$	13	24	3564
$(541^3) + (52^31)$	13	28	3520
$(532^2) + (4^21^2)$	13	30	4455
$(4^231) + (43^22)$	13	22	2970
(5321^2)*	14	68	7700
(4^22^2)*	14	28	2640
$(71^5) + (61^6)$	15	2	462
(621^4)*	16	16	2100

TABLE 3

LOWEST DEGREE CHIRALITY POLYNOMIAL

OF THE ICOSAHEDRON

$$
\begin{aligned}
X(A\ldots M) = {} & (A\text{-}M)^2\,[(B\text{-}K)^2 - (B\text{-}H)^2 + (B\text{-}L)^2 - (B\text{-}G)^2 + (C\text{-}L)^2 \\
& - (C\text{-}J)^2 + (C\text{-}G)^2 - (C\text{-}H)^2 + (D\text{-}G)^2 - (D\text{-}K)^2 + (D\text{-}H)^2 \\
& - (D\text{-}J)^2 + (E\text{-}H)^2 - (E\text{-}L)^2 + (E\text{-}J)^2 - (E\text{-}K)^2 + (F\text{-}J)^2 \\
& - (F\text{-}G)^2 + (F\text{-}K)^2 - (F\text{-}L)^2] + (B\text{-}J)^2\,[(A\text{-}K)^2 - (A\text{-}H)^2 \\
& + (A\text{-}E)^2 - (A\text{-}D)^2 + (C\text{-}E)^2 - (C\text{-}M)^2 + (C\text{-}D)^2 - (C\text{-}H)^2 \\
& + (G\text{-}D)^2 - (G\text{-}K)^2 + (G\text{-}H)^2 - (G\text{-}M)^2 + (L\text{-}H)^2 - (L\text{-}E)^2 \\
& + (L\text{-}M)^2 - (L\text{-}K)^2 + (F\text{-}M)^2 - (F\text{-}D)^2 + (F\text{-}K)^2 - (F\text{-}E)^2] \\
& + (C\text{-}K)^2\,[(A\text{-}L)^2 - (A\text{-}J)^2 + (A\text{-}F)^2 - (A\text{-}E)^2 + (D\text{-}F)^2 - (D\text{-}M)^2 \\
& + (D\text{-}E)^2 - (D\text{-}J)^2 + (H\text{-}E)^2 - (H\text{-}L)^2 + (H\text{-}J)^2 - (H\text{-}M)^2 + (G\text{-}J)^2 \\
& - (G\text{-}F)^2 + (G\text{-}M)^2 - (G\text{-}L)^2 + (B\text{-}M)^2 - (B\text{-}E)^2 + (B\text{-}L)^2 - (B\text{-}F)^2] \\
& + (D\text{-}L)^2\,[(A\text{-}G)^2 - (A\text{-}K)^2 + (A\text{-}B)^2 - (A\text{-}F)^2 + (E\text{-}B)^2 - (E\text{-}M)^2 \\
& + (E\text{-}F)^2 - (E\text{-}K)^2 + (J\text{-}F)^2 - (J\text{-}G)^2 + (J\text{-}K)^2 - (J\text{-}M)^2 + (H\text{-}K)^2 \\
& - (H\text{-}B)^2 + (H\text{-}M)^2 - (H\text{-}G)^2 + (C\text{-}M)^2 - (C\text{-}F)^2 + (C\text{-}G)^2 - (C\text{-}B)^2] \\
& + (E\text{-}G)^2\,[(A\text{-}H)^2 - (A\text{-}L)^2 + (A\text{-}C)^2 - (A\text{-}B)^2 + (F\text{-}C)^2 - (F\text{-}M)^2 \\
& + (F\text{-}B)^2 - (F\text{-}L)^2 + (K\text{-}B)^2 - (K\text{-}H)^2 + (K\text{-}L)^2 - (K\text{-}M)^2 + (J\text{-}L)^2 \\
& - (J\text{-}C)^2 + (J\text{-}M)^2 - (J\text{-}H)^2 + (D\text{-}M)^2 - (D\text{-}B)^2 + (D\text{-}H)^2 - (D\text{-}C)^2] \\
& + (F\text{-}H)^2\,[(A\text{-}J)^2 - (A\text{-}G)^2 + (A\text{-}D)^2 - (A\text{-}C)^2 + (B\text{-}D)^2 - (B\text{-}M)^2 \\
& + (B\text{-}C)^2 - (B\text{-}G)^2 + (L\text{-}C)^2 - (L\text{-}J)^2 + (L\text{-}G)^2 - (L\text{-}M)^2 + (K\text{-}G)^2 \\
& - (K\text{-}D)^2 + (K\text{-}M)^2 - (K\text{-}J)^2 + (E\text{-}M)^2 - (E\text{-}C)^2 + (E\text{-}J)^2 - (E\text{-}D)^2]
\end{aligned}
$$

Figure 1: The vertex labellings used for the polyhedra discussed in this paper.

Figure 2: The two chiral icosahedral carboranes $C_2B_{10}H_{11}X$. Large black circles indicate the locations of the carbon atoms.

END

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