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JAHN—TELLER EFFECTS IN SOME MOLECULAR POLYHEDRA

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Summary

The configurations of molecular polyhedra, exemplified by polynuclear metal carbonyls, and by boranes, carboranes and their metal ion complexes are interrelated by means of the second order Jahn—Teller effect.

Introduction

The observed structures of polyhedral molecules containing five or more cage atoms were first classified by Williams [1] into three series, *closo*, *nido* and *arachno*, which were subsequently rationalised by Wade [2] on the basis of the number of pairs of cage electrons: n pairs of cage electrons define an $(n-1)$-vertex polyhedron of which $(n-1)$, $(n-2)$, or $(n-3)$ vertices may be occupied, giving rise to the *closo*, *nido* and *arachno* series, respectively. The requirement that an $(n-1)$-vertex polyhedron gives rise to n cage-bonding molecular orbitals, regardless of whether the number of cage atoms participating is $(n-1)$, $(n-2)$ or $(n-3)$, has not been demonstrated in general terms, although the numbers of bonding orbitals have been derived for certain numbers of cage atoms in certain geometries [3,4], using an extended Hückel (EHMO) method: this method [3] does not necessarily predict as the most stable geometry that which is experimentally observed [4].

Four-atom polyhedra do not fit into this general classification [5], adopting tetrahedral structures in the presence of four or six pairs of electrons, and divacant octahedra when there are five or seven such pairs. The relationships between the several structures of four-atom polyhedra may be deduced either explicity or by means of the second order Jahn—Teller effect [6]: if the HOMO and LUMO of a molecular system are of symmetry classes Γ_0 and Γ_1, and binding energies E_0 and E_1 respectively, turn the restoring force constant f_q for a vibration along a coordinate q can for small $(E_1 - E_0)$ become negative, so that the system distorts spontaneously along the coordinate q whose symmetry class is, or is contained in, the direct product $\Gamma_1 \times \Gamma_0$. The purpose of this communica-

TABLE 1

MOLECULAR POLYHEDRA

Number	Polyhedron	Point-group	Symbol	N_0	N_1	N_2	Symmetry classes of bonding combinations	
1	Trigonal bipyramid	D_{3h}	$V4^2,3$	5	9	6	$A_1' + E' + A_2'' + E''$	(6)
2	Square pyramid	C_{4v}	—	5	8	5	$2A_1 + B_2 + 2E_1$	(7)
3	Plane pentagon	D_{5h}	5^2	5	5	2	$A_1' + E_1' + E_2' + A_1'' + E_1''$	(8)
4	—	C_s	—	5	8	5	$5A' + 3A''$	(8)
5	Octahedron	O_h	3^4	6	12	8	$A_{1g} + F_{2g} + F_{1u}$	(7)
6	Pentagonal pyramid	C_{5v}	—	6	10	6	$2A_1 + 2E_1 + E_2$	(8)
7	Plane hexagon	D_{6h}	6^2	6	6	2	$A_{1g} + E_{1g} + E_{2g} + A_{2u} + B_{2u} + E_{2u}$	(9)
8	Trigonal prism	D_{3h}	$4^2,3$	6	9	5	$2A_1' + 2E' + A_2'' + E''$	(9)
9	—	C_s	—	6	10	6	$5A' + 4A''$	(9)
10	Pentagonal bipyramid	D_{5h}	$V4^2,5$	7	15	10	$A_1' + E_1' + E_2' + A_2'' + E_1''$	(8)
11	Hexagonal pyramid	C_{6v}	—	7	12	7	$2A_1 + 2E_1 + B_2 + E_2$	(9)
12	Plane heptagon	D_{7h}	7^2	7	7	2	$A_1' + E_1' + E_2' + E_3' + A_2'' + E_1''$	(10)
13	Capped octahedron	C_{3v}	—	7	15	10	$3A' + 2E$	(7)
14	Capped trigonal prism	C_{2v}	—	7	13	8	$4A_1 + A_2 + 2B_1 + 2B_2$	(9)
15	Square antiprism	D_{4d}	$3^3,4$	8	16	10	$2A_1 + B_2 + E_1 + E_2 + E_3$	(10)
16	Tricapped trigonal prism	D_{3h}	—	9	21	14	$2A_1' + A_2' + 2E' + A_2'' + E''$	(10)
17	Bicapped square antiprism	D_{4d}	—	10	24	16	$2A_1 + B_2 + 2E_1 + E_2 + E_3$	(11)
18	Octadecahedron	C_{2v}	—	11	27	18	$5A_1 + 2A_2 + 3B_1 + 2B_2$	(12)
19	—	C_{5v}	—	11	25	16	$3A_1 + 3E_1 + 2E_2$	(13)
20	Icosahedron	I_h	3^5	12	30	20	$A_g + H_g + F_{1u} + G_u$	(13)

tion is to consider the structures of five-, six-, and seven-atom polyhedra in terms of this second order Jahn—Teller effect.

Results and discussion

The polyhedra to be considered here are set out in Table 1: possibly the most informative description of polyhedra, especially those of low or no symmetry is the numbers of elements of dimensionality j, N_j. In k-dimensional space, the N_j are related by:

$$\sum_{j=0}^{k} (-1)^j N_j = (-1)^k + 1$$

this relationship reduces for closed polyhedra in 3-dimensional space to the familiar relation of Euler:

$$N_0 - N_1 + N_2 = 2 \quad \text{i.e. } V - E + F = 2$$

The basis set for cage bonding is taken as three orbitals per atom, which are in the main factorised into mutually exclusive radial and tangential subsets. For p-block elements, the appropriate orbitals are p_0(radial) and $p_{\pm 1}$(tangential): for d-block elements, radial d_0 always transforms as radial p_0, and $d_{\pm 1}$ always transforms as $p_{\pm 1}$, for any order of rotation axis C_n. The symmetry classes of all the orbital combinations are readily obtained, and by examination of their explicit forms, the number of bonding combinations for each polyhedron can be ascertained: the symmetry classes of these bonding combinations are also set out in Table 1. The *closo* polyhedra (numbers 1, 5, 10) have $(n + 1)$ bonding combinations, those assignable to the *nido* series (numbers 2, 6, 11) have $(n + 2)$ bonding combinations, and members of the *arachno* series (numbers 3, 4, 7, 9, 12) have $(n + 3)$ bonding combinations, all in accordance with the Williams—Wade generalisations. Polyhedron 8, the trigonal prism, is unique among the isogonal polyhedra considered here in having exactly one bonding combination per edge ($N_1 = 9$); polyhedra 13 and 14, the capped octahedron and capped trigonal prism, have the same number of bonding combinations as their uncapped parents, as found [3] for the D_{3h} bicapped trigonal prism and the D_{4h} bicapped cube.

In a five-atom D_{3h} polyhedron, the ordering of the energy levels is:

$$(1a_1')(1a_2'')(1e')(1e'')/(2e')(1a_2')(2e'')$$

so that addition of a further pair of electrons into the LUMO $(2e')$ of a 12-electron species can subject the system to a distortion along a vibrational coordinate of symmetry $E' \times A_2' = E'$: the symmetry classes of the vibrations of a D_{3h} five-atom polyhedron are $2A_1' + 2E' + A_2'' + E''$, and a bend of class E' can convert the D_{3h} structure into C_{4v}. Examples of this are the notional conversion of the trigonal bipyramidal [7] 1,2-$C_2B_3H_5$ to the square pyramidal [8] 1,2-$C_2B_3H_7$; another such pair is represented by the trigonal bipyramidal $Os_5(CO)_{16}$ [9] and the square pyramidal $Os_5(CO)_{15}C$ [10]. In the resulting C_{4v} polyhedron, the ordering is:

$$(1a_1)(1e)(2a_1)(1b_2)(2e)/(1b_1)(3e)(1a_2)$$

and addition of an eighth pair of electrons into $(1b_1)$ may subject the system to a distortion of symmetry $B_1 \times E = E$: of the vibrations of a C_{4v} framework, of symmetry classes $2A_1 + 2B_1 + B_2 + 2E$, either component of the E bend lowers the symmetry from C_{4v} to C_s, as exemplified by B_5H_9 [11] and B_5H_{11} [12].

The ordering of the energy levels in a seven-atom polyhedron of D_{5h} symmetry may be written as:

$$(1a_1')(1e_1')(1a_2'')(1e_1'')(1e_2')/(1e_2'')(2e_1')(2e_1'')$$

and addition of a further pair of electrons into LUMO ($1e_2''$) of a closed 16-electron species (exemplified by 2,4-$C_2B_5H_7$ [13], $B_7H_7^{2-}$ [4], and $(CH_3Ga)C_2B_4H_6$ [14]) may subject the system to a distortion whose symmetry type is contained in $E_2'' \times E_1' = E_1'' + E_2''$. The vibrations of this polyhedron are of symmetry types $2A_1' + 2E_1' + 2E_2' + A_2'' + E_1'' + E_2''$, and these, the bend of E_2'' symmetry can convert the pentagonal bipyramid into a capped trigonal prism of C_{2v} symmetry: if the vertices of the pentagonal bipyramid are numbered in the conventional manner [15], the triangular faces of the trigonal prism are defined by the vertices (1, 2, 3) and (5, 6, 7), and the capped rectangular face by the vertices (1, 3, 7, 5) with vertex 4 becoming the capping vertex. In the capped octahedron (exemplified by $Os_7(CO)_{21}$ [16], and possibly also by B_7Cl_7 [17]), a plausible ordering of the energy levels is:

$$(1a_1)(2a_1)(1e)(3a_1)(2e)/(1a_2)(3e)(4e)$$

Addition of an eighth pair of electrons to the LUMO ($1a_2$) of a 14-electron species may destabilise the system with respect to a distortion of symmetry $A_2 \times E = E$: addition of two further pairs to a 14-electron species may subject the system to a distortion whose symmetry class is contained in $E \times E = A_1 + A_2 + E$. The vibrations of a capped octahedron are of symmetry classes $3A_1 + 2A_2 + 5E$: of these, a bend of symmetry class E can convert the capped octahedron into a pentagonal bipyramid (whose axial vertices are numbers 2 and 6 of the capped octahedron), while one of the A_1 modes can give rise to a hexagonal pyramid: in each of these perturbations from the capped octahedron, the polyhydron predicted is one of those set out in Table 1. Representative of the hexagonal pyramid is $(\eta^6\text{-}C_6H_6)Cr(CO)_3$ [18]: while no example of the capped trigonal prism has yet been identified, plausible examples of the capped octahedron to pentagonal bipyramid transformation would be $Os_7(CO)_{21} \rightarrow Os_7(CO)_{21}^{2-}$ and $B_7Cl_7 \rightarrow B_7Cl_7^{2-}$. It is perhaps noteworthy that the planar geometries, idealised in D_{5h} for five vertices and D_{7h} for seven vertices, which appear to be exemplified only by such species as $C_5X_5^-$ and $C_7X_7^+$, cannot be attained by Jahn—Teller distortions of three dimensional structures: in a similar way, the 12-electron species $(CH)_4$ appears to be of lower potential energy in the planar than in the tetrahedral configuration [19], despite the tetrahedral configuration adopted by other 12-electron M_4 species (M = Si, Ge, Sn, Pb, P, As).

For a six-atom polyhedron of C_{5v} symmetry, the ordering of the energy levels is:

$$(1a_1)(1e_1)(2a_1)(1e_2)(2e_1)/(2e_2)(3e_1)(1a_2)$$

and addition of two further electrons to the LUMO ($2e_2$) of a 16-electron species may induce a distortion along a vibration whose symmetry classes contained in $E_2 \times E_1 = E_1 + E_2$. The vibrations of the polyhedron span the symmetry classes

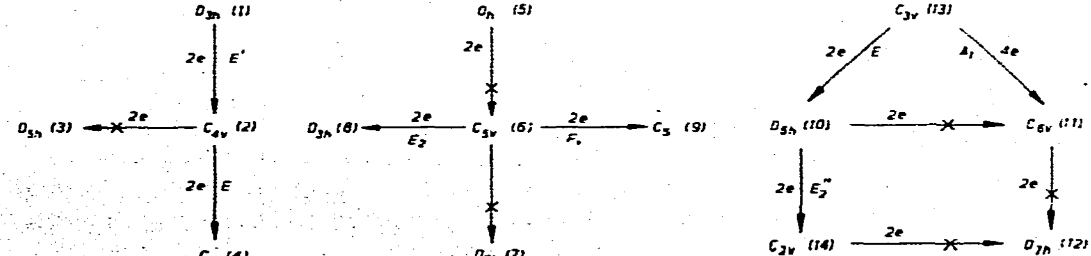
$2A_1 + 2E_1 + 3E_2$, and of these a bend of class E_1 converts the C_{5v} structure to C_s (polyhedron 10), while a bend of class E_2 converts C_{5v} to the D_{3h} trigonal prism. C_{5v} is typified by B_6H_{10} [20], and it is not impossible [21] that the C_s structure is adopted by B_6H_{12}. Known trigonal prismatic species containing 18 cage electrons include Te_6^{6+} [22] and $Rh_6(CO)_{15}C^{2-}$ [23]: analogous species in higher oxidation levels, having correspondingly different configurations, may await preparation. Addition of either two or four further electrons to a 14-electron O_h polyhedron e.g. $B_6H_6^{2-}$ [24] or $Os_6(CO)_{18}^{2-}$ [25] the order of whose energy levels is:

$$(1a_{1g})(1f_{1u})(1f_{2g})/(1f_{2u})(1f_{1g})(2f_{1u})(1e_g)$$

will populate $(1f_{2u})$: consequently the system should be subject to a first order distortion along a non-totally symmetric vibrational coordinate whose symmetry class is contained in $[F_{2u}]^2 = A_{1g} + E_g + F_{1g} + F_{2g}$. The molecular vibrations of such a six-atom O_h polyhedron are of symmetry classes $A_{1g} + E_g + F_{2g} + F_{1u} + F_{2u}$: both of the allowed vibrations (E_g and F_{2g}) maintain the initial centrosymmetry, so that none of the other polyhedra in Table 1 can be achieved in a first-order distortion from O_h. A distortion along the F_{2g} coordinate would reduce the symmetry to D_{2h} while the two components of the E_g distortion would reduce the symmetry to D_{4h} and D_{2h} respectively, but in neither case would there be an increase in the number of bonding electrons. As with the five- and seven-atom polyhedra, the planar D_{6h} structure, exhibited only by benzene [26] and its analogues, cannot be attained by Jahn—Teller distortion of any of the other six-atom geometries. The distortions of five-, six-, and seven-atom polyhedra are summarised in Scheme 1.

For the larger polyhedra, especially those of low symmetry, it is not possible to establish, even roughly, the order of the energy levels merely qualitatively. Calculations of these levels have however been published for polyhedra of nine vertices in D_{3h} using the EHMO method [27] and for ten and twelve vertices in D_{4d} and I_h respectively [28] using an SCF method: the SCF calculations also show that in $B_{10}H_{10}^{2-}$ and $B_{12}H_{12}^{2-}$ the gap between the HOMO and LUMO is large, so that these systems are stable to Jahn—Teller distortions, but that the gap between the lowest two unoccupied orbitals is small, so that $B_{10}H_{10}^{4-}$ and $B_{12}H_{12}^{4-}$ may be unstable to such distortion.

SCHEME 1. JAHN—TELLER DISTORTIONS IN FIVE-, SIX- AND SEVEN-ATOM POLYHEDRA (POLYHEDRA ARE NUMBERED AS IN TABLE 1)



The molecular vibrations of a square antiprismatic M_8 polyhedron span the symmetry classes $2A_1 + B_1 + B_2 + 2E_1 + 3E_2 + 2E_3$. Of these, the B_2 mode can convert the square antiprism into the bicapped trigonal prism (C_{2v}): if the symmetries of the appropriate energy levels support a second-order Jahn—Teller distortion along such a vibrational coordinate, then an example is furnished by the notional reduction of the *closo* ion $B_8H_8^{2-}$, which probably has D_{4d} symmetry in solution [4], to the *nido* species B_8H_{12}, whose boron framework approximates to a bicapped trigonal prism [29]. For an M_9 polyhedron in D_{3h}, a plausible ordering of the cage energy levels is [27]:

$$(1a_1')(1e')(1a_2'')(2a_1')(1e'')(2e')(1a_2')/(2a_2'')(2e'')(1a_1'')$$

so that addition of two further electrons into the LUMO ($2a_2''$) of a 20-electron species may give rise to distortion along a vibration of symmetry $A_2'' \times E'' = E'$. The vibrations of such a polyhedron are of symmetry classes $3A_1' + A_2' + 4E' + A_1'' + 2A_2'' + 3E''$: of these, one of the E' bends can convert the *closo* tricapped prism into the *nido* monocapped square antiprism (C_{4v}). An example of this transformation is provided by $B_9H_9^{2-}$ [27] and B_9H_{13}, whose boron framework in its mono-adduct with acetonitrile is a somewhat distorted monocapped square antiprism [3]. Another of the E' bends can give rise to the *arachno* di-vacant octadecahedron, typified by B_9H_{14} [31] and occasioned by addition of two further pairs of electrons into $2a_2''$ and $2e''$ ($E'' \times A_1'' = E'$).

For a bicapped square antiprismatic M_{10} polyhedron (D_{4d}) a plausible ordering is:

$$(1a_1)(1b_2)(1e_1)(1e_2)(1e_3)(2a_1)(2e_1)/(2e_2)(1b_1)(3e_1)$$

and addition of either two or four further electrons to a 22-electron species, exemplified by $B_{10}H_{10}^{2-}$ [32] may subject the system to a distortion along a vibration whose symmetry is $E_2 \times B_1 = E_2$. Although such a vibration can convert the D_{4d} structure into a di-vacant icosahedron, exemplified by the *arachno* ion $B_{10}H_{14}^{2-}$ [33], the *nido* univacant octadecahedron, typified by $B_{10}H_{14}$ [34] cannot be attained along any of the vibrations of the D_{4d} polyhedron. The vibrations of the C_{2v} eleven-vertex octadecahedron span the symmetry classes $9A_1 + 5A_2 + 7B_1 + 6B_2$, and of these, one of the B_2 modes can convert the C_{2v} polyhedron into the univacant icosahedron of C_{5v} symmetry: an example of this transformation is the notional conversion of the *closo* $(MeC)_2B_9H_9$ [35] to the *nido* $C_2B_9H_{11}^{2-}$, structurally characterised in its metal-ion complexes [36—39]: the distortions occasioned by the electronic structures of the metal-ions in these dicarbolide complexes have been discussed previously [40]. The structure of the anion $B_{11}H_{11}^{2-}$ is not unambiguously known, but its solution NMR spectra have been interpreted [41] in terms of a C_{2v} ground state in which all the boron atoms are rendered equivalent via intermediates of approximately C_{5v} symmetry, suggesting that in this species, for which no SCF calculation has yet appeared the HOMO—LUMO gap is small (cf. MX_5 [42]): in its reduction product $B_{11}H_{13}^{2-}$, the B_{11} framework is a C_{5v} univacant icosahedron [43].

The icosahedral framework of twelve atoms occurs in $B_{12}H_{12}^{2-}$ [44] and in a number of metal borides [45—47] as well as in B_4C ($\equiv B_{12}C_3$) [48] and in α-tetragonal [49] and α-rhombohedral [50] boron. The ordering of the energy levels is [3]:

$(1a_g)(1f_{1u})(1h_g)(1g_u)/(1g_g)(1h_u)(2f_{1u})$

and addition of two further electron to a 26-electron species may subject the systems to a distortion whose symmetry class is contained in $G_g \times H_u = F_{1u} + F_{2u} + G_u + 2H_u$. The vibrations of this polyhedron span the symmetry classes $A_g + G_g + 2H_g + F_{1u} + F_{2u} + G_u + H_u$: so that a range of univacant thirteen-vertex polyhedra are accessible.

Finally, some apparent exceptions to the William—Wade generalisation are noted: in $Pt_6(CO)_{12}^{2-}$, the Pt_6 group is expected to be octahedral, but is found [51] to approximate toa D_{3h} prism, but with the triangular faces slipped: in the carbide $Rh_8(CO)_{19}C$, the 18-electron framework might be expected to adopt a square antiprismatic structure, but in fact the Rh_8 group is found [52] to be a very irregularly bicapped trigonal prism. The 22-electron ion Bi_9^{5+} may be expected to adopt a *nido* structure, the monocapped square antiprism: however it is found to adopt a tricapped prismatic structure in both $(Bi^+)(Bi_9^{5+})(HfCl_6^{2-})_3$ [53] and in $(Bi_9^{5+})_2(BiCl_5^{2-})_4(Bi_2Cl_8^{2-})$ [54], although in the latter it could plausibly be described as a capped antiprism. EHMO calculations [55] indicate that this D_{3h} ion has eleven rather than ten bonding orbitals: however the quantitative and hence predictive reliability of this calculation is possibly diminished by its lack of a large HOMO—LUMO gap, as found by more sophisticated methods [28]. The icosaborane $B_{20}H_{20}$ is found [28] not to be a dosed shell species when dinegative, $B_{20}H_{20}^{2-}$, as with the smaller $(BH)_n^{2-}$ polyhedra, but only when tetranegative, $B_{20}H_{20}^{4-}$.

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