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The heptakisoctahedral group and its relevance to carbon allotropes with negative curvature

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We introduce the pollakispolyhedral groups and describe in detail the representational structure of PSL(2, 7) or ^{7}O, the automorphism group of the Klein graph composed of 56 trivalent vertices arranged in 24 heptagonal faces. Leapfrog and quadruple transformations of the graph are described and their eigenvalue spectra derived. Considered as carbon frameworks on the "*plumber's nightmare*" surface these chiral structures exhibit significant steric strain which prevents the molecular realisation of the Klein symmetry.

1. Introduction

The most familiar applications of group theory in chemistry use point groups which describe the spatial symmetry of molecules [20,21]. In this context the groups of the regular polyhedra are of particular interest because of their high symmetry. This paper presents a novel view of these regular polyhedral groups as subgroups of larger permutation groups, which themselves are subgroups of the corresponding symmetric groups S_n. This approach uses classical mathematics, some dating back to the 19th century, which is generally unfamiliar to chemists and physicists. Of particular relevance to chemists is the suggestion [22] that these groups may be used to describe carbon allotrope structures with negative curvature constructed from hexagons and heptagons of sp^2-hybridized carbon atoms [22,23,28].

2. The three pollakispolyhedral permutation groups: ^{5}T, ^{7}O, ^{11}I

The elements of the point groups used to describe the symmetry of objects in three-dimensional space include only the standard symmetry operations, namely the identity (E), proper rotations (C_n), reflections (σ), inversion (i), and improper rotations (S_n). The concepts of group theory can also be applied to more abstract sets

such as the permutations of a set of n objects. A set of permutations of n objects with the structure of a group is called a permutation group of degree n, and the number of permutations in the set is the order of the group [2]. The standard operations in symmetry point groups can be considered to be special types of permutations applied to discrete sets of points or lines such as the vertices or edges, respectively, of polyhedra. In this context, symmetry point groups appear as special cases of permutation groups.

Let G be a permutation group acting on the set X and let g be any operation in G and x be any object in the set X. The subset of X obtained by the action of all operations in G on x is called the orbit of x. A permutation group is transitive on a set if that set is a single orbit of the group.

Let A and X be two elements in a group G. Then $X^{-1}AX = B$ is equal to some element in the group, B is called the similarity transform of A by X, and A and B are said to be conjugate. The complete set of elements of a group that are conjugate to one another is called a class (or, more precisely, a conjugacy class) of the group G. A normal subgroup N of G is a subgroup that consists only of *entire* conjugacy classes of G. A normal chain of a group G is a sequence of normal subgroups going from G down to the trivial group C_1 consisting only of the identity. A simple group is a group having no normal subgroups other than the identity group. Simple groups correspond to the transitive groups of "highest symmetry" and are particularly important in the theory of finite groups. The only nontrivial simple group found as a symmetry point group is the icosahedral pure rotation group I of order 60.

The concept of pollakispolyhedral[1] groups arises from an alternative definition of the icosahedral rotation group I. Thus, consider a prime number p and let F_p denote the finite field of p elements, which can be represented by the p integers $0, \ldots, p-1$; larger integers can be converted to an element in this finite field by dividing by p and taking the remainder (i.e., the number is taken "mod p"). For example, the finite field F_5 contains five elements represented by the integers 0, 1, 2, 3 and 4 and other integers are converted to one of these five integers by dividing by 5 and taking the remainder. The group SL$(2, p)$ is defined to be the group of all 2×2 matrices with entries in F_p having determinant 1. It has order $p(p^2-1)$ [10]. The subgroup PSL$(2, p)$ for odd p of SL$(2, p)$ is defined to be the quotient group of SL$(2, p)$ modulo its centre. In the case of the groups SL$(2, p)$ where $p \geqslant 5$, the centre has only two elements and the quotient group PSL$(2, p)$ is a simple group. The group PSL$(2, 5)$ contains 60 elements and is isomorphic to the icosahedral pure rotation group I.

An important property of the PSL$(2, p)$ permutation groups for the three primes $p = 5$, 7, and 11 is that they can function as transitive permutation groups on sets of either p or $p+1$ objects, a property not shared by the groups for primes larger than 11, where the corresponding PSL$(2, p)$ permutation groups are transitive on sets of $p+1$ objects, but not on sets of p objects. The properties of the three PSL$(2, p)$ groups of

[1] We have taken the prefix *pollakis* from the Greek $\pi o\lambda\lambda\alpha\kappa\iota\varsigma$ meaning "many times", in analogy to prefixes such as bis, tris, tetrakis, etc.

Table 1
The three pollakispolyhedral groups (G is the polyhedral subgroup).

PSL(2, p)	Symbol	Order	Conjugacy classes	G
5	${}^5T$	60	$E + 12C_5 + 12C_5^2 + 20C_3 + 15C_2$	T
7	${}^7O$	168	$E + 24C_7 + 24C_7^3 + 56C_3 + 21C_2 + 42C_2$	O
11	${}^{11}I$	660	$E + 60C_{11} + 60C_{11}^2 + 110C_3$ $+ 55C_2 + 132C_5 + 132C_5^2 + 110C_6$	I

interest in this paper (i.e., $p = 5$, 7, and 11) are summarized in table 1. All three of these groups are simple groups.

In the case of PSL(2, 5) the transitive permutations on five and six objects can be visualized as permutations of parts of an icosahedron, since PSL(2, 5) is isomorphic to the pure icosahedral rotation group. Thus, the PSL(2, 5) group acts transitively on the *six* diameters of an icosahedron, where a diameter of an icosahedron is defined as a line drawn between a pair of antipodal vertices. The transitive permutations of PSL(2, 5) on *five* elements of an object of icosahedral symmetry can be visualized by taking the dual of the icosahedron, namely the regular dodecahedron, and partitioning its 20 vertices into five sets of four vertices each so that each set of four vertices forms a regular tetrahedron (figure 1). The PSL(2, 5) permutation group viewed as the icosahedral pure rotation group or as the isomorphic alternating group A_5 permutes transitively these five subtetrahedra of the regular dodecahedron. This relates to the fact that the tetrahedral rotation group T is a subgroup of index 5 of the icosahedral rotation group I, and arises by removal from I of all elements of period 5 (i.e., the five-fold rotations C_5) while retaining the group structure. Conversely, the icosahedral rotation group can be constructed by adding a generator of period 5 to the tetrahedral rotation group. This generation of the icosahedral group from the tetrahedral group can be indicated by the alternative designation of $I = \mathrm{PSL}(2, 5)$ as the *pentakistetrahedral group* or ${}^5T$. The icosahedral group is thus the first member of a series of three pollakispolyhedral groups which are isomorphic with the three groups PSL(2, p) (for $p = 5$, 7, and 11). Paradoxically, whereas the icosahedral group is the *largest* of the regular polyhedral groups and indeed the largest nontrivial symmetry point group, the isomorphic PSL(2, 5) group is the *smallest* of the three pollakispolyhedral groups (table 1). The second such pollakispolyhedral group, namely the heptakisoctahedral group [18,24,30] or ${}^7O$, will be considered in detail in this paper.

Geometrical models, albeit less obvious, are available for the PSL(2, 7) or heptakisoctahedral group of order 168, which depict its transitive permutations on sets of 7 and 8 objects, although the heptakisoctahedral group is no longer isomorphic with any symmetry point group in three dimensions. A set of seven objects permuted transitively by the heptakisoctahedral group can be obtained from the seven-point-seven-line geometry presented in D_3 symmetry when a circle is inscribed into an equilateral triangle with its three altitudes [26] (figure 2). Thus the permutations of the seven vertex

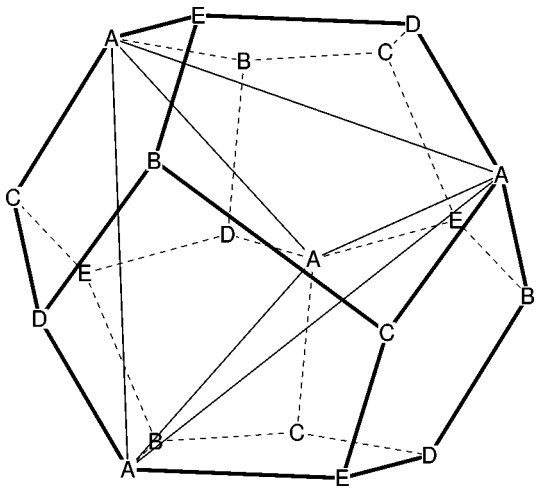

Figure 1. Five regular tetrahedra in a regular dodecahedron.

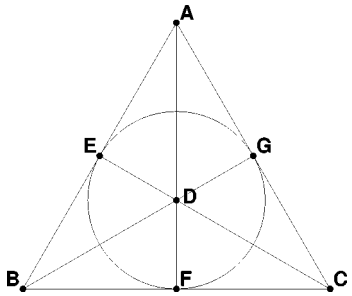

Figure 2. Seven-point-seven-line geometry.

labels that preserve the seven collineations (AEB, BFC, AGC, ADF, BDG, CDE, EFG) form the heptakisoctahedral group. Note that in this presentation the inscribed circle is treated on an equal footing with the six straight lines forming the three edges and the three altitudes of the triangle. Eight objects permuted transitively by the heptakisoctahedral group are the vertex labels of a cuboid of D_2 point group symmetry which give a set of 168 nonsuperimposable cuboids. In analogy to the relationship between the tetrahedral and pentakistetrahedral (= icosahedral) group discussed above, the octahedral rotation group O can be generated from the heptakisoctahedral group ${}^7O$ by deleting all seven-fold symmetry elements.

The final pollakispolyhedral group is the PSL(2, 11) or undecakisicosahedral group of order 660, conveniently abbreviated as ${}^{11}I$. This group has the icosahedral group as a subgroup of index 11. Kostant [25] has suggested that this group is relevant to understanding some aspects of the permutational symmetry of the truncated icosahedral structure of C_{60}. The undecakisicosahedral group is considerably more complicated than ${}^7O$ and will not be discussed in detail in the present paper.

The existence of only three PSL(2, p) groups (p = 5, 7, and 11) that can act transitively on sets of cardinality p or $p + 1$ appears to be intimately related to the existence of only three rotation groups for the Platonic polyhedra in three-dimensional space [26].

3. The heptakisoctahedral group

In this section we describe in some detail the structure and representations of ${}^7O$. The group has 168 elements with orders 1, 2, 3, 4 and 7. These symmetry elements can most conveniently be represented as automorphisms on the heptagonal faces in the 56-vertex polyhedron shown in figures 3a and 3b.

A C_7 generator can be obtained by performing a sevenfold rotation around the central heptagon. This leads to the following automorphism:

$$C_7 \rightarrow (1), (23), (24), (2, 3, 4, 5, 6, 7, 8), (9, 10, 11, 12, 13, 14, 15), (16, 18, 20, 17, 19, 21, 22). \quad (1)$$

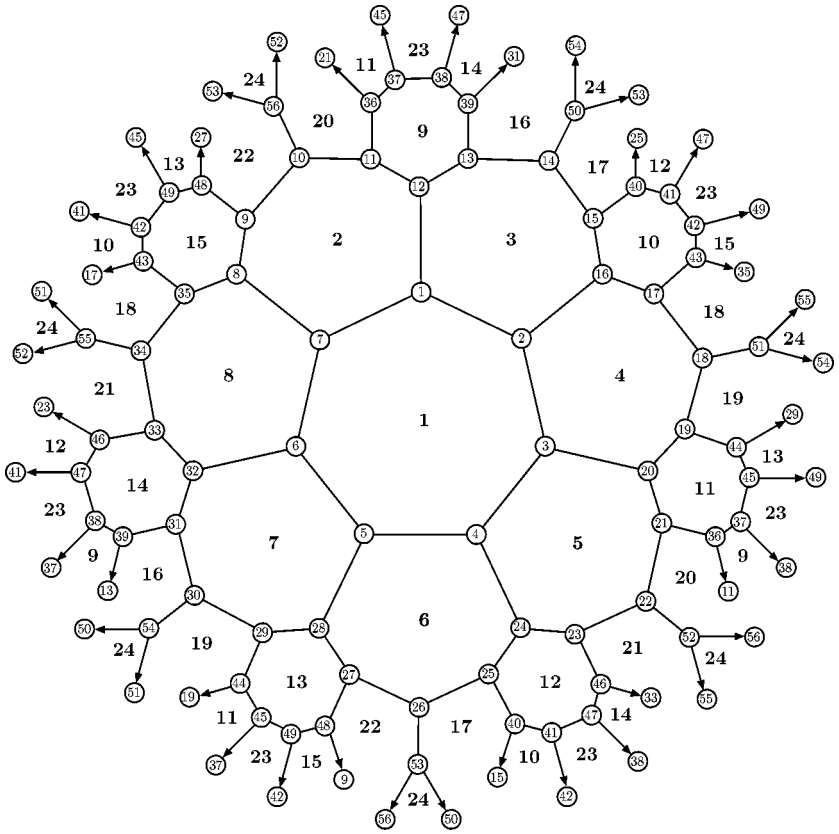

Figure 3a. Schlegel-like diagram of the 56-vertex Klein polyhedron viewed from an inner heptagonal face.

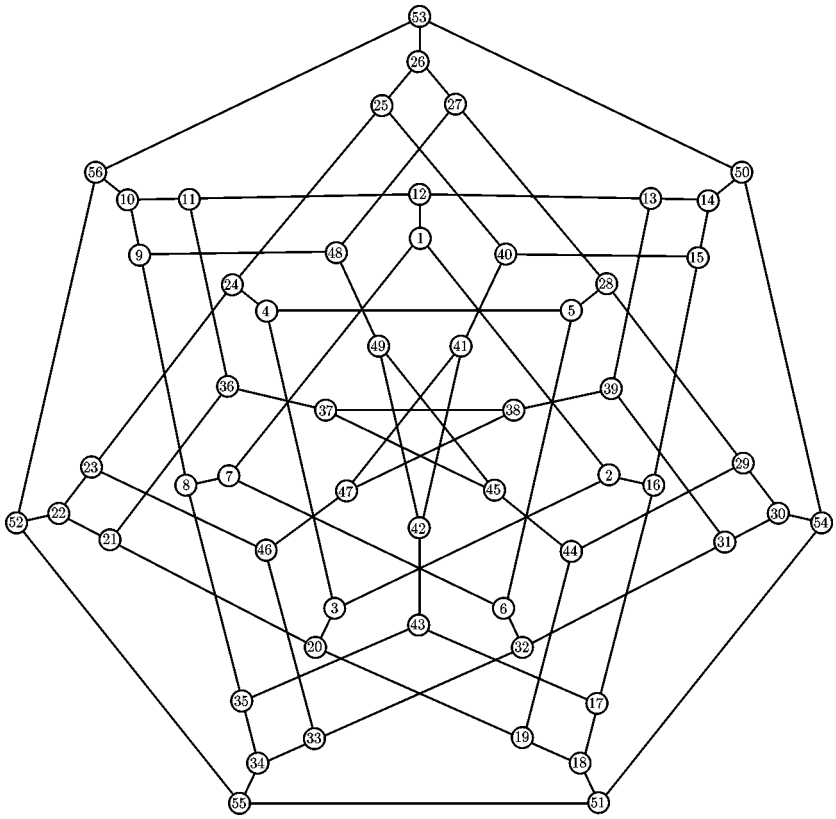

Figure 3b. The same Schlegel-like diagram as in figure 3a but viewed from an outer heptagonal face.

Here the mapping is denoted as a cyclic permutation of all heptagons: 1, 23 and 24 are invariant, 2 goes to 3, 3 goes to 4, etc. This permutation conserves all bond pairs and therefore corresponds to an automorphism. We will refer to this generator as a C_7 rotation, although it should be clear that it cannot be represented by an actual rotation in ordinary space. Each C_7 generator leaves three faces of the polyhedron invariant. In this way the 24 heptagons give rise to eight rotation elements of this type.

The trivalent vertices are stabilised by threefold symmetry elements. We choose as a C_3 generator the threefold rotation through the common vertex of heptagons 1, 2, 3:

$$C_3 \rightarrow (1,2,3),(4,8,9),(5,15,16),(6,22,17),\\ (7,20,10),(11,18,14),(12,13,24),(19,21,23). \qquad (2)$$

Under this operation two vertices remain invariant: $(1,2,3)$ and $(6,22,17)$, with vertex numbers **1** and **26**, respectively. Such a pair of vertices will be called *antipodal*. In this way the 56 vertices give rise to 28 antipodal pairs, and an equal number of C_3 elements.

The two generators can now be combined to yield C_2 and C_4 operations, in the following way:

$$C_2 = C_7 \times C_3, \qquad C_4 = C_7^4 \times C_3. \tag{3}$$

The C_2 element in this equation can be associated with a twofold rotation through the common edge of heptagons 1 and 3. In this way three adjacent symmetry elements may be combined to yield the unit element, $C_7 \times C_3 \times C_2 = E$, in exactly the same way as for neighbouring C_5, C_3, and C_2 axes in the icosahedron [19]. The twofold rotation is seen to leave four edges invariant: (1–3), (11–20), (12–14), (15–18). In this way the 84 edges of the polyhedron give rise to 21 twofold symmetry elements:

$$\begin{aligned} C_2 \rightarrow\ & (1,3),(2,4),(5,9),(6,16),(7,17),(8,10),(11,20),(12,14), \\ & (13,24),(15,18),(19,22),(21,23). \end{aligned} \tag{4}$$

Finally, the fourfold rotation groups the heptagons together in six 4-cycles:

$$\begin{aligned} C_4 \rightarrow\ & (1,6,17,3),(2,7,22,16),(4,5,12,10),(8,13,24,9), \\ & (11,21,23,18),(14,15,19,20). \end{aligned} \tag{5}$$

The squares of the fourfold generators correspond to the C_2 elements, so that there will be 21 of them too.

In table 2 we show the character table of ${}^7O$, taken with some revision of notation form the *Atlas of Finite Groups* [11]. The symmetry elements constitute six classes. Note that the C_7 operations are in two separate classes, as are the C_5 elements in the icosahedral group. There are six irreducible representations which we have labeled A, T_1, T_2, I, J, K. As is common practice in the chemical literature, the letters refer to the representational degeneracies: A means nondegenerate and T triply degenerate. Since G and H in the icosahedral group usually refer to fourfold and fivefold degeneracies we have continued in alphabetical order as I, J, and K for sixfold, sevenfold, and eightfold degeneracies, respectively.

The T_1 and T_2 representations are complex conjugate, inducing a common sixfold degenerate representation in the covering symmetric group of rank seven. The icosahedral group has a somewhat similar pair of T-representations, which are however irrational conjugates connected by $\sqrt{5} \rightarrow -\sqrt{5}$.

Table 2
Character table for ${}^7O$.

		E	$21C_2$	$56C_3$	$42C_4$	$24C_7$	$24C_7^3$
Γ_1	A	1	1	1	1	1	1
Γ_2	T_1	3	-1	0	1	$\frac{1}{2}(-1+\mathrm{i}\sqrt{7})$	$\frac{1}{2}(-1-\mathrm{i}\sqrt{7})$
Γ_3	T_2	3	-1	0	1	$\frac{1}{2}(-1-\mathrm{i}\sqrt{7})$	$\frac{1}{2}(-1+\mathrm{i}\sqrt{7})$
Γ_4	I	6	2	0	0	-1	-1
Γ_5	J	7	-1	1	-1	0	0
Γ_6	K	8	0	-1	0	1	1

It is clear from the drawing that our polyhedral graph has a further reflection symmetry (see also [12]), which can be generated by a vertical symmetry plane:

$$\sigma_v \rightarrow (1),(6),(9),(18),(23),(24),(2,3),(4,8),(5,7),\\ (10,15),(11,14),(12,13),(16,20),(17,22),(19,21). \quad (6)$$

This generator is an odd permutation which will double the parent group. The product group will be denoted as ${}^7O_d$, since its construction is similar to the extension of rotation groups by dihedral symmetry planes. The symmetry plane contains the poles of two sevenfold axes. Since there are eight C_7 elements and each heptagon is cut by seven planes the total number of planes equals $7 \cdot 8/2 = 28$.

The combination of the C_7 generator with a symmetry plane that does not pass through its poles yields another type of symmetry element, which we will denote as S_6, since it is a cyclic element of order 6 which is similar to an improper sixfold rotation axis in the point groups:

$$S_6 = \sigma_v' \times C_7. \quad (7)$$

Let σ_v' be the symmetry element that bisects the edge between heptagons 2 and 3. Then one obtains

$$S_6 \rightarrow (1,9,17,19,21,15),(2,3,16,24,18,8),\\ (5,23,6,11,12,13),(4,14,22),(7,20,10). \quad (8)$$

The square of this element is a threefold axis. There is thus one S_6 axis along each of the 28 threefold directions. The inverse elements S_6^5 belong to the same symmetry class.

Finally, the combination of the σ_v and C_4 generators yields a cyclic element of order 8, which we will denote as S_8:

$$S_8 = \sigma_v \times C_4. \quad (9)$$

One has

$$S_8 \rightarrow (1,6,22,20,11,19,16,3),(2,5,13,24,9,4,7,17),\\ (8,12,15,21,23,18,14,10). \quad (10)$$

These elements are associated with the fourfold axes, so that there will be 21 of them. The resulting 21×4 improper rotations form two classes of 42 elements, containing S_8, S_8^7, and S_8^3, S_8^5, respectively.

When constructing the character table for the full group it must be noted that the two classes of sevenfold elements are merged by the reflection elements. The class structure of ${}^7O_d$ thus corresponds to

$${}^7O_d = E + 21C_2 + 56C_3 + 42C_4 + 48C_7 + 28\sigma_v + 56S_6 + 42S_8 + 42S_8^3. \quad (11)$$

Its character table can easily be constructed using the cyclic subgroups of orders six and eight, and is displayed in table 3. Since all C_7 elements are similar the two T

Table 3
Character table for ^7O_d.

		E	$21C_2$	$56C_3$	$42C_4$	$48C_7$	$28\sigma_v$	$56S_6$	$42S_8$	$42S_8^3$
Γ_1	A	1	1	1	1	1	1	1	1	1
Γ_2	B	1	1	1	1	1	-1	-1	-1	-1
Γ_3	I_1	6	-2	0	2	-1	0	0	0	0
Γ_4	I_2	6	2	0	0	-1	0	0	$\sqrt{2}$	$-\sqrt{2}$
Γ_5	I_3	6	2	0	0	-1	0	0	$-\sqrt{2}$	$\sqrt{2}$
Γ_6	J_1	7	-1	1	-1	0	1	1	-1	-1
Γ_7	J_2	7	-1	1	-1	0	-1	-1	1	1
Γ_8	K_1	8	0	-1	0	1	2	-1	0	0
Γ_9	K_2	8	0	-1	0	1	-2	1	0	0

Table 4
Multiplication table.

	A	T_1	T_2	I	J	K
A	A	T_1	T_2	I	J	K
T_1		T_2+I	$A+K$	T_2+J+K	$I+J+K$	$T_1+I+J+K$
T_2			T_1+I	T_1+J+K	$I+J+K$	$T_2+I+J+K$
I				$A+2I+J+2K$	$T_1+T_2+I+2J+2K$	$T_1+T_2+2I+2J+2K$
J					$A+T_1+T_2+2I+2J+2K$	$T_1+T_2+2I+2J+3K$
K						$A+T_1+T_2+2I+3J+3K$

representations of the rotational subgroup combine into a single sixfold degenerate representation which is denoted as I_1.

While the use of point group terminology proves to be very convenient for describing ^7O and ^7O_d, it must be kept in mind that these groups refer to automorphisms of a graph. A generator such as σ_v shares with a true symmetry plane its cyclic nature and odd character, but cannot be identified with a crystallographic symmetry plane of the periodic lattice on which the polyhedron can be mapped. Also there is no element that is similar to a centre of inversion, since the transposition of *antipodal* points is not an automorphism here.

In the further treatment we will mainly be concerned with the rotational subgroup ^7O, which incorporates the essential group theoretical structure of the Klein map. Extensions of the results to the full group are usually straightforward. The direct products of the irreducible representations of ^7O are listed in the multiplication table 4. Note the occurrence of product multiplicities, which means that the heptakisoctahedral group is not simply reducible. Interestingly, the product of I with the direct sum of all representations reduces to the regular representation:

$$I \times (A + T_1 + T_2 + I + J + K) = \Gamma_{reg}. \tag{12}$$

Table 5
Subduction table of ^7O representations to subgroups representations.

^7O	O	M_7	C_7	C_3
A	A_1	A_1	A	A
T_1	T_1	T_1	$E_1+E_2+E_3$	$A+E$
T_2	T_2	T_2		$A+E$
I	A_1+E+T_2	T_1+T_2	$E_1+E_2+E_3$	$2A+2E$
J	$A_2+T_1+T_2$	$A_1+T_1+T_2$	$A+E_1+E_2+E_3$	$3A+2E$
K	$E+T_1+T_2$	$A_2+A_3+T_1+T_2$	$2A+E_1+E_2+E_3$	$2A+3E$

The genealogical tree of subgroups of ^7O is shown in figure 4 whilst table 5 describes the subduction of the parent irreducible representations upon decrease in symmetry. Coset expansion of the group into its subgroup gives rise to symmetric orbits, some of which can be represented by polyhedral structures, with interesting chemical perspectives. In the next section we will discuss some of these in more detail.

4. The orbits of ^7O

4.1. The 7-orbit

The group ^7O contains fourteen subgroups of order 24 which constitute two distinct conjugacy classes (O' and O'' in figure 4) of seven O groups, each isomorphic to the rotations of an octahedron. The 56 vertices of the Schlegel diagram can therefore be decomposed into seven cubes in two different ways. As shown in figures 5a and 5b, these would interconvert on reflection of the diagram in any one of the 28 mirror planes of the covering ^7O_d group. Each C_4 axis of ^7O is common to two cubes, one from each set; each C_2 axis of ^7O appears three times within each set of seven cubes, as C_4^2 of one cube and C_2' of two others. The induced representations corresponding to both orbits are identical and can be obtained at once by applying the Frobenius reciprocity theorem [1] to the subduction table 5. The totally symmetric representation of the octahedron is present only in the heptakisoctahedral A and I representations, implying that these will be the only symmetries of the 7-vertex graph of figure 2:

$$\Gamma_{A_1}\left(O \uparrow {}^7O\right) = A + I. \tag{13}$$

As the genealogical tree in figure 4 shows, the separate octahedral subgroups O' and O'' have distinct subgroups T' and T'', corresponding to orbits of 14 tetrahedra from each set of seven cubes, and distinct D_2 subgroups for orthorhombic deformations of these tetrahedra. D_4, C_4, D_3, C_3 and C_2 subgroups are, however, common to O' and O''.

4.2. The 8-orbit

The heptakisoctahedral group also contains a hemi-metacyclic group, M_7, of order 21. Its orbit contains eight elements. This metacyclic group is generated by

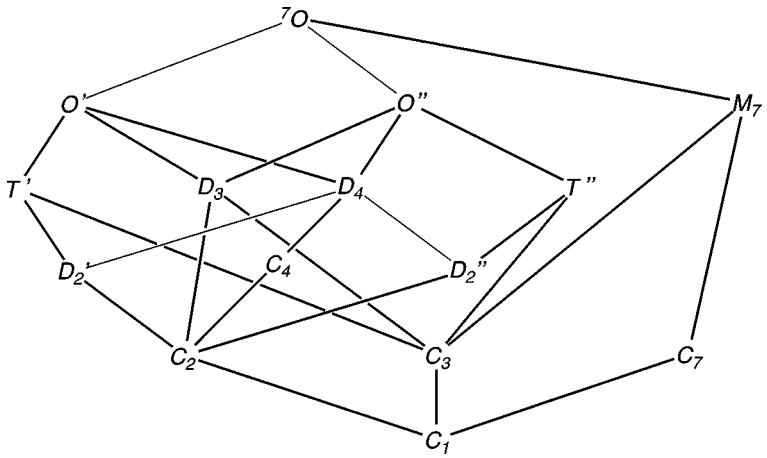

Figure 4. The genealogical tree of subgroups of ${}^7O$.

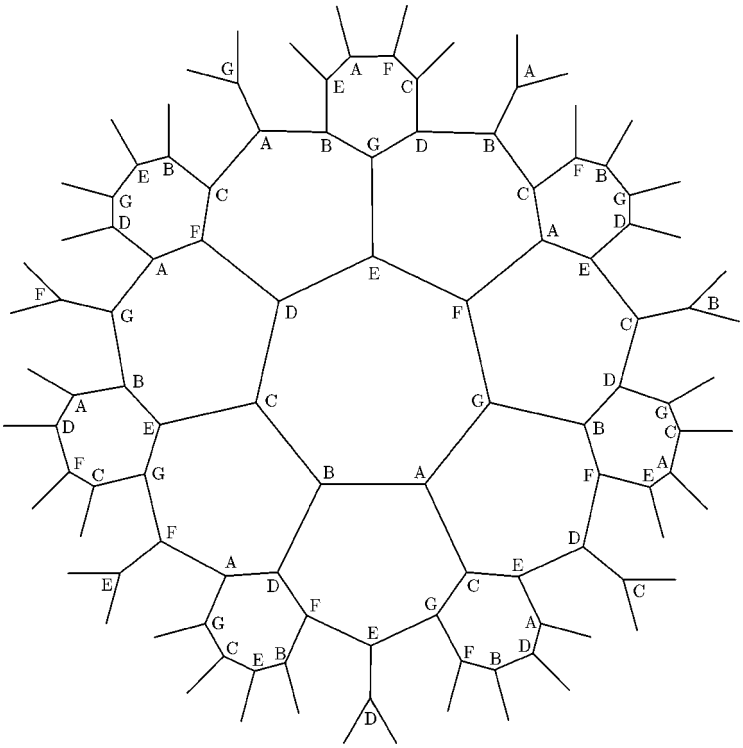

Figure 5a. The seven cubes of the O' orbit of ${}^7O$; each letter $A, B, \ldots, G$ denotes vertices belonging to one set of 8.

the direct product of a sevenfold and threefold cyclic group. If one chooses as a generator the C_7 element through heptagons 1, 23, 24 there will be seven threefold symmetry axes that stabilise this triplet of heptagons, and thus can be combined with

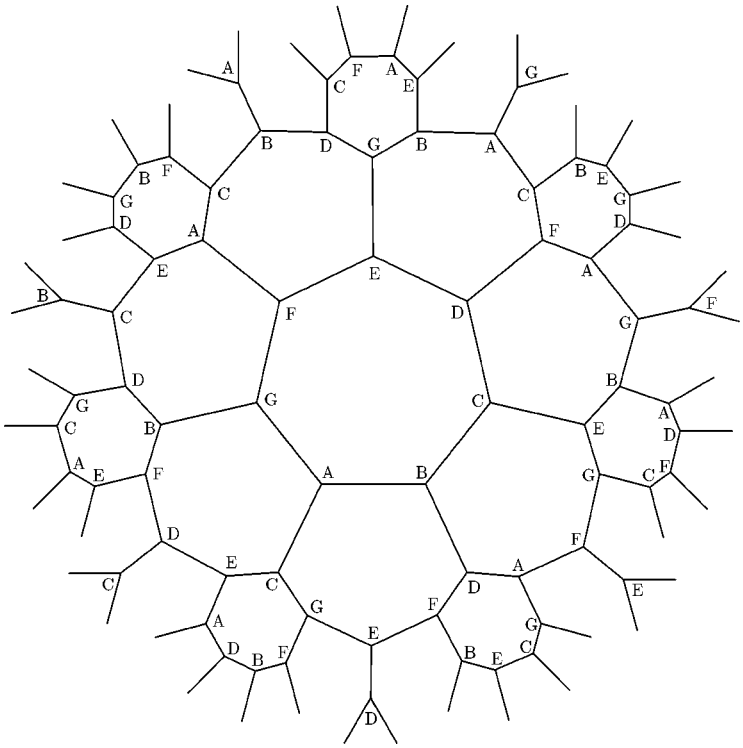

Figure 5b. The seven cubes of the O'' orbit, produced by reflecting cubes A to G of figure 5a in the vertical mirror plane of ${}^7O_d$.

the sevenfold generator to yield a subgroup of order 21. Its character table is represented in table 6. There are 3 nondegenerate and 2 triply-degenerate representations, which we have labeled as A_1, A_2, A_3 and T_1, T_2, respectively. A_2 and A_3 are one-dimensional complex conjugate nondegenerate representations, which each directly induce the K representation of ${}^7O$ in irreducible form:

$$\begin{aligned} \Gamma_{A_2}\big(M_7 \uparrow {}^7O\big) &= K, \\ \Gamma_{A_3}\big(M_7 \uparrow {}^7O\big) &= K. \end{aligned} \tag{14}$$

This remarkable property again also occurs in the icosahedral group, where the H representation can be obtained in irreducible form by direct induction from one of the one-dimensional complex conjugate representations of the tetrahedral subgroup. It implies that both H and K representational matrices can be obtained in monomial form [3], i.e., with only one unimodular number in each row and column.

4.3. The 24-orbit

This orbit is generated through coset expansion of the cyclic subgroup of order 7 and contains 24 points. These points correspond to the centers of the 24 heptagonal

Table 6
Character table for M_7.

		E	$3C_7$	$3C_7^3$	$7C_3$	$7C_3^2$
Γ_1	A_1	1	1	1	1	1
Γ_2	A_2	1	1	1	$\frac{1}{2}(-1+\mathrm{i}\sqrt{3})$	$\frac{1}{2}(-1-\mathrm{i}\sqrt{3})$
Γ_3	A_3	1	1	1	$\frac{1}{2}(-1-\mathrm{i}\sqrt{3})$	$\frac{1}{2}(-1+\mathrm{i}\sqrt{3})$
Γ_4	T_1	3	$\frac{1}{2}(-1+\mathrm{i}\sqrt{7})$	$\frac{1}{2}(-1-\mathrm{i}\sqrt{7})$	0	0
Γ_5	T_2	3	$\frac{1}{2}(-1-\mathrm{i}\sqrt{7})$	$\frac{1}{2}(-1+\mathrm{i}\sqrt{7})$	0	0

faces and form the dual of the 56-graph. The icosahedral analogue corresponds to the regular icosahedron. From the subduction table one obtains

$$\Gamma_A\big(C_7 \uparrow {}^7O\big) = A + J + 2K. \tag{15}$$

The spectrum of this graph has eigenvalues 7 (A), $\sqrt{7}$ (K), -1 (J), $-\sqrt{7}$ (K), and again resembles closely the spectrum of the icosahedron with its pair of $\pm\sqrt{5}$ roots.

4.4. The 56-orbit

Finally we consider the 56-graph itself (see figure 3). Its trivalent vertices are stabilized by threefold operations. This polyhedron constructed entirely of heptagons can be considered to be an analogue of the regular pentagonal dodecahedron. The induced representation of its 56 vertices is given by

$$\Gamma_A\big(C_3 \uparrow {}^7O\big) = A + T_1 + T_2 + 2I + 3J + 2K. \tag{16}$$

The spectrum of eigenvalues is listed in table 7 and shown in figure 6. The T_1 and T_2 levels both have eigenvalue -2. Their degeneracy is due to the reflection symmetry of the covering ${}^7O_d$ group. A further characteristic feature, which is again reminiscent of the dodecahedron, is the occurrence of nonbonding orbitals in the centre of the spectrum. These orbitals can be generated by induction from a nonbonding orbital which transforms as the A_1 representation of M_7, and is obtained by putting $+1$ on vertices **11**, **15**, **19**, **23**, **27**, **31** and **35** and -1 on vertices **9**, **13**, **17**, **21**, **25**, **29** and **33**. In ${}^7O_d$ the induced representation transforms as $B + J_1$, but since the orbital basis of the 56-polyhedron does not contain a B representation, the nonbonding orbital shown has irreducible J_1 symmetry and hence a seven-fold degeneracy. A similar explanation has been found [8] for the fourfold degeneracy of the nonbonding orbital of the dodecahedron in terms of nonbonding orbitals on the five cubes inside the dodecahedron.

5. Leapfrog and quadrupling transformations of the heptakisoctahedron

Since the heptakisoctahedral graph has the topology of a surface of genus 3 (e.g., a sphere with three handles) it can be realized in three-dimensional space without intersection as an infinite periodic lattice. In this paper we consider only the most

Table 7
Eigenvalue spectra and symmetries of 56-, 168- and 224-orbits of ^7O.

56	J	$(-1-\sqrt{17})/2$	I	$-\sqrt{2}$	I	$\sqrt{2}$	K	$1+\sqrt{2}$
	T_1	-2	K	$1-\sqrt{2}$	J	$(-1+\sqrt{17})/2$	A	3
	T_2	-2	J	0				
168	J	$-(1+\sqrt{21})/2$	K	-1.5165^{c}	I	0.1859^{b}	J	1.4626^{a}
	T_1	$(-\sqrt{5}-3)/2$	J	-1	I	$\sqrt{2}-1$	J	$(\sqrt{21}-1)/2$
	T_2	$(-\sqrt{5}-3)/2$	J	-1	T_1	1	K	2
	I	$-1-\sqrt{2}$	K	-1	T_2	1	I	2.2283^{b}
	K	-2	K	-0.5524^{c}	K	1	J	2.4728^{a}
	J	-1.9354^{a}	T_1	$(\sqrt{5}-3)/2$	K	1.2873^{c}	K	2.7816^{c}
	I	-1.7746^{b}	T_2	$(\sqrt{5}-3)/2$	I	1.3604^{b}	A	3
224	J	-2.8339^{d}	J	-1.3793^{d}	I	0.9229^{f}	I	1.6269^{f}
	T_1	-2.6996^{e}	I	-1	A	1	K	1.6566^{g}
	T_2	-2.6996^{e}	J	-1	T_1	1	J	1.7559^{d}
	I	-2.5498^{f}	K	-1	T_2	1	J	2.0472^{d}
	K	-2.2361^{g}	T_1	-0.7609^{e}	I	1	K	2.2361^{g}
	J	-2.1598^{d}	T_2	-0.7609^{e}	K	1	I	2.4004^{f}
	I	-2.0240^{f}	K	-0.4450^{g}	K	1.2470^{g}	J	2.5957^{d}
	K	-1.8019^{g}	I	-0.3763^{f}	T_1	1.4605^{e}	K	2.8342^{g}
	K	-1.4909^{g}	J	-0.0529^{d}	T_2	1.4605^{e}	A	3
	J	-1.4648^{d}	J	0.4919^{d}				

[a] Roots of $x^3-2x^2-4x+7=0$.
[b] Roots of $x^4-2x^3-3x^2+6x-1=0$.
[c] Roots of $x^4-2x^3-4x^2+4x+3=0$.
[d] Roots of $x^9+x^8-15x^7-13x^6+73x^5+55x^4-128x^3-78x^2+53x+3=0$.
[e] Roots of $x^3+2x^2-3x-3=0$.
[f] Roots of $x^6-10x^4+2x^3+25x^2-10x-7=0$.
[g] Roots of $x^8-2x^7-12x^6+20x^5+49x^4-62x^3-77x^2+60x+35=0$.

symmetrical primitive lattice, the P minimal surface, known as the *plumber's nightmare*. The decoration of this surface by the 56-graph is shown in figure 7. These drawings represent the smallest unit cell that forms a trivalent realization of the ^7O automorphism group. Homologues where the heptagonal contacts have been removed by surrounding each heptagon by hexagons can be achieved both by the leapfrog and quadrupling operations.

5.1. *The 168-leapfrog*

The leapfrog transform of a polyhedron is obtained by performing the following instructions consecutively [16]: first omnicap, and then take the dual. This results in an expansion to a polyhedron with three times as many vertices as the original. In this way the 56-graph is expanded to one with 168 vertices (see figure 8) [29], which is the analogue of the C_{60} structure formed by leapfrogging C_{20} in the fullerene family. This structure exemplifies the full 168-orbit of the heptakisoctahedral group.

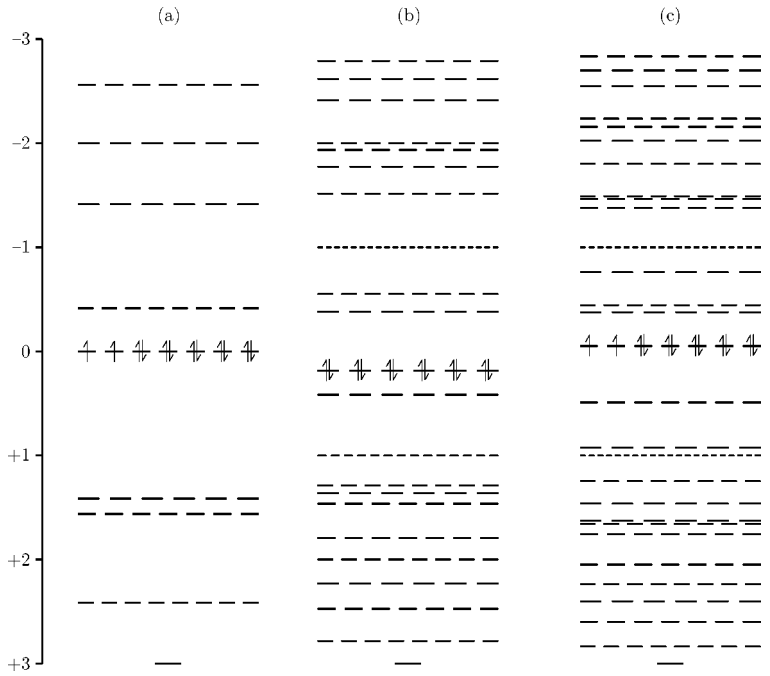

Figure 6. Graphical representation of the eigenvalue spectra of the 56-, 168- and 224-orbits of ^7O. Arrows indicate the occupation of the HOMO-levels.

Each symmetry element maps a given vertex to a different image, in such a way that vertices can be put in one-to-one correspondence with group elements. This property can be used to calculate the eigenvalue spectrum from the character table [14]. The spectrum is listed in table 7 and shown in figure 6; it spans the regular representation, and therefore a single orbit of ^7O, since

$$\Gamma_A\left(C_1 \uparrow {}^7O\right) = A + 3T_1 + 3T_2 + 6I + 7J + 8K. \tag{17}$$

A characteristic feature of the leapfrog transformation on fullerenes and certain other polyhedra [16], which also is observed for the present example, is that the number of bonding eigenvalues is equal to half the number of vertices. This means that occupation of these bonding orbitals by two electrons per orbital will yield a closed-shell structure.

Upon closer inspection one notices the presence of twelve almost nonbonding orbitals, transforming as $2I$ and with eigenvalues 0.1859 and 0.4142. Again this reminds us of the characteristic presence of six almost nonbonding orbitals in the centre of the spectrum of all leapfrog fullerenes, transforming as $T_{1u} + T_{1g}$ [6]. In the case of fullerenes these $2T$ orbitals are the lowest unoccupied (LUMO), while for the present polyhedron the $2I$ pair are the highest occupied (HOMO). These levels are directly related to the presence of pentagonal or heptagonal "defects" in an otherwise regular hexagonal plane, and draw their LUMO or HOMO character from the chemical bonding in pentagons and heptagons. Pentagons can form a closed shell structure by

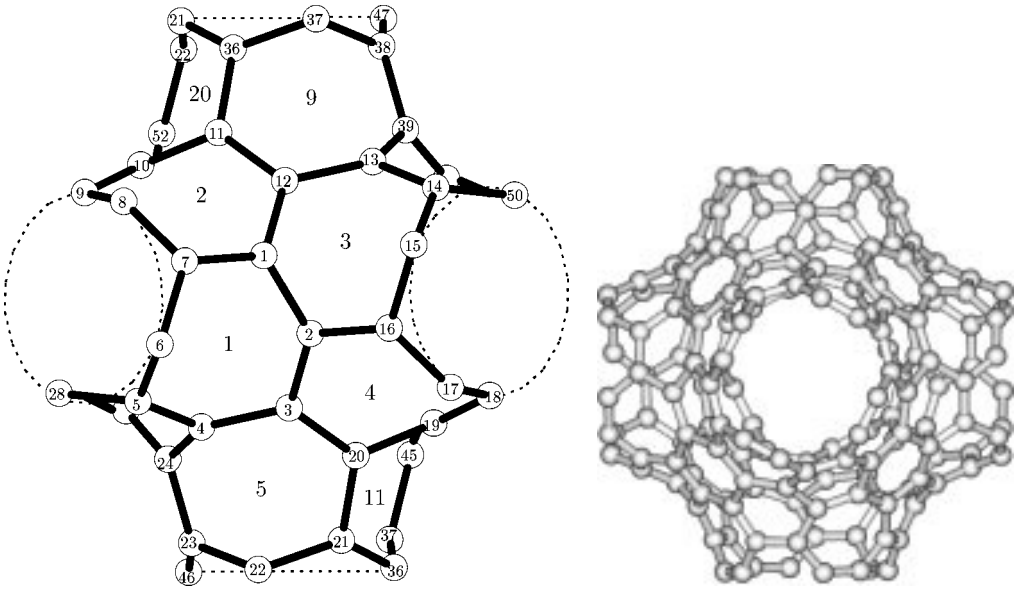

Figure 7. (a) A segment for the decoration of the "plumber's nightmare" surface with an all-heptagon periodic lattice. This unit is chiral and embodies a twist of a few degrees between the top and bottom 8-cycles. In addition, note also that the vertex identification necessary for the Klein graph imply a further 90° twist between top and bottom of this unit (compare, e.g., vertices marked 36). The vertex and ring numbering scheme is consistent with that used in figure 3. (b) The full octahedral unit, formed from sections of (a).

taking up one additional electron, thus forming the typical aromatic sextet of organic chemistry. The six $2T$ orbitals provide precisely the room to accommodate the twelve electrons associated with the twelve pentagonal defects. In contrast, heptagons reach sextet stability by loss of one electron each. The 24 heptagon defects in the leapfrog thus explain the presence of twelve orbitals close to zero energy, from which up to 24 electrons can readily be withdrawn. In a chemical sense C_{60} is thus a typical electron-deficient compound, which can accept extra electrons [6], while the C_{168} polyhedron is expected to be an electron-rich species, with electron-donating properties. This has consequences for possible attempts to prepare such structures, as the presence of electron withdrawing agents such as halogens could perhaps facilitate the synthesis.

The bonding analysis does not explain why the defect orbitals should transform precisely as $2I$. This characteristic symmetry can be derived from an extension of Euler's theorem as will be explained in section 6.

5.2. The 224-quadruple

An alternative expansion which also removes the heptagonal contacts by surrounding all seven-membered rings with hexagons while maintaining the heptakisoctahedral symmetry is the quadrupling transformation. This transformation multiplies

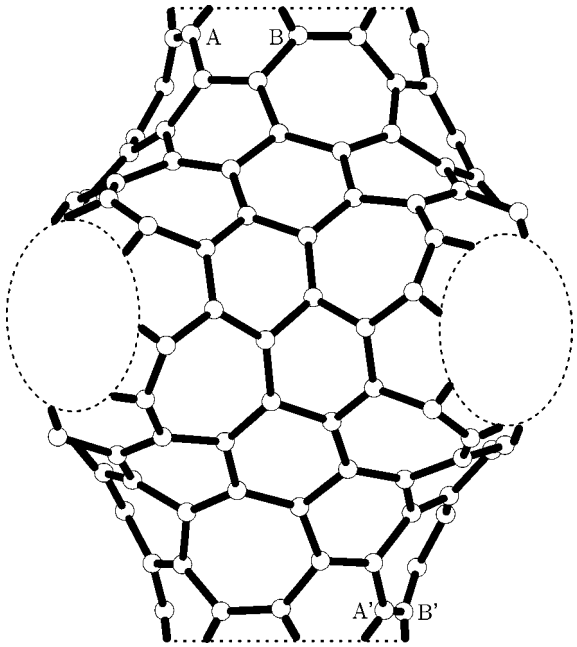

Figure 8. The leapfrog transform of the structure in figure 7. In this structure, the boundary between octahedral units intersects bonds. Note again the 90° twist in making the connections across the boundary, from A to A', B to B', etc.

the number of vertices by four. It was applied by Fowler et al. [15] to generate the C_{80} fullerene by quadrupling the C_{20} parent dodecahedron and simply corresponds to a bevelling of every edge in which every edge is replaced by a hexagon. In the work of Deza, following Goldberg, it is referred to as the "chamfering" transformation [13,17]. Quadrupling of the 56-vertex polyhedron leads to a 224-vertex structure with the heptakisoctahedral symmetry of the parent, as shown in figure 9. Its eigenvalue spectrum is included in table 7 and figure 6. Unlike leapfrogs, quadruples do not generally have closed-shell structures. Thus, in the case of the icosahedral C_{80} the neutral form has a fourfold degenerate HOMO which is occupied by only two electrons [15]. This pattern is in fact characteristic for the parent dodecahedron, the vertices of which still form an orbit inside the quadrupled cage. Similarly, in the present symmetry group the quadrupled structure C_{224} has an open shell with two holes in the J-level at -0.0529, a pattern which is also found in the parent C_{56} polyhedron with two holes in the nonbonding J-level (cf. table 7 and figure 6).

6. The symmetry of the Euler characteristic

The Euler theorem relates the numbers of vertices (v), edges (e), and faces (f) to an invariant that is characteristic of the topology of the surface on which the polyhedron

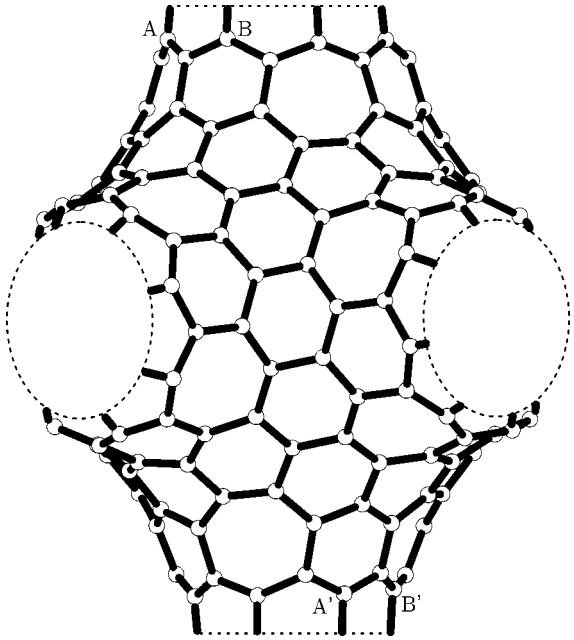

Figure 9. Quadruple transform of the structure in figure 7. As in the leapfrog, some bonds cross the boundary of the octahedral unit, and as in both leapfrog and parent structures, a 90° twist relates equivalent positions at top and bottom of the segment.

is constructed, according to the celebrated rule

$$v - e + f = \chi, \tag{18}$$

where χ is the Euler characteristic. For all polyhedra that have been considered here the Euler characteristic is equal to -4, e.g., for the 56-heptakisoctahedron one has $56 - 84 + 24 = -4$. This value complies with the characteristic of a sphere with three handles, on which the Klein figure can indeed be mapped. Behind the simple dimensional relationship lies a deeper symmetry connection which can be expressed by irreducible representations as follows [5,9]:

$$\Gamma_\sigma(v) - \Gamma_\parallel(e) + \Gamma_\odot(f) = \sum_{p=0,1,2} (-1)^p \Gamma_{H_p}. \tag{19}$$

The Γ symbols on the left-hand side of this equation refer to induced representations of the polyhedral group: $\Gamma_\sigma(v)$ simply corresponds to the representation of the set of vertex points. It corresponds to the symmetry of a basis set of σ-type orbitals, each symmetric with respect to all symmetry elements that pass through the vertex sites. $\Gamma_\parallel(e)$ spans the set of arrows on the edges, and $\Gamma_\odot(f)$ is the symmetry representation of circular arrows on the faces. On the right-hand side are the symmetries of the topological invariants, which are described by the homology groups H_p, where $p = 0, 1, 2$ refers to vertices, edges and faces, respectively.

We can identify at once the symmetries of these invariants by forming the alternating sum over the induced representations. As an example, for the 24-orbit the induced representations in ^7O_d read

$$\begin{aligned}\Gamma_\sigma(v) &= A + J_1 + 2K_1,\\ \Gamma_\parallel(e) &= 2I_1 + I_2 + I_3 + 2J_1 + 2J_2 + 2K_1 + 2K_2,\\ \Gamma_\odot(f) &= B + I_1 + I_2 + I_3 + J_1 + 2J_2 + 2K_2.\end{aligned} \tag{20}$$

From these results the symmetries of the invariant part follow at once:

$$\begin{aligned}\Gamma_{H_0} &= A,\\ \Gamma_{H_1} &= I_1,\\ \Gamma_{H_2} &= B.\end{aligned} \tag{21}$$

The dimensions of these representations explain the Euler characteristic as

$$\chi = \dim(A) - \dim(I_1) + \dim(B) = 1 - 6 + 1 = -4. \tag{22}$$

The three homology groups follow distinct irreducible representations. Vertex and face homologies transform respectively according to the scalar (A) and pseudo-scalar (B) representation, which is also the case for a spherical surface. In contrast, the appearance of an edge homology is related to the existence of handles. Topologically, these correspond to circuits on the surface than cannot be shrunk to a point, because of the presence of holes. For the case of a sphere with one handle, which is equivalent to a torus, there are two such edge modes [7], as compared to six in the present case of a sphere with three handles. From a physical point of view the edge homologies are directly related to the existence of topology-sustained through-bond currents [4]. In the case of the torus of genus 1 these can be identified as the magnetic dipole and anapole moment. No fewer than six independent moments are thus expected to be sustained by the present topology.

Apart from the general Euler theorem and its symmetry extension, several corollaries can be derived which apply to specific polyhedra. As an example, for trivalent polyhedra on surfaces of genus 3 the number of edges is linked to the number of faces by the rule

$$e = 3f + 12. \tag{23}$$

This rule is obtained by combining the general Euler theorem with the special result, $3v = 2e$, valid for trivalent cages. Again this result can be extended to a relationship between induced representations, viz.:

$$\Gamma_\sigma(e) = \Gamma_\sigma(f) + \Gamma_\pi(f) + I_2 + I_3. \tag{24}$$

As before, the Γ_σ symbols denote induced representations over symmetric objects on the specified sites. $\Gamma_\pi(f)$ stands for the induced representation of a set of two orthogonal in-plane arrows in the centre of each face. In a chemical context such arrows often symbolize a set of in-plane p_x, p_y orbitals which transform as the

π representation of the cylindrical group. The position of the arrows is completely defined by the contours of the faces, and for this reason those automorphisms of the vertices that preserve polyhedral faces induce well-defined symmetry transformations of this π basis.

We will now illustrate this symmetry extension for the case of the 56-polyhedron, which has 24 faces and 84 edges. One has

$$\begin{aligned}\Gamma_\sigma(e) &= A + I_1 + 2I_2 + 2I_3 + 2J_1 + J_2 + 3K_1 + K_2,\\ \Gamma_\sigma(f) &= A + J_1 + 2K_1,\\ \Gamma_\pi(f) &= I_1 + I_2 + I_3 + J_1 + J_2 + K_1 + K_2.\end{aligned} \tag{25}$$

The derivation of the induced $\Gamma_\pi(f)$ representation requires some caution. As an example, for the C_7 generator three faces are stabilized and hence three sets of face arrows will contribute to the character of the induced representation. The arrows in the centre of face 1 will contribute $2\cos 2\pi/7$ to the character, since this face is rotated over one seventh of a full circle. In contrast the two remaining poles of the generator on faces 23 and 24 perform respective rotations over four and two sevenths of a full circle. This is easily demonstrated by considering the local environment of these polygons and applying the permutations associated with the C_7 generator. In this way the character of $\Gamma_\pi(f)$ becomes

$$\chi_\pi = 2\cos 2\pi/7 + 2\cos 4\pi/7 + 2\cos 8\pi/7 = -1. \tag{26}$$

When we subtract the face terms from the edge term, all representations apart from $I_2 + I_3$ cancel, in agreement with equation (24).

This corollary to Euler's theorem for trivalent polyhedra can be connected directly to chemical bonding in leapfrogs. We will follow here a strategy which was already succesfully applied to the case of leapfrog fullerenes [6]. Perfect bond alternation in a leapfrog can be satisfied by making double bonds on all edges that originate from edges on the parent structure, and single bonds on all others. This bonding extreme is denoted as the Fries structure. Clearly the symmetry representation of these bonding orbitals will correspond to the representation spanned by symmetric objects on the edge centres of the parent polyhedron. For the 168-leapfrog this is precisely the $\Gamma_\sigma(e)$ term of the 56-parent.

An alternative bonding scheme can be realized by distributing double bonds over the faces of the leapfrog that coincide with original faces of the parent. Such face bonds are known as aromatic sextets, and the corresponding bonding scheme is called the Clar structure. In the 168-leapfrog these sextets span precisely the face terms $\Gamma_\sigma(f)+\Gamma_\pi(f)$ for the parent 56-polyhedron. Fries and Clar structures are complementary, in the sense that all Clar face bonds are single bonds in the Fries structure and all double bonds of the Fries structure are single bonds in the Clar picture. The Euler result of equation (24) simply compares the symmetries of the bonding orbitals in both schemes. It shows that both symmetries match, except for twelve orbitals, transforming as $I_2 + I_3$, which are bonding in the Fries scheme but are missing in the Clar scheme. To the extent

that the actual bonding situation is intermediate between both extremes we can thus predict that there will be a set of twelve orbitals that are almost nonbonding as a result of their bonding Fries but antibonding Clar character. These orbitals are indeed found as the HOMOs in the centre of the leapfrog spectrum, with eigenvalues 0.1859β and 0.4142β. As was already indicated, they are responsible for the electron donating character of the 168-leapfrog.

7. Carbon allotropes and the heptakisoctahedral group

Several hypothetical network allotropes of carbon have been constructed as decorations of the negatively curved minimal surfaces [27,29]. It has been suggested [22] that those decorating the genus-3 P surface (the so-called "plumber's nightmare") share the ^7O automorphism group of the Klein graph.

However, these embeddings in 3D periodic lattices present some chemically significant steric problems. As figures 7 and 9 show, the embeddings of the 24-heptagon Klein graph and its expansions on the plumber's nightmare surface require a twist of 90° between opposite arms of the hexaskelion unit. If the embedded unit were to incorporate this twist, then the heptagonal (and hexagonal) rings of carbon atoms must take up the distortion (see figure 10). In fact, construction of figure 10 as a molecular model with flexible connections, or as a computer model to be optimised by molecular mechanics, leads to spontaneous untwisting which cause the structures to revert

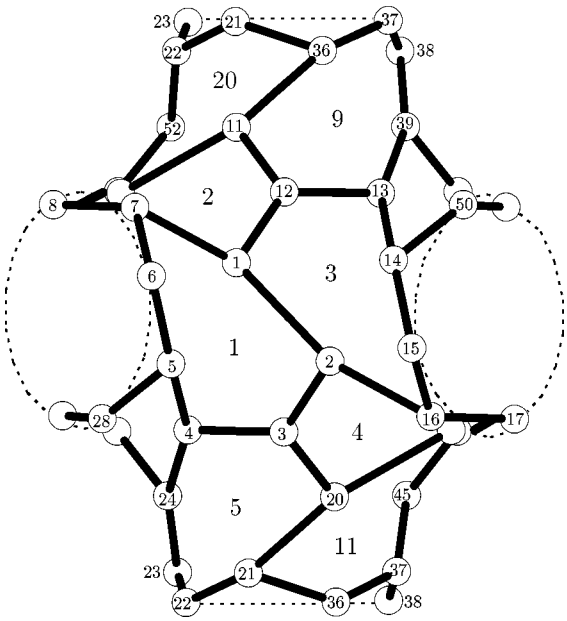

Figure 10. A version of the 56-orbit polyhedron of ^7O in which equivalent vertices at top and bottom of the segment are now related by a pure translation parallel to a C_4 axis, at the cost of considerable ring strain. The numbering scheme is taken from figure 7.

to those in figures 7–9, which do not themselves have the correct set of atom-atom adjacencies for the Klein graph if connected unit-to-unit by pure translations.

The heptakisoctahedral group therefore describes not the ground state structure of these P-schwarzite networks, but a stationary point of higher order. Direct application of PSL(2, 7) symmetry to plumber's nightmare schwarzites should therefore be made with some caution, as large steric barriers appear to push the structures into less symmetrical topologies.

In addition to the decorations of the P minimal surface considered here, other candidates for negatively curved analogues of graphite include the decorated D surface, for which Vanderbilt and Tersoff [29] found a tetrahedrally symmetric structure with 168 vertices per unit cell. This is a leapfrog of a 24-heptagon decoration made up of two enantiomeric tetrahedral "joints" composed of 12 heptagons which can be realised with moderate steric strain, but in fact is not based on the Klein graph; the difference is simply proved, by noting that, for example, of the 7 neighbours of any one heptagon, H_i, two meet in an edge that has no vertex in common with H_i. Such a configuration of faces, which corresponds in the dual to a *separating triangle* whose removal would disconnect the graph, is not present in the Klein graph, which is therefore not the correct descriptor for these decorations of D surfaces.

8. Conclusions

The icosahedral symmetry group I is the largest proper point group of three-dimensional space and at the same time isomorphic to the pentakistetrahedral group ${}^5T$, which is the smallest member of the triad of pollakispolyhedral groups. In this paper we have studied the orbits and representations of the next member of this group: the heptakisoctahedral group, ${}^7O$, and its companion ${}^7O_d$. Many points of correspondence between the two family members have been noted.

While the icosahedral group plays a prominent role in the chemistry of fullerenes, the heptakisoctahedral group has been advocated as automorphism group of schwarzite structures [22]. The actual realization of this claim in the molecular world remains an open challenge. In the meantime the study of structural patterns which are common to fullerenes and schwarzites is of direct relevance to fullerene research by providing a deeper understanding of its group theoretical basis.

Two such common aspects have been discussed in the present paper: the closed-shell structure of leapfrogs and the open-shell structure of chamfered polyhedra. Leapfrog structures such as C_{60} fullerene and C_{168} schwarzite typically have a closed-shell structure with specific sets of nearly nonbonding orbitals. The chamfered structures such as C_{80} fullerene and C_{224} schwarzite in contrast have an open-shell structure which is similar to that of the respective parents. The leapfrog result is explained by the symmetry extension of the Euler theorem for trivalent polyhedra, but the regular pattern for the chamfered structures still awaits a full explanation.

Acknowledgements

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