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A Descriptor System and Suggested Numbering Procedures for Closed Boron Polyhedra Belonging to D_n, T, and C_s Symmetry Point Groups

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Received April 24, 1981

The system proposed for describing closed, fully triangulated boron polyhedra having at least one rotational symmetry axis and one symmetry plane is applied to boron polyhedra belonging to the D_n, T, and C_s symmetry point groups, which have only one of these symmetry elements. Extensions to the procedure for numbering closed polyhedra previously published are suggested to accommodate these polyhedral structures.

Introduction

In a previous report,[2] a method for definitively describing structures of closed polyboron polyhedra with at least one rotational symmetry axis and one symmetry plane, closely associated with the general procedure for numbering coordination and boron polyhedra,[3] was proposed. This method involves a four-part descriptor for fully triangulated polyboron polyhedra consisting of (1) the point group symmetry symbol for the homogeneous polyboron framework, (2) a description of the arrangement and type of vertices, enclosed in parentheses or brackets, (3) the symbol Δ^n, where Δ indicates triangular faces and n gives the number of faces of the polyhedron, and (4) the familiar descriptor "*closo*-".

Although this procedure is quite adequate for the known closed, fully triangulated boron polyhedra, and most of the hypothetical ones, there are a number of hypothetical fully triangulated polyhedral structures[4] that lack one of the symmetry elements required by the proposed method. For example, polyhedral structures belonging to D_n and T symmetry point groups have rotational symmetry axes but no symmetry plane and those belonging to the C_s symmetry point group have a symmetry plane but no rotational symmetry axis.

This report applies the proposed method[2] to fully triangulated polyhedral systems of the D_n, T, and C_s symmetry point groups and suggests extensions to the procedure for numbering polyhedral structures to accommodate these polyhedra.

Discussion

The first step in numbering symmetric polyhedra is to select three structural features: a reference axis, a preferred terminal plane of symmetrically equivalent vertices perpendicular to the reference axis, and a reference plane containing the reference axis. These features are identified schematically in Figure 1. For polyhedra of high symmetry, a number of criteria must be applied to select the reference axis and the preferred terminal and reference planes, as discussed in our earlier report. The next step in numbering is to orient the polyhedron by looking down the reference axis from the preferred end and rotating the reference plane until it is vertical. The vertices of the polyhedron are then numbered consecutively, clockwise or anticlockwise, beginning with vertices in the preferred terminal plane and proceeding successively to succeeding planes of vertices working down the reference axis from the preferred end. The vertices in each plane are numbered in the same direction, beginning in each plane with a vertex in the reference plane at the top of the projection derived from the preferred orientation or with the first vertex encountered in the direction chosen for numbering from the top of the projection.

D_n Polyhedra. Polyhedral structures of the D_n symmetry point group have rotational symmetry axes, and therefore, except when $n = 2$, the reference axis for describing and numbering these polyhedra can be selected according to the procedure given in our earlier report. Also, as discussed for the more symmetrical polyhedra of our earlier study, parallel planes of polyhedral vertices perpendicular to the reference axis can be defined by symmetrically equivalent vertices. However, since D_n polyhedra do not have a symmetry plane, the reference plane for numbering must be arbitrarily defined.

D_3 Polyhedra. The reference axis in a D_3 polyhedron is the C_3 rotational symmetry axis, and because the terminal planes of polyhedral vertices are the same, either can be the preferred terminal plane. To define the reference plane in a D_3 polyhedron, we suggest that it not only contain the reference axis, as required by the previous procedure,[2] but also contain one of the vertices in a terminal plane. If there is only one polyhedral vertex in a terminal plane, the reference plane should also contain a vertex in the adjacent parallel plane of vertices.[5]

Numbering the vertices of these D_n polyhedra is done as with the more symmetric polyhedra[2] (see also above), except, since the polyhedra are chiral, the direction of numbering must be specified in order to distinguish between the enantiomers. We propose to specify the direction of numbering using the criterion of proximity to the reference plane of one of the symmetrically equivalent vertices in the terminal plane of vertices at the end of the reference axis opposite to the preferred terminal plane. If this terminal plane contains only one vertex, then the perpendicular plane of symmetrically equivalent vertices immediately adjacent to it is used. The plane used to choose the direction for numbering is called the directional plane (see Figure 1) and the vertex nearest to the reference plane is called the directional vertex. To illustrate, if a D_3 polyhedron is oriented so that the directional plane is observed from the preferred terminal plane by looking down the reference axis with the reference plane vertical, one of the vertices in the directional plane, i.e., the directional vertex, will be closer to the top of the reference plane than the other vertices. The direction of this vertex from the reference plane, clockwise or anticlockwise, determines the direction of numbering for the polyhedron. With a clock as a model with the reference plane of a D_3 polyhedron bisecting the face at 12 o'clock and 6 o'clock, the three symmetrically equivalent vertices in the

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(2) Casey, J. B.; Evans, W. J.; Powell, W. H. *Inorg. Chem.* **1981**, *20* (5), 1333-1341.

(3) (a) The International Union of Pure and Applied Chemistry. "Nomenclature of Inorganic Chemistry (1970)", 2nd ed.; Butterworths: London, 1971; Rule 7.514, p 63. (b) American Chemical Society. "The Nomenclature of Boron Compounds". *Inorg. Chem.* **1968**, *7* (10), 1945-1964. (c) The International Union of Pure and Applied Chemistry. "Nomenclature of Inorganic Boron Compounds". *Pure Appl. Chem.* **1972**, *30* (3-4), 684-710.

(4) (a) Brown, L. D.; Lipscomb, W. N. *Inorg. Chem.* **1977**, *16* (12), 2989-2996. (b) Bicerano, J.; Marynick, O. S.; Lipscomb, W. N. *Ibid.* **1978**, *17* (7), 2041-2042; **1978**, *17* (12), 3443-3453.

(5) In polyhedra without symmetry planes it is much more convenient to define the reference plane in terms of specific vertices. For application of the criterion of fewest vertices contained in the reference plane, used for polyhedra with symmetry planes,[2] many more considerations would be required in order to define a single plane from the larger number of planes containing the reference axis that can pass through an edge.

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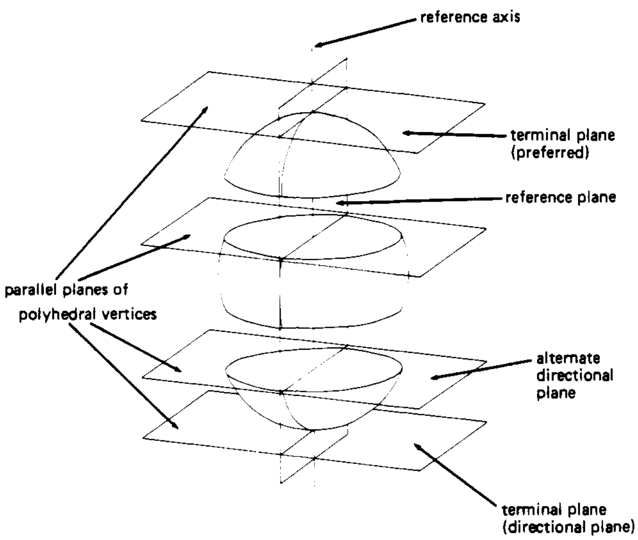


Figure 1. Schematic representation of the features for numbering a polyhedron.

directional plane may occur at 1, 5, and 9 o'clock, for example. Since the vertex at 1 o'clock is closer to the reference plane at the top of the projection (12 o'clock) than the vertex at 9 o'clock, the 1 o'clock vertex is the directional vertex beginning the numbering in that plane and the direction of numbering for the polyhedron is clockwise. If the vertices in the directional plane occur at 3, 7, and 11 o'clock (as in the enantiomer), the 11 o'clock vertex is the directional vertex, which is numbered first in that plane, and the direction of numbering for the polyhedron is anticlockwise. Since the numbering of the vertices in each plane must be in the same direction, the choice of direction for numbering the entire polyhedron is made in the directional plane. Stated more concisely, the direction of numbering for D_n polyhedra is determined by the directional vertex, i.e., the vertex nearest to the reference plane at the top of the projection in the directional plane.[6] We suggest that the *direction of numbering* be specified by prefixing the italic letter *C* or *A* to the descriptor, derived by the method given in our earlier report,[2] according to whether the direction is *clockwise* or *anticlockwise*. Finally, it must be emphasized that the direction of numbering chiral D_n structures is determined by the polyhedron and cannot be changed by the presence of heteroatoms, ligands, or other structural features in specific compounds.

Four D_3 polyhedra are shown in Figure 2. The 17-vertex D_3 polyhedron, structure A in Figure 2, was proposed recently as the basis for the structure of an undecaarsenide (3–) ion.[7] The other three D_3 polyhedra have been discussed by Brown and Lipscomb.[4a]

The reference axis of the 18-vertex D_3 polyhedron shown as structure B in Figure 2 is the C_3 axis passing through the faces defined by the vertices 1,2,3 and 16,17,18. The polyhedron has six sets of three symmetrically equivalent vertices in planes perpendicular to the reference axis. The reference plane, which must contain the reference axis, is arbitrarily defined as passing through a vertex in one of the identical terminal planes, thus defining the preferred terminal plane. In this structure, the reference plane also passes through vertices 5 and 7. This polyhedron is then oriented for numbering by looking down the C_3 axis from the preferred terminal plane and rotating the structure until the vertex in the preferred terminal plane and also in the reference plane is at the top. This vertex is assigned the locant number 1. Before the numbering of other vertices can be done, the direction for numbering must be determined. In this polyhedron this depends on locating the directional vertex, i.e., a vertex in the directional plane on one side of the reference plane that is closer to the top of the reference plane than a vertex on the other side. In structure B(1) of Figure 2, vertex 16 is closer than vertex 18 to the top of the reference plane, and since vertex 16 is clockwise from the reference plane, the polyhedron must be numbered clockwise, as shown. In structure B(2), vertex 16 is anticlockwise from the top of the reference plane; therefore the polyhedron must be numbered anticlockwise and locants are assigned to the vertices as shown.

***D_2* Polyhedra.** Like D_{2d} and D_{2h} polyhedra,[2] D_2 polyhedra have three "highest order" C_2 rotational symmetry axes; thus criteria for selecting one as the reference axis are necessary. For the D_{2d} and D_{2h} polyhedra, this was done[2] by specifying that (a) the reference axis should have a terminal plane with the fewest number of vertices and (b) the reference axis must lie in the reference plane. However, D_2 polyhedra, like other D_n polyhedra, do not have symmetry planes and thus a reference plane must be defined. Hence, for D_2 polyhedra, both a reference axis and a reference plane must be chosen and the requirements introduced for other D_n polyhedra above are not sufficient.

This insufficiency for D_2 polyhedra can be removed by further defining the reference plane as that plane having the fewest number of perpendicular planes defining sets of polyhedral vertices that are either symmetrically equivalent or equivalent in skeletal connectivity (i.e., equivalent in that they have the same number of polyhedral edges associated with the vertex[9]). These additional requirements for choosing a reference plane are included in the full procedure for numbering polyhedra given in the Appendix.

Two D_2 polyhedra have been discussed by Lipscomb et al.[4] Descriptors and our proposed numbering for these polyhedra are shown in Figure 3.

Structure A, Figure 3, has three C_2 rotational symmetry axes, one passing through edges connecting a pair of v^6 polyhedral vertices and two passing through edges connecting pairs of v^5 polyhedral vertices. The latter two axes are eliminated because they lie in arbitrary planes that have more perpendicular planes defined by sets of polyhedral vertices (8 vs. 6). Thus, the C_2 axis passing through edges connecting the pairs of v^6 polyhedral vertices is the reference axis, and the reference plane contains a pair of these vertices.

Each of the three C_2 rotational symmetry axes of structure B, Figure 3, passes through a pair of edges connecting v^6 polyhedral vertices. Citation of symmetrically equivalent or connectively equivalent vertices in parallel planes perpendicular to each of these C_2 axes gives the descriptions

(B-I) $2v^62222v^62v^62v^62v^62222v^6$

(B-II) $2v^6244v^64v^6422v^6$

(B-III) $2v^624v^6444v^622v^6$

(6) An alternative method for determining the direction of numbering was explored, namely, to number clockwise or anticlockwise (*C* or *A*) according to the helicity of the system, i.e., Δ or Λ, respectively. Helicity was identified by rotating the structure around the reference axis and noting whether it turned like a right hand (Δ) or left hand (Λ) screw. For polyhedra A and C in Figure 2, this method gives the same numbering as that favored in the text, but for polyhedra B and D it is the opposite. The method described in the text was selected because it seems much more straightforward and the visualization of helicity in these large polyhedra is not an easy task.

(7) Belin, C. H. E. *J. Am. Chem. Soc.* **1980**, *102* (19), 6036–6040.

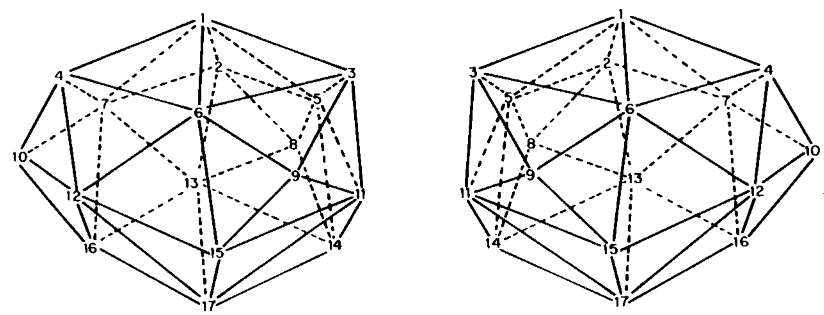
(8) In the notation for the reference axis and reference plane, two or three numbers, separated by commas enclosed in parentheses, indicate polyhedral edges and faces, respectively. Numbers enclosed in square brackets in the notation for the reference plane indicate polyhedral vertices that may not be rigorously in the reference plane but, for numbering purposes, are considered to be in the reference plane.

(9) The fewest number of perpendicular planes was chosen to make the structures easier to visualize from the descriptor.

A. $n = 17$

Descriptors

(1) C-[D_3-($1\upsilon^6 33\upsilon^6 3\upsilon^4 3\upsilon^6 31\upsilon^6$)-$\Delta^{30}$-*closo*] (2) A-[D_3-($1\upsilon^6 33\upsilon^6 3\upsilon^4 3\upsilon^6 31\upsilon^6$)-$\Delta^{30}$-*closo*]

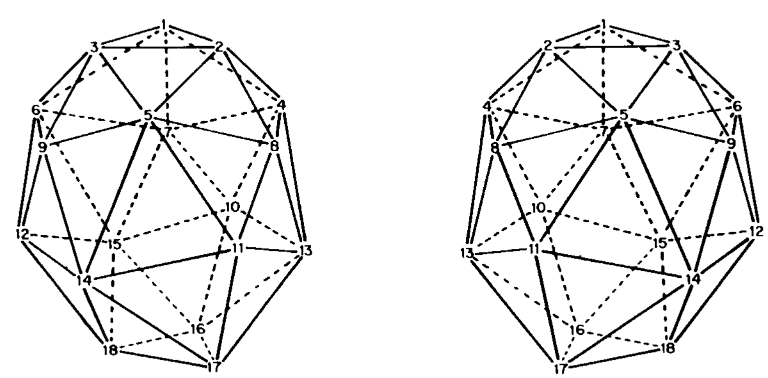


Ref. Axis: 1-17
Ref. Plane: 1-2-6-(8,13)-(12,15)-(13,14)-17
Dir. Plane: 14-15-16
Dir. Vertex: 14

B. $n = 18$

Descriptors

(1) C-[D_3-($33\upsilon^6 333\upsilon^6 3$)-$\Delta^{32}$-*closo*] (2) A-[D_3-($33\upsilon^6 333\upsilon^6 3$)-$\Delta^{32}$-*closo*]

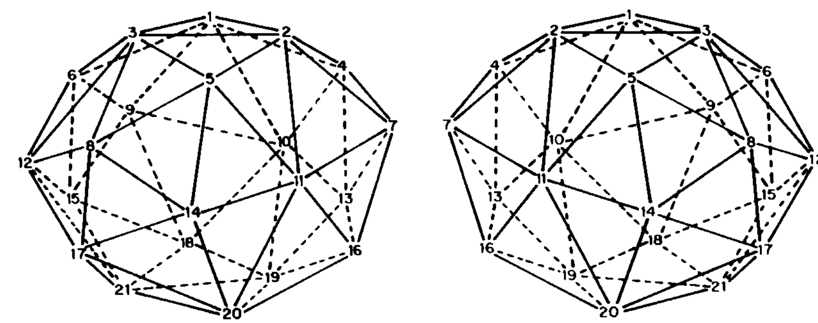


Ref. Axis: (1, 2, 3)-(16,17,18)
Ref. Plane: 1-(2,3)-5-7-(10,15)-(11,14)-(16,18)-(17,18)
Dir. Plane: 16-17-18
Dir. Vertex: 16

C. $n = 21$

Descriptors

(1) C-[D_3-($3\upsilon^6 333\upsilon^6 333\upsilon^6$)-$\Delta^{38}$-*closo*] (2) A-[D_3-($3\upsilon^6 333\upsilon^6 333\upsilon^6$)-$\Delta^{38}$-*closo*]

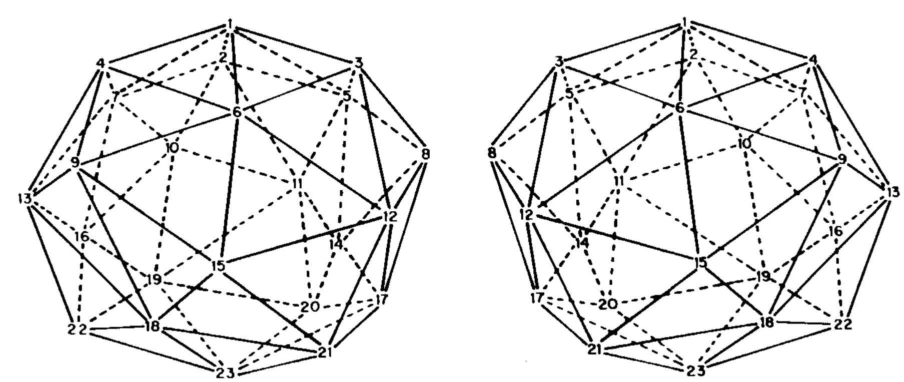


Ref. Axis: (1, 2, 3)-(19,20,21)
Ref. Plane: 1-(2,3)-5-(9,10)-(10,18)-(11,14)-(14,20)-(18,19)-(19,21)-(20,21)
Dir. Plane: 19-20-21
Dir. Vertex: 19

D. $n = 23$

Descriptors

(1) C-[D_3-($1\upsilon^6 33\upsilon^6 33\upsilon^6 33\upsilon^6 31\upsilon^6$)-$\Delta^{42}$-*closo*] (2) A-[D_3-($1\upsilon^6 33\upsilon^6 33\upsilon^6 33\upsilon^6 31\upsilon^6$)-$\Delta^{42}$-*closo*]



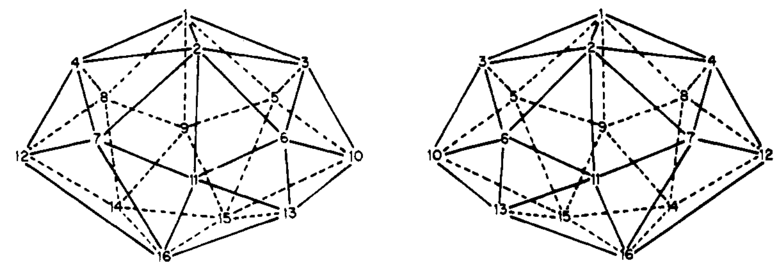
Ref. Axis: 1-23
Ref. Plane: 1-2-6-(10,11)-(11,19)-(12,15)-(15,21)-(18,21)-(19,20)-23
Dir. Plane: 20-21-22
Dir. Vertex: 20

Figure 2. D_3 $[B_nH_n]^{2-}$ polyhedra.[8]

A. $n = 16$

Descriptors

(1) C-[D_2-($2v^6 24422v^6$)-Δ^{28}-*closo*] (2) A-[D_2-($2v^6 24422v^6$)-Δ^{28}-*closo*]

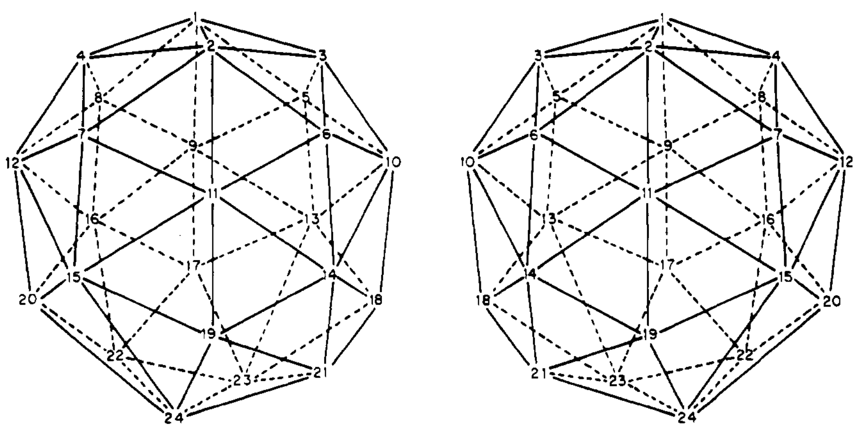


Ref. Axis: (1,2)-(15,16)
Ref. Plane: 1-2-[9]-[11]-(13,16)-(14,15)-(15,16)
Dir. Plane: 15-16
Dir. Vertex: 15

B. $n = 24$

Descriptors

(1) C-[D_2-($2v^6 244v^6 4v^6 422v^6$)-Δ^{44}-*closo*] (2) A-[D_2-($2v^6 244v^6 4v^6 422v^6$)-Δ^{44}-*closo*]



Ref. Axis: (1,2)-(23,24)
Ref. Plane: 1-2-[9]-[11]-[17]-[19]-(21,24)-(22,23)-(23,24)
Dir. Plane: 23-24
Dir. Vertex: 23

Figure 3. D_2 $[B_nH_n]^{2-}$ polyhedra.[8]

C_2 axis B-I is eliminated because it lies in an arbitrary plane that has more perpendicular planes defined by sets of polyhedral vertices. C_2 axis B-II is preferred over C_2 axis B-III because it has vertices with fewer skeletal connectivities in the third plane of polyhedral vertices; i.e., vertices with fewer skeletal connectivities have lower locant numbers.

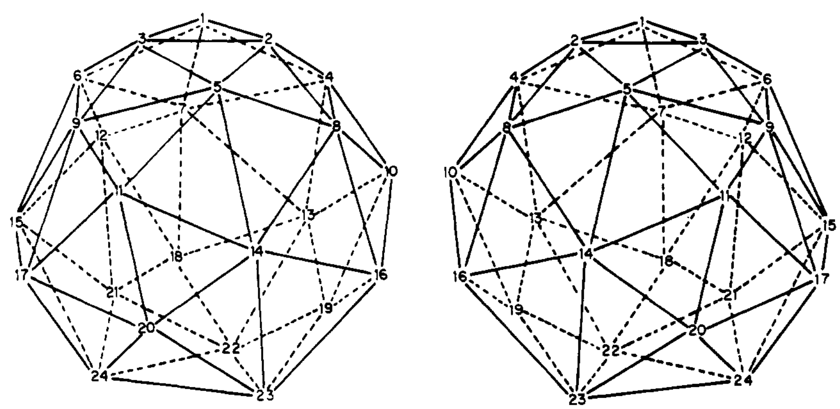
As shown in Figure 3, assignment of the directional descriptors C and A and numbering of the vertices for these D_2 polyhedra follow closely the procedure described above for D_3 polyhedra. However, there is one additional feature of the numbering shown for these D_2 polyhedra that must be explained. In these examples, there are vertices that are very close to the reference plane but are not coplanar. With our models, it is very difficult to detect whether those vertices do in fact lie in the reference plane. If structural models are not constructed with great precision, different assignments for numbering will result in such chiral structures depending on whether the vertex is assumed coplanar with, to the left of, or to the right of the reference plane. In the D_2 structures discussed here, vertices 9 and 11 in structure A (Figure 3) and vertices 9, 11, 17, and 19 in structure B (Figure 3) fall into this category. The same problem can also occur in other D_n and T polyhedra. To avoid this problem, we have chosen to treat these vertices as if they were in the reference plane; thus the numbering in the appropriate plane of symmetrically equivalent vertices begins with vertex 9 in structure A and vertices 9 and 17 in structure B (Figure 3). In the descriptions of the reference plane in the figures, this situation is identified by enclosing such vertices in square brackets.

***T* Polyhedra.** These polyhedra are quite similar to the D_3 polyhedra discussed above. All C_3 rotational symmetry axes are identical, and the reference plane must be defined arbitrarily as described for the D_3 polyhedra. However, for the T polyhedron shown in Figure 4, described by Brown and Lipscomb,[4a] it is also necessary to select a preferred terminal plane. For this, the same criteria can be used as previously described;[2] i.e., the preferred terminal plane has the fewest number of polyhedral vertices and, if these are the same (as in this T polyhedron), the fewer total number of polyhedral edges (skeletal connectivities). The descriptor and numbering of this 24-vertex T polyhedron are shown in Figure 4.

***C*$_s$ Polyhedra.** These polyhedra have a symmetry plane, which must be the reference plane, but they do not have a rotational symmetry axis. Hence, it is necessary to define, arbitrarily, a reference axis. Since there are an infinite number of axes in the reference plane that could be used as a reference

Descriptors

(1) C-[T-($33v^6 3v^6 33v^6 333v^6$)-Δ^{44}-*closo*] (2) A-[T-($33v^6 3v^6 33v^6 333v^6$)-Δ^{44}-*closo*]

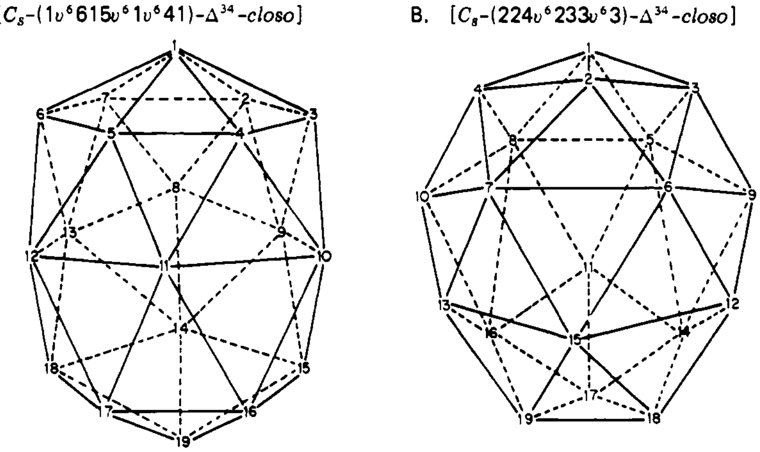


Ref. Axis: (1,2,3)-(22,23,24)
Ref. Plane: 1-(2,3)-5-7-(11,14)-(13,18)-(14,20)-(18,22)-(20,23)-(21,22)-(22,24)-(23,24)
Dir. Plane: 22-23-24
Dir. Vertex: 22

Figure 4. A T $[B_{24}H_{24}]^{2-}$ polyhedron.[8]

Descriptors

A. [C_s-($1v^6 615v^6 1v^6 41$)-Δ^{34}-*closo*] B. [C_s-($224v^6 233v^6 3$)-Δ^{34}-*closo*]



	A	B
Ref. Axis:	1-(14,19)	(1,2)-(17,18,19)
Ref. Plane:	1-(2,7)-(4,5)-8-11-14-(16,17)-19	1-2-(5,8)-(6,7)-11-15-17-(18,19)

Figure 5. C_s $[B_{19}H_{19}]^{2-}$ polyhedra.[8]

axis, a large number of possibilities must be investigated. Even if the choice of reference axis is limited to an axis that passes through a structural element, several possibilities still exist. For example, it could pass through a vertex in the symmetry plane, an edge in the plane, an edge perpendicular to the plane, or a triangular face bisected by the plane. Because only the two C_s polyhedra discussed by Brown and Lipscomb[4a] were used in this initial study, it is premature to suggest definitive rules for numbering such polyhedra. Therefore, the descriptor and numbering of the two C_s polyhedra shown in Figure 5 are rather arbitrary, describing what we consider at this time to be the "best" representation, i.e., the orientation leading to the easiest visualization of the structure and the least ambiguity in assigning coplanar sets of vertices.

For structure A in Figure 5, the arbitrarily defined reference axis passes through vertex number 1 and is perpendicular to the plane defined by the six adjacent five-coordinate vertices (numbers 2–7 in the structure). This choice allows the largest number of vertices to be specified in the first two planes. As for the D_2 polyhedra discussed above, the parallel planes perpendicular to the reference axis are defined by vertices having equivalent skeletal connectivities, which may not be necessarily symmetrically equivalent.

For structure B in Figure 5, the arbitrarily defined reference axis bisects the edge defined by vertices 1 and 2, is perpendicular to the plane defined by vertices 5, 6, 7, and 8, and passes through the face defined by vertices 17, 18, and 19.

Summary

The system developed for describing closed, fully triangulated boron polyhedra having at least one rotational symmetry axis and one symmetry plane[2] has been applied to boron polyhedra belonging to D_n, T, and C_s symmetry point groups. Other C_s polyhedra are being studied and extensions of the system to capped and encapsulating polyhedra are being developed. Modifications to the rules for numbering polyhedral systems have been suggested to handle the chiral D_n and T polyhedra.

Appendix. Procedure for Numbering Closed Polyhedral Frameworks

1. Select the reference axis, i.e., a rotational symmetry axis of highest order that lies in a symmetry plane of the polyhe-

dron. If a further choice is needed, the following should be applied in sequence:

a. The reference axis should have a terminal plane with the fewest number of polyhedral vertices.

b. The reference axis should lie in the reference plane (see principle 3, below).

2. Select the preferred terminal plane of symmetrically equivalent vertices, which defines the preferred end of the reference axis. The preferred terminal plane (a) contains the fewer number of polyhedral vertices, and if these are the same, (b) contains the vertices with the fewer total number of skeletal connectivities, i.e., the fewer number of polyhedral edges associated with the vertex.

If a further choice is needed, the preferred terminal plane is nearer to the parallel plane of symmetrically equivalent vertices preferred by applying criteria 2(a) and 2(b), above, successively to pairs of parallel planes proceeding inward from each terminal plane.

3. Select the reference plane, i.e., a symmetry plane or, if none, an arbitrarily defined plane containing the reference axis and at least one vertex not on the reference axis in a terminal plane or adjacent parallel plane. If there is more than one such plane containing the reference axis, or if selection of a reference axis was not effected by principle 1, above, the reference plane is chosen by applying the following criteria, sequentially, until a decision is made:

a. (i) If the polyhedron has at least one symmetry plane, the reference plane passes through the fewest number of polyhedral vertices. (ii) If the polyhedron does not have a symmetry plane, the reference plane has the fewest number of perpendicular planes defined by sets of polyhedral vertices that are either symmetrically equivalent or connectively equivalent, i.e., that have the same number of polyhedral edges associated with the vertex.

b. The reference plane passes through a polyhedral vertex that is nearer to the preferred terminal plane (see principle 2, above); i.e., polyhedral vertices in the reference plane have lower locant numbers when assigned according to principles 4–6, below.

c. The reference plane passes through a polyhedral vertex with the fewest number of associated polyhedral edges; i.e., polyhedral vertices with the lowest skeletal connectivity in the reference plane have the lower locant numbers when assigned according to principles 4–6, below.

4. Orient the polyhedron, in order to provide a consistent reference point for numbering, by looking down the reference axis from the preferred end (see principle 2, above) and rotating the polyhedron until the reference plane (see principle 3, above) is vertical. If a choice is needed, the preferred orientation has a polyhedral vertex of the preferred terminal plane, or in a parallel plane nearest to it, at the top of the orientation in the reference plane.

5. Determine the direction for numbering, if the reference plane of the polyhedron is *not* a symmetry plane, by noting the direction from the reference plane of the directional vertex, i.e., the vertex in the directional plane nearest to the top of the projection of the reference plane. The directional plane is the terminal plane at the end of the reference axis opposite to the preferred terminal plane, or if this terminal plane contains only one vertex, the directional plane is a parallel plane of polyhedral vertices adjacent to it.

6. Number the vertices of the polyhedron consecutively, clockwise or anticlockwise, starting with vertices in the preferred terminal plane and proceeding successively to succeeding planes of vertices working down the reference axis from the preferred end. The vertices in each plane are numbered in the same direction as the preceding and/or following planes, beginning in each plane with a vertex at the top of the preferred orientation (see principle 4, above), in the reference plane, or with the first vertex encountered, in the direction chosen, or required, for numbering, from the top of the preferred orientation. For chiral polyhedra in which the reference plane is arbitrarily defined, a vertex at the top of the preferred orientation need not be exactly in the reference plane but should be very close.

Notes

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Carbon-13 NMR Spectrum of $[Ir(bpy)_2H_2O(bpy)]Cl_3$: Further Indication of a Monodentate Bipyridine Structure

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Received September 3, 1980

In this report we present NMR spectra of the hydrated tris(bipyridyl)iridium complex whose synthesis and UV–visible spectra were reported in 1977 and whose structure has been debated.[1-3] The most likely candidates for the structure are represented in Figure 1: (A) one which features a monodentate bipyridine and a water bound directly to the metal; (B) a "covalent hydrate" in which water is added across a carbon–nitrogen double bond. In view of the detailed structural information obtained from NMR spectra of transition-metal complexes of 2,2′-bipyridine (bpy) and 1,10-phenanthroline (phen),[4-8] we consider the structural implications of ^1H and

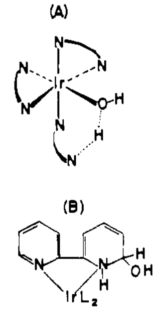

Figure 1. Possible solution structures of $[Ir(bpy)_2H_2O(bpy)]Cl_3$: (A) monodentate bipyridine with H_2O bound to the metal; (B) Covalent hydrate.

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