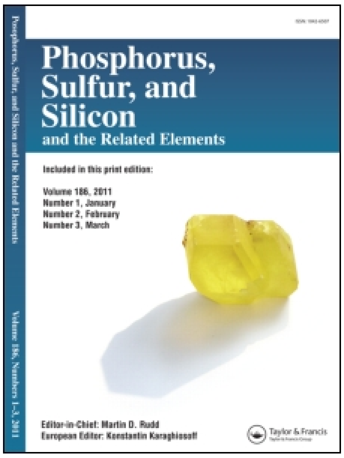

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# Closo Boron Hydrides and Carbon Fullerenes

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# CLOSO BORON HYDRIDES AND CARBON FULLERENES

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The dual (reciprocal) relationship between closo boranes and carbon fullerenes, e.g. between $B_{12}H_{12}^{-2}$ and $C_{20}$, or between a proposed $B_{32}H_{32}$ and $C_{60}$, is extended to plausible multicage closo structures.

*Key words:* Boranes, fullerenes, multicage structures

## INTRODUCTION

Preceding the discovery[1,2] of $C_{60}$ there were several proposals for its possible existence and structure[3-6]. The parallel dual or reciprocal[7] structure related to $C_{60}$ is the proposed icosahedral $B_{32}H_{32}$ borane[8] (or ion). This relationship between fullerenes and closoboranes, which extends to other proposed polyhedral species[9], has been based upon the Descartes-Euler equation[7]

$$P + F = C + 2$$

which relates the number of vertices (points), the number of faces and the number of edges (curves). The replacement of vertices by new faces or of faces by new vertices is the dual (reciprocal) conceptual transformation of, for example, the $C_{60}$ to the $B_{32}$ polyhedron[8,9] (Figure 1). The earlier comparison referred to almost spherical species. Here, we make a modest extension of less spherical molecules which do not have internal bonding contacts and which we conjecture will satisfy the Descartes-Euler equation.

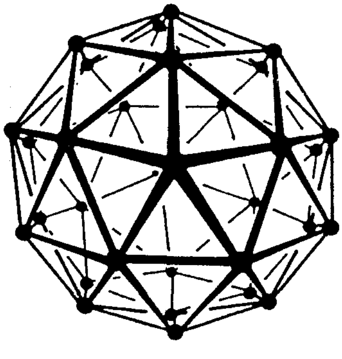

FIGURE 1 The proposed $B_{32}H_{32}$ species of icosahedral symmetry, the dual (reciprocal) polyhedron of $C_{60}$ (buckminsterfullerene). The drawing shows the position of boron each of which has a hydrogen atom extending outward from the center of the polyhedron.

## RESULTS AND DISCUSSION

Of the many ways that polyhedral fragments bind to make a larger molecule[10-13], we begin by examining the joining of near-icosahedral fragments (Table I, Figures 2 and 3).

TABLE I

Multicage polycarbon species and boron analogues

| Carbon species | P | F | C | Symmetry | Boron species | P | F |
|---|---|---|---|---|---|---|---|
| $C_{20}$ | 20 | 12 | 30 | $I_h$ | $B_{12}H_{12}$ | 12 | 20 |
| $C_{35}$ | 35 | 22 | 55 | $D_{5h}$ | $B_{22}H_a$ | 22 | 35 |
| $C_{47}$ | 47 | 30 | 75 | $D_{3h}$ | $B_{30}H_b$ | 30 | 47 |
| $C_{56}$ | 56 | 36 | 90 | $T_d$ | $B_{36}H_c$ | 36 | 56 |

The number of hydrogen atoms may be less (a, b, c, in Table 1) than the number of boron atoms in certain regions where the polyhedral surface is less convex, or even concave as it is in the known $B_{20}H_{16}$ molecule[14]. Of course, the $B_{12}H_{12}$ is a dinegative

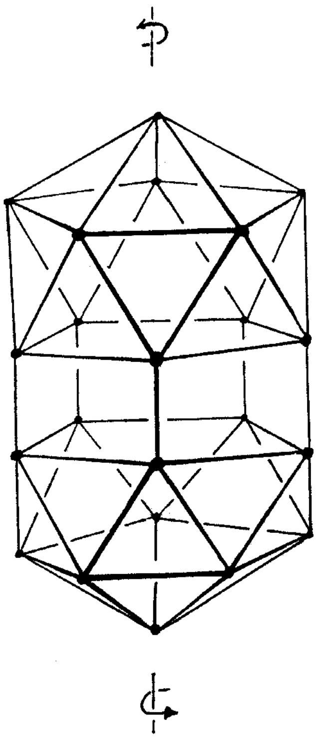

FIGURE 2 A $B_{22}$ polyhedron of $D_{5h}$ symmetry, the dual of a 35-vertex polyhedron ($Zr_{13}C_{22}$ proposal) having 5 square faces. Each vertex is connected to five others.

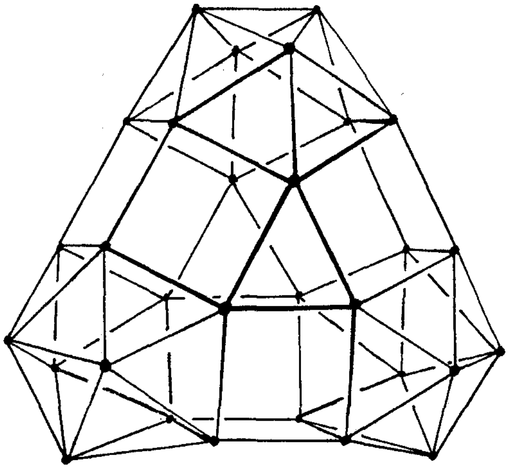

FIGURE 3 A $B_{30}$ polyhedron of $D_{3h}$ symmetry, the dual of a 47-vertex polyhedron ($Zr_{18}C_{29}$ proposal) having 9 square faces. A rotational distortion about the threefold axis gives fully triangulated faces and a dual which is a candidate for a $C_{56}$ polyhedron of $C_3$ symmetry.

ion. However, we leave a study of the probable charges of the other boron species for later. The first three $C_n$ species in Table 1 are like the polyhedra suggested[15] for $Zr_8C_{12}$, $Zr_{13}C_{22}$ and $Zr_{18}C_{29}$, whereas the $C_{56}$ species differs from the $Zr_{22}C_{35}$ analogue of a $C_{57}$ which has internal bonds and does not yield a dual polyhedron satisfying the Descartes-Euler formula. Of course, this difference does not exclude the 57-vertex proposal as a reasonable suggestion.

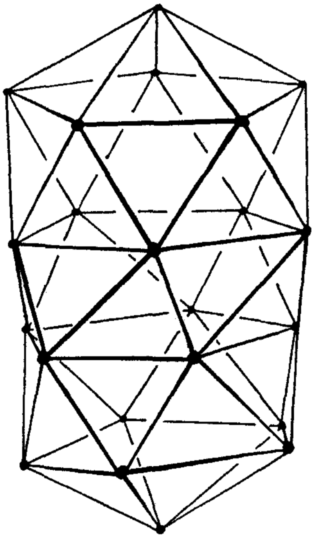

FIGURE 4 A rotational distortion of the $B_{22}$ polyhedron in which the five square faces become two base sharing triangular faces. The dual polyhedron is a candidate for a $C_{40}$ polyhedron of $D_{5d}$ symmetry. Each of the ten nearly equatorial vertices is connected to six other vertices.

The boron polyhedra of the $B_{22}$,$B_{30}$ and $B_{36}$ types have square faces which, at least conceptually, can make a square-diamond collapse[16] (framework rearrangement) as shown in Figure 4. This 22-vertex triangulated polyhedron has 40 faces, and its dual is candidate for a $C_{40}$. A similar twist about the threefold axes of the $B_{30}$ polyhedron gives a molecule which has 56 triangulated faces, and its dual is a possible $C_{56}$. The twist of the tetrahedral $B_{36}$ similarly to lower symmetry (T) yields 68 triangular faces, thus implying the dual $C_{68}$.

Since other types of condensed polyhedral species have been achieved by oxidative coupling[17-20], we suggest that this method be tried on the nido or conjuncto species of borane or carborane, either with single metal or small clusters of metal ions.

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