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Univalent (Monodentate) Substitution on Convex Polyhedra

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Pólya's enumeration theorem has been used to evaluate, by computer, the numbers N of distinct configurations (= positional isomers) produced by univalent (monodentate) substitution at the vertices of convex polyhedra of crystallographic or stereochemical interest. The values of N are tabulated for a large variety of polyhedra of up to $V=120$ vertices and for up to V kinds of structureless substituents. The N have been evaluated not only for the maximum point-group symmetry of each polyhedron but also, for $V\le 24$, for *all* the subgroup symmetries of the maximum point group. For $V>24$ only polyhedra of cubic and icosahedral symmetries are included. An example shows how the tables of N can be used to enumerate pairs of enantiomorphs. The effect of symmetry on N for large values of V is examined.

Symbols and abbreviations

a	axial digyre (see text)
$\mathscr{A}$	Archimedean polyhedron (isogonal)
$\mathscr{A}^*$	Catalan polyhedron (dual to $\mathscr{A}$, isohedral)
$\mathscr{C}_1$	number of all non-isomorphic convex polyhedra of maximum p.g. symmetry C_1 and a given V
d	diagonal digyre (see text)
$\mathscr{D}$	dual polyhedron
E	number of edges
F	number of faces
i	centre of symmetry; inversion
$\mathscr{K}a$	Kasper polyhedron
m	mirror plane
ma	axial mirror plane (also in combinations maa and mad; see text)
md	diagonal mirror plane (also in mdd; see text)
mh	horizontal mirror plane (also in combinations mha and mhd; see text)
N	number of distinct configurations
$\mathscr{N}$	number of all non-isomorphic convex polyhedra of a given V
$p(\mathbf{G})$	order of the point group $\mathbf{G}$
p.g.	point group
$\mathscr{P}\ell$	Platonic polyhedron
v', v''	nonequivalent (vertical) mirror planes
V	number of vertices
$\mathscr{V}$	vertex-figure derivative
Z	cycle index
$\mathscr{Z}$	number of Z-isomorphic classes
Δ	deltahedron (Freudenthal & van der Waerden, 1947)
Π	partition
8–2	running number of polyhedron of $V=8$ and maximum p. g. symmetry in Table 5
8–2 (*20*)	running number of polyhedron of $V=8$ obtained from, or related to, **8–2** by lowering the p.g. symmetry from the maximum possible for **8–2**, *32*, to *20*
45, *109*	running number of a p.g. in Table 3

A problem of some importance in various branches of science is the determination of the number N of distinct‡ positional isomers that can be obtained by

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‡ Distinct positional isomers are not congruent with respect to rotation.

univalent substitution at the vertices of convex polyhedra or their isomorphs; in coordination chemistry such substitution is called monodentate.* The numbers N are well known for small polyhedra of high symmetry that occur as coordination figures. They have been determined by calculation or by inspection, and tabulated for the square, the regular tetrahedron and octahedron (Main Smith, 1924; Trimble, 1954); the cube, the square antiprism, the dodecadeltahedron, and the bicapped trigonal prism (Marchi, Fernelius & McReynolds, 1943), always for the maximum p.g. symmetry. However, explicit listing of all the possible distinct configurations and their classification by symmetry is a task of some magnitude even for small values of V. Thus when V is large and when there are more than two kinds of substituents, knowledge of N is a prerequisite to enumeration: it provides an advance measure of the practicability of listing and serves as a check in attempts to generate the configurations exhaustively by computer methods. The need to know N is even greater when substitution is considered on polyhedra that derive from the regular or semiregular bodies by the various reductions of the p.g. symmetry. In the following we list the values of N for a large variety of polyhedra in dependence on the maximum and subgroup symmetries of each polyhedron and, wherever practical, for all distinct partitions of V, *i.e.* for up to V kinds of substituents. The results have been obtained, or verified, by machine computation.

The determination of N without construction is a combinatorial problem taking due account of reduction, by symmetry, of the number of distinct permutations. A method of solution which concerns itself explicitly with chemical isomerism was described as early as 1929 by Lunn & Senior; it was subsequently used by Marchi *et al.* (1943). However, a more powerful and elegant enumeration method is the *cycle-index* method due to Redfield (1927) and to Pólya (1936, 1937). This is the method used to obtain the present results. Pólya's original presentations were not concerned directly with polyhedra and their symmetries. The first to apply the method to substitution on crystallographic polyhedra of full and reduced p.g. symmetries seems to have been Niggli (1941, 1945). It was employed, independently, for enumeration of three-dimensional chemical isomers by Hill (1943) and again, in more detail, by Kennedy, McQuarrie & Brubaker (1964) [*cf.* also the clear summary by Salthouse & Ware (1972)]. A concise general account of Pólya's enumeration theorem will be found in Harary & Palmer (1973).

For our purposes the cycle index† Z will be a polynomial that specifies the permutation group of V positions in E^3, some or all of which may be equivalent by symmetry. For a set of V positions (points) forming a configuration of p.g. symmetry $\mathbf{G}$, Z is given by

$$Z=[1/p(\mathbf{G})]\,(h_a s_{a_1}^{i_1} s_{a_2}^{i_2} s_{a_3}^{i_3} + h_b s_{b_1}^{j_1} s_{b_2}^{j_2} s_{b_3}^{j_3} + h_c s_{c_1}^{k_1} s_{c_2}^{k_2} s_{c_3}^{k_3} + \ldots)\,, \quad (1)$$

$$i_1a_1+i_2a_2+i_3a_3=j_1b_1+j_2b_2+j_3b_3=\ldots=V\,, \quad (2)$$

$$h_a+h_b+h_c+\ldots=p(\mathbf{G})\,, \quad (3)$$

where $s_{a_1}^{i_1}$ represents i_1 permutation cycles of length a_1, and similarly for $s_{b_1}^{j_1}, s_{c_1}^{k_1}$ *etc*. The first term of each of the s-products in equation (1) refers to a symmetry operation contained in one of the classes of $\mathbf{G}$, and its length is the order of that operation. That is, the operation represented by s_{a_1} permutes points in each of the i_1 subsets of a_1 points. If $i_1a_1=V$, $s_{a_2}^{i_2}s_{a_3}^{i_3}=1$. If $i_1a_1<V$, some or all of the remaining $V-i_1a_1$ points may lie on the symmetry element $\mathscr{S}_{a_1}$ represented by s_{a_1}, and the s-product contains more than one s-term. If *all* the $V-i_1a_1$ points lie on $\mathscr{S}_{a_1}, a_2=1$ or 2, $i_1a_1+i_2a_2=V$, and $i_3=0$. Otherwise the $V-i_1a_1$ points fall in i_2 subsets of a_2 points, the points of each subset being permuted by $\mathscr{S}_{a_2}\subset\mathscr{S}_{a_1}$, plus i_3 subsets of a_3 points permuted by $\mathscr{S}_{a_3}\subset\mathscr{S}_{a_1}$; $a_2=1$ or 2, $i_2\geq 0$, $a_3>a_2$. The coefficients h_a, h_b *etc.* are the numbers of symmetry operations contained in the particular classes of $\mathbf{G}$. Thus if $\mathscr{S}_{a_1}$ is a threefold rotation axis, $h_a=2$.

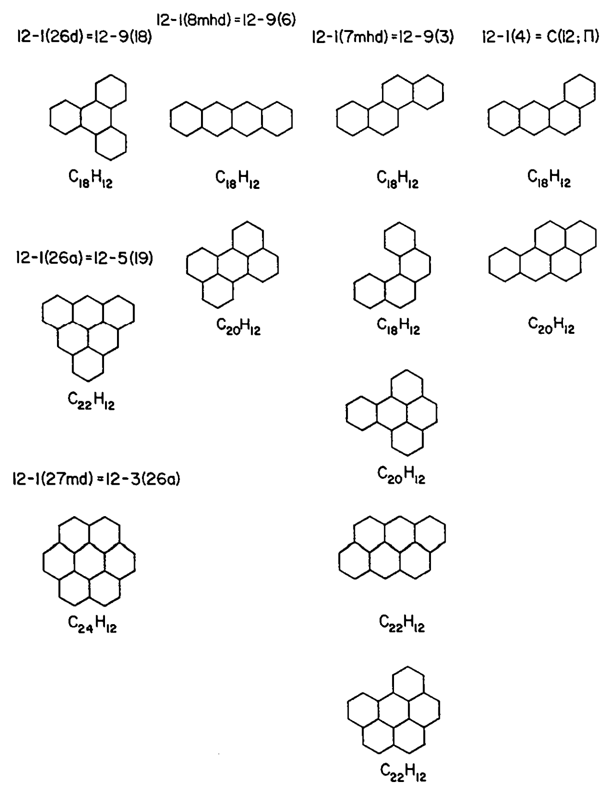

Fig. 1. Z-equivalent molecules of aromatic hydrocarbons with rigid condensed-ring systems containing twelve potentially replaceable hydrogen atoms (*cf.* Example 4 in text).

* In this paper a substituent will always be considered as having spherical symmetry and thus not giving rise to additional configurations by virtue of its own structure.

† Redfield (1927) called this polynomial a 'group-reduction function'.

The construction of a cycle index is shown in examples 1 to 3. Note that, following standard practice, the order of the s-terms in these examples, in Table 1 and elsewhere in the text, is reversed from that in the preceding paragraph; the s-terms in a product are arranged in the order of their *increasing* length.

Example 1. The symmetry elements, h coefficients and s-products of a hexagonal bipyramid **8–6** of symmetry $6/mmm$ (D_{6h}) are listed in Table 1. The two-term s-products arise from the circumstance that some of the vertices are situated on a symmetry element and are thus self-permuted relative to the corresponding symmetry operation, or at least are not subject to it to the full extent, *e.g.* $s_2^1 s_6^1$. While the threefold inversion axis corresponds to an operation of order six, its operation on a vertex located in the horizontal mirror plane m would produce a set of only three equivalent vertices in m. Hence the vertex permutation is of order three and the corresponding s-product is $s_2^1 s_3^2$ and not $s_2^1 s_6^1$. Collecting the s-terms yields $Z = (\frac{1}{24})(s_1^8 + 4s_2^4 + 7s_1^2 s_2^3 + 3s_1^4 s_2^2 + s_1^6 s_2^1 + 2s_1^2 s_3^2 + 2s_2^1 s_3^2 + 2s_1^2 s_6^1 + 2s_2^1 s_6^1)$.

Table 1. *The symmetry elements, h coefficients, and s-products of a hexagonal bipyramid of symmetry* $6/mmm$ (D_{6h}) (**8–6**)

Number	Type	h	s-product
1	onefold axis	1	s_1^8
1	sixfold axis (two vertices on 6)	2	$s_1^2 s_6^1$
1	sixfold inversion axis (two vertices on $\bar{6}$)	2	$s_2^1 s_3^2$
1	threefold axis $C_3 \subset C_6$ (two vertices on 3)	2	$s_1^2 s_3^2$
1	threefold inversion axis (two vertices on $\bar{3}$)	2	$s_2^1 s_6^1$
1	twofold axis $C_2 \subset C_6$ (two vertices on 2)	1	$s_1^2 s_2^3$
3	axial twofold axes (two vertices on 2)	3	$s_1^2 s_2^3$
3	diagonal twofold axes	3	s_2^4
3	axial mirror planes (four vertices in m)	3	$s_1^4 s_2^2$
3	diagonal mirror planes (two vertices in m)	3	$s_1^2 s_2^3$
1	horizontal mirror plane (six vertices in m)	1	$s_1^6 s_2^1$
1	centre of symmetry	1	s_2^4

Example 2. The bicapped tetrakaidecadeltahedron **11–5** of symmetry $\bar{6}m2$ (D_{3h}) may be visualized as a bicapped trigonal prism + 3. It is one of the two polyhedra listed in Table 5 whose Z contain a triple product: $Z = (\frac{1}{12})(s_1^{11} + 3s_1^1 s_2^5 + s_1^3 s_2^4 + 3s_1^5 s_2^3 + 2s_1^2 s_3^3 + 2s_2^1 s_3^1 s_6^1)$; the other polyhedron is **14–10**. The triple product corresponds to the simultaneous permutation of two vertices *on* $\bar{6}$ by $\bar{1} \subset \bar{6}$, three vertices in $m \perp \bar{6}$ by $3 \subset \bar{6}$, and six vertices forming a set about the $\bar{6}$ axis by $\bar{6}$.

Example 3. The difference between the Platonic pentagonal dodecahedron **20–1** of symmetry $53m$ (I_h) and the corresponding 'crystallographic' solid **20–1** (*29*) of the reduced symmetry $m3$ (T_h) (pyritohedron) is clearly displayed in the cycle indices:

20–1: $$(\tfrac{1}{120})(s_1^{20} + 16s_2^{10} + 15s_1^4 s_2^8 + 20s_1^2 s_3^6 + 24s_5^4 + 20s_2^1 s_6^3 + 24s_{10}^2)$$

20–1(*29*): $$(\tfrac{1}{24})(s_1^{20} + 4s_2^{10} + 3s_1^4 s_2^8 + 8s_1^2 s_3^6 + 8s_2^1 s_6^3)\,.$$

To obtain N, a generating function f is substituted for each s in Z. This function takes account of the extent of equivalence of the V objects (substituents) placed one each in the V positions related through Z. It is a polynomial whose number of terms is equal to the number of substituent types and whose degree is equal to the length of the cycle s. For example, a partition Π of $V = 14$ is specified by $3+3+3+2+2+1 = 3^3 2^2 1^1$, *i.e.* there are six types of substituents distributed as 3A, 3B, 3C, 2D, 2E, and one F. The generating function is then

$$f_{a_1} = x_A^{a_1} + x_B^{a_1} + x_C^{a_1} + x_D^{a_1} + x_E^{a_1} + x_F^{a_1}\,,$$

so that $s_{a_1}^{i_1} = f_{a_1}^{i_1}$ and similarly for a_2 *etc.* The value of $N(\Pi)$, *i.e.* the number of distinct positional isomers for the combination of substituents (='chemical composition'), $A_3B_3C_3D_2E_2F$, is then equal to the coefficient of the term $x_A^3 x_B^3 x_C^3 x_D^2 x_E^2 x_F$ in the expanded $Z[f(\Pi)]$ polynomial and will be tabulated under the partition $3^3 2^2 1^1$.

Example 4. The formulae in Fig. 1 represent aromatic hydrocarbons with rigid condensed-ring systems whose molecules contain 12 potentially replaceable hydrogen atoms. Configurations of the H atoms in these molecules are Z-isomorphic with the dodecagon **12–1** of various subgroup symmetries of $12/mmm$ (D_{12h}). The Z-equivalences shown in Fig. 1 do not require the molecule to be planar. The results remain unchanged when the horizontal m is omitted from the symmetry assumed for the molecule. To the molecules shown in Fig. 1 one may add the as yet unknown polyhedrane $C_{12}H_{12}$ and prismane $C_{12}H_{12}$, which would be Z-isomorphic with **12–2** and **12–3** respectively. This example shows how consideration of Z-isomorphism extends the usefulness of the tabulation of N.

The cycle-index method for determining N is applicable to any assembly of V points, regardless of whether or not the points form a convex hull.* However, many of the sets of points considered here can conveniently be visualized as convex polyhedra. Although in some cases two or more non-isomorphic polyhedra can be constructed from a given set of V points, it is clear that N is independent of the edge-connectivity of such polyhedra. For example, for $V = 14$ and $m3m$ (O_h), the 14 points can be joined to form a tetrahexadron $\{h0l\}$ (**14–3**), a trisoctahedron $\{hhl\}$ $h > l$ (**14–3′**), or a rhombic dodecahedron $\{101\}$ (**14–3″**). The three polyhedra are not edge-isomorphic, but they are Z-isomorphic. Such polyhedra are distinguished in Table 5 by primes and double primes.

* For example, the small stellated dodecahedron, a Kepler solid, is Z-isomorphic with the pentakisdodecahedron **32–3** if the inner as well as the outer vertices are counted, and the isomorphism extends over all the subgroups of **32–3**.

For V discrete points to form a convex polyhedron, the maximum p.g. symmetry of their configuration is restricted by the requirement that

$V=0,1,2 \pmod{n}$ for rotations through $2\pi/n$, $n \geq 2$,
$V=0,2 \pmod{2n}$ for rotary inversions, $n \geq 2$, and
$V=0 \pmod{2}$ for a centre of symmetry.

The minimum condition for $V=2 \pmod{n}$ and $2 \pmod{2n}$ is that two of the points be located on the rotation axis in such a way that the remaining $V-2$ points are confined between two parallel planes perpendicular to the rotation axis and each passing through one of the two points. Similarly, for $V=1 \pmod{n}$ the n-axis is polar and contains one of the V points; this point defines a plane perpendicular to the rotation axis and having the property that the remaining $V-1$ points are on one side of this plane. Additional requirements come from Euler's theorem and other theorems of combinatorial topology [*cf.* for example Grünbaum (1967)].

Selection of polyhedra

The assortment of polyhedra treated in this work is based on an arbitrary selection. The numbers $\mathcal{N}$ of *all* non-isomorphic convex polyhedra are large even for small values of V (Grünbaum, 1967), but the numbers $\mathcal{Z}$ of the Z-isomorphic classes among which the polyhedra are distributed are much smaller (Table 2). Our Tables 6 to 46 thus cover many more polyhedra than those named explicitly in Table 5, though of course the coverage decreases with increasing V. The $\mathcal{N}$ are known up to $V=8$. An exhaustive listing of the corresponding polyhedra has been provided by Britton & Dunitz (1973). For $V=8$ the 257 polyhedra† are distributed among only 19 Z-isomorphic classes, all of which are included in this work, and further, 140 of these polyhedra have p.g. symmetry C_1. The trends for $\mathcal{Z}/\mathcal{N}$ and $\mathcal{C}_1/\mathcal{N}$ in Table 2 show that for some of the $V>8$ the number of cycle indices evaluated here may include *all* the $\mathcal{Z}$ possible Z-isomorphic classes. The probability of this happening is greater for V that are prime or at least odd. The numbers of cycle indices evaluated are, for example,

V	9	10	11	12	13	14
Number of Z	28	50	28	65	30	78.

The selection in Table 5 includes polygons (a special class of two-dimensional polyhedra), the five Platonic polyhedra $\mathcal{P}\ell$, and all the cubic and icosahedral Archimedean polyhedra $\mathcal{A}$ and their duals $\mathcal{A}^*$.‡ Semi-regular polyhedra of the infinite $\mathcal{A}$ and $\mathcal{A}^*$ classes (Table 4) have been considered up to $V=24$, though not exhaustively. Polyhedra of reduced p.g. symmetry that have well-established names are listed under the corresponding parent polyhedron of maximum p.g. symmetry. For example, the rhombohedron **8–2**(*20*) and the tetragonal prism **8–2**(*15*) are listed under the cube **8–2**. Some general relationships are shown in Table 4.

† Maximum possible p.g. symmetry is assigned to every polyhedron in Britton & Dunitz's list.

‡ For illustrations of the $\mathcal{P}\ell$ and $\mathcal{A}$ polyhedra see, for example, Cundy & Rollett (1961) or Wells (1956). For the $\mathcal{A}^*$ polyhedra see Niggli (1941), Wells (1956) or Nowacki (1933).

Table 2. *The numbers of all non-isomorphic convex polyhedra of a given V* ($\mathcal{N}$), *of the corresponding Z-isomorphic classes* ($\mathcal{Z}$), *of the polyhedra of p.g. symmetry* C_1 ($\mathcal{C}_1$), *and of cycle indices evaluated*

V	$\mathcal{N}$	$\mathcal{Z}$	$100\mathcal{Z}/\mathcal{N}$	$\mathcal{C}_1$	$100\mathcal{C}_1/\mathcal{N}$	Number of Z
4	1	1	100	0	0	11
5	2	2	100	0	0	14
6	7	6	~86	0	0	30
7	34	8	~23·5	7	~21	18
8	257	19	~7·4	140	~55	45

Six of the eight convex deltahedra Δ bounded by congruent equilateral triangles (Freudenthal & van der Waerden, 1947) are members of the classes already mentioned: **3–1**, **4–2**, **5–3**, **6–4**, **7–3**, and **12–9**. The remaining three are **8–2**(*14*), **9–5**, and **10–9**.

The Kasper polyhedra $\mathcal{K}\alpha$ are generalized deltahedra. They are favoured as coordination polyhedra in crystal structures of metallic phases (Kasper, 1956). The three $\mathcal{K}\alpha$ polyhedra considered here are **14–7**, **15–5**, and **16–6**; $\mathcal{K}\alpha$-12 is the icosahedron **12–9**.

Among polyhedra of chemical interest are those of the 3-connected isogonal polyhedra whose vertex angles fall within the ranges consistent with potentially admissible C–C–C and H–C–C bond angles in the two classes of saturated hydrocarbons C_nH_n, the polyhedranes and the prismanes (Schultz, 1965). Apart from tetrahedrane and cubane, both of which have $\mathcal{P}\ell$ geometries all the other polyhedrane skeletons are $\mathcal{A}$ (**12–2**, **20–1**, **24–1**, **24–2**, **48–1**, **60–1**, **60–2**, **120–1**). Of the prismane skeletons seven are included here: **6–2**, **10–2**, **12–3**, **14–2**, **16–2**, **20–2**, **24–3**.

Derivative polyhedra were generated from the parent polyhedra mostly by methods that preserve p.g. symmetry. Regular truncation (complete or partial) of the vertices, augmentation by associating additional vertices with the faces (capping) or edges of the parent figure in a p.g. preserving manner, construction of duals $\mathcal{D}$ and vertex-figure derivatives $\mathcal{V}$ are such processes. In Table 5 the term *singly-capped* refers to augmentation by one vertex and *bicapped* to augmentation by two vertices on a principal axis of rotation. Other types of augmentation on faces are described by names like 'singly-capped trigonal prism + 1' *etc.*

Schematic projections of some of the less common polyhedra of Table 5 are shown in Fig. 2. It is useful to note that the $\mathcal{V}$ derivative of an n-sided bipyramid is an n-sided prism $+n$, that of an n-sided pyramid is a tapered antiprism (top basal face smaller than the bottom basal face), and that of an n-sided prism is a *completely truncated* n-sided prism (a class of its own, related to the prisms as the cuboctahedron is to the cube).

Partitions

Every partition $\Pi(V)$ of V corresponds to a combination of univalent (monodentate) substituents, *i.e.* to a 'chemical composition'. The number of partitions grows rapidly with V and so do the values of $N[\Pi(V)]$. It is then necessary to decide at which point tabulation can no longer be viewed as practical and potentially useful. In the present tabulation unrestricted partitions are included for $V \le 8$. Partitions up to quinary are included for $V=9$; up to quaternary for $V=10,11,12$; and up to ternary for V from 13 to 16. For $V \ge 17$ only binary partitions are listed. When $V>26$ the numbers $N[\Pi(V)]$ become very large even for binary

Table 3. *Sequence of point groups*

Only those settings are listed that appear in Tables 5 to 46; see text for conventions.

No.	P.g. and setting	No.	P.g. and setting	No.	P.g. and setting
1	1 (C_1)	*39*	$5/m$ (C_{5h})	*78*	11 (C_{11})
2	$\bar{1}$ ($C_i=S_2$)	*40*	$10/m$ (C_{10h})	*79*	11.2 (D_{11})
3	2 (C_2); *3v, 3a, 3d*	*41*	10.2 (D_{10})	*80*	$11m$ (C_{11v})
4	m (C_s); *4mh, 4ma, 4md*	*42*	$10m$ (C_{10v})	*81*	$\overline{22}$ (C_{11h})
5	$2/m$ (C_{2h}); *5v, 5a, 5d*	*43*	$\overline{10}m2$ (D_{5h}); *43a, 43d*	*82*	$\overline{22}m2$ (D_{11h})
6	222 (D_2); *6va, 6vd*	*44*	$10/mmm$ (D_{10h})	*83*	12 (C_{12})
7	$2mm$ (C_{2v}); *7mha, 7mhd, 7maa, 7mdd, 7mad*	*45*	532 (I)	*84*	$\overline{12}$ (S_{12})
8	mmm (D_{2h}); *8mha, 8mhd*	*46*	$53m$ (I_h)	*85*	$12/m$ (C_{12h})
9	4 (C_4)	*47*	7 (C_7)	*86*	$12.2.2$ (D_{12}); *86a, 86d*
10	$\bar{4}$ (S_4)	*48*	$\bar{7}$ ($C_{7i}=S_{14}$)	*87*	$12m$ (C_{12v})
11	$4/m$ (C_{4h})	*49*	72 (D_7)	*88*	$12m2$ (D_{6h}); *88a, 88d*
12	422 (D_4); *12a, 12d*	*50*	$7m$ (C_{7v})	*89*	$12/mmm$ (D_{12h})
13	$4mm$ (C_{4v}); *13ma, 13md*	*51*	$\bar{7}m$ (D_{7d}); *51a, 51d*	*90*	13 (C_{13})
14	$\bar{4}m2$ (D_{2d}); *14a, 14d*	*52*	14 (C_{14})	*91*	13.2 (D_{13})
15	$4/mmm$ (D_{4h}); *15ma, 15md*	*53*	$\overline{14}$ (C_{7h})	*92*	$13m$ (C_{13v})
16	3 (C_3)	*54*	$14/m$ (C_{14h})	*93*	$\overline{26}$ (C_{13h})
17	$\bar{3}$ ($C_{3i}=S_6$)	*55*	14.2 (D_{14})	*94*	$\overline{26}m2$ (D_{13h})
18	32 (D_3); *18a, 18d*	*56*	$14m$ (C_{14v})	*95*	15 (C_{15})
19	$3m$ (C_{3v}); *19ma, 19md*	*57*	$\overline{14}m2$ (D_{7h}); *57a, 57d*	*96*	15.2 (D_{15})
20	$\bar{3}m$ (D_{3d}); *20a, 20d*	*58*	$14/mmm$ (D_{14h})	*97*	$15m$ (C_{15v})
21	6 (C_6)	*59*	8 (C_8)	*98*	$\overline{30}$ (C_{15h})
22	$\bar{6}$ (C_{3h})	*60*	$\bar{8}$ (S_8)	*99*	$\overline{30}m2$ (D_{15h})
23	$6/m$ (C_{6h})	*61*	$8/m$ (C_{8h})	*100*	16 (C_{16})
24	622 (D_6); *24a, 24d*	*62*	822 (D_8)	*101*	$\overline{16}$ (S_{16})
25	$6mm$ (C_{6v}); *25ma, 25md*	*63*	$8mm$ (C_{8v}); *63ma, 63md*	*102*	$16/m$ (C_{16h})
26	$\bar{6}m2$ (D_{3h}); *26a, 26d*	*64*	$\bar{8}m2$ (D_{4d}); *64a, 64d*	*103*	16.2 (D_{16})
27	$6/mmm$ (D_{6h}); *27ma, 27md*	*65*	$8/mmm$ (D_{8h}); *65ma, 65md*	*104*	$16mm$ (C_{16v})
28	23 (T)	*66*	9 (C_9)	*105*	$\overline{16}m2$ (D_{8d}); *105a, 105d*
29	$m3$ (T_h)	*67*	$\bar{9}$ ($C_{9i}=S_{18}$)	*106*	$16/mmm$ (D_{16h})
30	432 (O)	*68*	92 (D_9)	*107*	17 (C_{17})
31	$\bar{4}3m$ (T_d)	*69*	$9m$ (C_{9v})	*108*	17.2 (D_{17})
32	$m3m$ (O_h)	*70*	$\bar{9}m2$ (D_{9d}); *70a, 70d*	*109*	$17m$ (C_{17v})
33	5 (C_5)	*71*	18 (C_{18})	*110*	$\overline{34}$ (C_{17h})
34	$\bar{5}$ ($C_{5i}=S_{10}$)	*72*	$\overline{18}$ (C_{9h})	*111*	$\overline{34}m2$ (D_{17h})
35	52 (D_5); *35a, 35d*	*73*	$18/m$ (C_{18h})	*112*	19 (C_{19})
36	$5m$ (C_{5v}); *36ma, 36md*	*74*	18.2 (D_{18})	*113*	19.2 (D_{19})
37	$\bar{5}m$ (D_{5d}); *37a, 37d*	*75*	$18mm$ (C_{18v})	*114*	$19m$ (C_{19v})
38	10 (C_{10})	*76*	$\overline{18}m2$ (D_{9h})	*115*	$\overline{38}$ (C_{19h})
		77	$18/mmm$ (D_{18h})	*116*	$\overline{38}m2$ (D_{19h})

Table 4. *General relationships of some classes of convex polyhedra*

	Polyhedron	V	F		E/V	–	
P.g.		F	V	E	–	E/V	Dual polyhedron
D_{nh}	n-gons†	n	2	n	1	–	
C_{nv}	n-sided pyramids	$n+1$	$n+1$	$2n$	<2	<2	n-sided pyramids
D_{nh}	n-sided prisms ($\mathscr{A}$)	$2n$	$n+2$	$3n$	$\frac{3}{2}$	<3	n-sided bipyramids ($\mathscr{A}$*)
D_{nd}	Antiprisms projecting to regular $2n$-gons ($\mathscr{A}$)	$2n$	$2n+2$	$4n$	2	<2	Streptohedra projecting to regular $2n$-gons as contours ($\mathscr{A}$*)
D_{nh}	Bicapped n-sided prisms	$2n+2$	$3n$	$5n$	$<\frac{5}{2}$	$\frac{5}{3}$	Basally truncated n-sided bipyramids
D_{nd}	Bicapped antiprisms projecting to regular $2n$-gons as contours	$2n+2$	$4n$	$6n$	<3	$\frac{3}{2}$	Basally truncated streptohedra projecting to regular $2n$-gons as contours
	Deltahedra (triangular faces only)	V	$2(V-2)$	$3(V-2)$	$3-(6/V)$‡	–	

† $Z(C_{nv})=Z(D_n)=Z(D_{nh})$, $Z(C_n)=Z(C_{nh})$, $Z(4ma)=Z(3a)=Z(7mha)$, $Z(4mh)=Z(1)$.
‡ This is the upper limit of the E/V ratio for convex polyhedra

Table 5. *List of polyhedra*

No.	P.g.	F	E	Polyhedron	Table
3–1	*26*	2	3	Triangle	19
4–1	*15*	2	4	Square	46
4–2	*31*	4	6	Tetrahedron, ($\mathscr{P}\ell$, Δ), self-dual, $\mathscr{V}$ = **6–4**	8
4–2 (*19*)	*19*	4	6	Trigonal pyramid, $\mathscr{V}$ = **6–4** (*19*)	8
4–2 (*14*)	*14*	4	6	Bisphenoid, $\mathscr{V}$ = **6–4** (*14*)	8
5–1	*43*	2	5	Pentagon	19
5–2	*13*	5	8	Square pyramid, $\mathscr{V}$ = **8–1** (*15ma*)	21
5–3	*26*	6	9	Trigonal bipyramid (Δ), $\mathscr{D}$ = **6–2**, $\mathscr{V}$ = **9–5** (*26*)	21
6–1	*27*	2	6	Hexagon	46
6–2	*26*	5	9	Trigonal prism, $\mathscr{D}$ = **5–3**	46
6–3	*36*	6	10	Pentagonal pyramid	20
6–4	*32*	8	12	Octahedron ($\mathscr{P}\ell$, Δ), $\mathscr{D}$ = **8–2**, $\mathscr{V}$ = **12–5**	9
6–4 (*20*)	*20*	8	12	Trigonal antiprism, $\mathscr{D}$ = **8–2** (*20*)	9
6–4 (*15*)	*15*	8	12	Tetragonal bipyramid, $\mathscr{D}$ = **8–2** (*15*)	9
6–4 (*14*)	*14*	8	12	Tetragonal scalenohedron [= **6–4** (*14d*)]	9
7–1	*57*	2	7	Heptagon	19
7–2	*25*	7	12	Hexagonal pyramid	22
7–2 (*19*)	*19*	7	12	Singly-capped trigonal prism [= **7–2** (*19ma*)]	22, 46
7–2 (*19*)	*19*	10	15	Singly-capped trigonal antiprism [= **7–2** (*19ma*)]	22, 46
7–2 (*7*)	*7*	8	13	Trigonal prism + 1 [= **7–2** (*7mad*)]	22, 46
7–3	*43*	10	15	Pentagonal bipyramid (Δ)	22
8–1	*65*	2	8	Octagon	23
8–1 (*64*)	*64*	10	16	Square antiprism [= **8–1** (*64a*)]	23, 46
8–1 (*7*)	*7*	11	17	Trigonal prism + 2 [= **8–1** (*7maa*)]	23, 46
8–2	*32*	6	12	Cube ($\mathscr{P}\ell$), $\mathscr{D}$ = **6–4**, $\mathscr{V}$ = **12–5**	12
8–2 (*31*)	*31*	12	18	Tristetrahedron ($\mathscr{A}^*$), $\mathscr{D}$ = **12–2**	12, 46
8–2 (*20*)	*20*	6	12	Rhombohedron (trigonal streptohedron, $\mathscr{A}^*$), $\mathscr{D}$ = **6–4** (*20*)	12, 46
8–2 (*15*)	*15*	6	12	Tetragonal prism, $\mathscr{D}$ = **6–4** (*15*)	12, 46
8–2 (*14*)	*14*	12	18	Dodecadeltahedron (Δ) [= **8–2** (*14d*)]	12, 46
8–2 (*8*)	*8*	8	14	See Fig. 2 [= **8–2** (*8mha*)]	12, 46
8–3	*50*	8	14	Heptagonal pyramid	20
8–4	*14*	8	14	See Fig. 2	46
8–5	*26*	9	15	Bicapped trigonal prism	46
8–5 (*4*)	*4*	10	16	Singly-capped trigonal prism + 1 [= **8–2** (*4ma*)]	12
8–6	*27*	12	18	Hexagonal bipyramid	23
8–6 (*20*)	*20*	12	18	Hexagonal (ditrigonal) scalenohedron [= **8–6** (*20d*) = **8–2** (*20*)]	12
9–1	*76*	2	9	Nonagon	24
9–2	*63*	9	16	Octagonal pyramid	24
9–2 (*13*)	*13*	13	20	Singly-capped square antiprism [= **9–2** (*13ma*)]	24, 46
9–3	*13*	9	16	Singly-capped cube	25
9–4	*7*	12	19	Bicapped trigonal prism + 1	25
9–5	*26*	14	21	Tetrakaidecadeltahedron (Δ)	25
9–5 (*26*)	*26*	8	15	$\mathscr{D}$ (**8–5**) = basally truncated **5–3**	25
9–5 (*26*)	*26*	11	18	$\mathscr{V}$(**6–2**) = $\mathscr{V}$(**5–3**)	25
9–5 (*26*)	*26*	14	21	Trigonal prism + 3 (faces not all equilateral)	25
9–5 (*19*)	*19*	14	21	Octahedron + 3 (symmetric)	25, 46
9–5 (*4*)	*4*	13	20	Singly-capped trigonal prism + 2 [= **9–5** (*4ma*) = **9–2** (*4ma*)]	24
9–6	*57*	14	21	Heptagonal bipyramid	25
10–1	*44*	2	10	Decagon	27
10–2	*43*	7	15	Pentagonal prism	46
10–3	*69*	10	18	Nonagonal pyramid	28
10–4	*37*	12	20	Pentagonal antiprism	46
10–5	*15*	12	20	Bicapped cube	28
10–6	*7*	15	23	Bicapped trigonal prism + 2	46
10–7	*65*	16	24	Octagonal bipyramid	26
10–7 (*64*)	*64*	8	16	Streptohedron ($\mathscr{A}^*$) [= **10–7** (*64d*)], $\mathscr{D}$ = **8–1** (*64*)	26, 46
10–8	*19*	16	24	Singly-capped trigonal prism + 3	46
10–9	*64*	16	24	Hexakaidecadeltahedron (Δ)	46
10–10	*64*	16	24	Bicapped square antiprism [= **10–9**]	46
10–11	*31*	16	24	Tetrahedron with broken edges (= octahedron + 4)	27
11–1	*82*	2	11	Hendecagon	19
11–2	*42*	11	20	Decagonal pyramid	30
11–2 (*36*)	*36*	16	25	Icosahedron − 1 (= singly-capped pentagonal antiprism) [= **11–2** (*36ma*)]	30, 46
11–3	*7*	15	24	Cube + 3 (equatorial)	46
11–4	*76*	18	27	Nonagonal bipyramid	29
11–5	*26*	18	27	Bicapped tetrakaidecadeltahedron	30
11–5 (*19*)	*19*	15	24	Cube + 3 (vicinal)	30, 46
11–6	*7*	12	21	See Fig. 2	46
12–1	*89*	2	12	Dodecagon	32
12–2	*31*	8	18	Truncated tetrahedron ($\mathscr{A}$), $\mathscr{D}$ = **8–2** (*31*)	46

Table 5 (*cont.*)

No.	P.g.	F	E	Polyhedron	Table
12–3	*27*	8	18	Hexagonal prism	32
12–4	*80*	12	22	Hendecagonal pyramid	20
12–5	*32*	14	24	Cuboctahedron ($\mathscr{A}$), $\mathscr{D}$ = **14–3″**	13
12–6	*88*	14	24	Hexagonal antiprism	46
12–7	*15*	18	28	Cube + 4 (equatorial)	46
12–8	*7*	18	28	Cube + 4 (vicinal)	46
12–9	*46*	20	30	Icosahedron ($\mathscr{P}\ell$, Δ), $\mathscr{D}$ = **20–1**, $\mathscr{V}$ = **30–1**	6
12–9 (*37*)	*37*	20	30	Bicapped pentagonal antiprism	6
12–10	*44*	20	30	Decagonal bipyramid	31
12–11	*20*	8	18	Basally truncated rhombohedron [= **12–9**]	6
12–12	*15*	10	20	Basally truncated tetragonal bipyramid	32
12–13	*14*	12	22	See Fig. 2	46
12–14	*8*	12	22	See Fig. 2	46
12–15	*43*	15	25	Bicapped pentagonal prism	46
12–16	*14*	16	26	See Fig. 2	46
13–1	*94*	2	13	Tridecagon	19
13–2	*87*	13	24	Dodecagonal pyramid	33
13–3	*25*	13	24	Singly-capped hexagonal prism	33
13–4	*13*	21	32	Cube + 5	33
13–5	*82*	22	33	Hendecagonal bipyramid	33
14–1	*58*	2	14	Tetradecagon	36
14–2	*57*	9	21	Heptagonal prism	46
14–3	*32*	24	36	Tetrahexahedron ($\mathscr{A}$*), $\mathscr{D}$ = **24–2**	10, 11
14–3 (*31*)	*31*	24	36	Hextetrahedron	10, 11, 46
14–3′	*32*	24	36	Trisoctahedron ($\mathscr{A}$*) [= **14–3**], $\mathscr{D}$ = **24–1**	10, 11
14–3″	*32*	12	24	Rhombic dodecahedron ($\mathscr{A}$*) [= **14–3**], $\mathscr{D}$ = **12–5**	10, 11
14–3″ (*31*)	*31*	12	24	Deltohedron [= **14–3** (*31*)]	10, 11, 46
14–4	*92*	14	26	Tridecagonal pyramid	20
14–5	*27*	18	30	Bicapped hexagonal prism	37
14–6	*89*	24	36	Dodecagonal bipyramid	34, 35
14–7	*88*	24	36	Bicapped hexagonal antiprism ($\mathscr{K}a$-14)	46
14–8	*20*	24	36	Bicapped icosahedron	46
14–9	*51*	18	30	Heptagonal antiprism	46
14–10	*26*	9	21	$\mathscr{D}$(**9–5**)	36
15–1	*99*	2	15	Pentadecagon	38
15–2	*43*	12	25	Basally truncated pentagonal bipyramid	40
15–3	*26*	17	30	Hexagonal prism + 3 (alternating)	40
15–4	*94*	26	39	Tridecagonal bipyramid	39
15–5	*26*	26	39	Kasper-15 ($\mathscr{K}a$)	40
16–1	*106*	2	16	Hexadecagon	41
16–2	*65*	10	24	Octagonal prism	42
16–2 (*64*)	*64*	10	24	Basally truncated **10–7** (*64d*) = $\mathscr{D}$(**10–9**) [= **16–2** (*64d*)]	42, 46
16–3	*31*	16	30	Tristetrahedron with truncated trivalent vertices	42
16–4	*64*	18	32	$\mathscr{V}$[**8–1** (*64*)] [= **16–1** (*64d*)]	41
16–5	*105*	18	32	Octagonal antiprism [= **16–1** (*105d*)]	41
16–6	*19*	28	42	Kasper-16 ($\mathscr{K}a$)	46
17–1	*111*	2	17	Heptadecagon	*19*
18–1	*77*	2	18	Octadecagon	43
18–2	*26*	11	27	See Fig. 2	46
18–3	*32*	32	48	Cuboctahedron + 6 (above square faces)	15
19–1	*116*	2	19	Nonadecagon	19
20–1	*46*	12	30	Pentagonal dodecahedron ($\mathscr{P}\ell$), $\mathscr{D}$ = **12–9**, $\mathscr{V}$ = **30–1**	6
20–1 (*29*)	*29*	12	30	Pyritohedron	6
20–1 (*28*)	*28*	12	30	Tetartoid	6
20–1′ (*29*)	*29*	24	42	See Fig. 2	6
20–2	*44*	12	30	Decagonal prism	44
20–3	*32*	30	48	Cuboctahedron + 8 (above triangular faces)	16
24–1	*32*	14	36	Truncated octahedron ($\mathscr{A}$), $\mathscr{D}$ = **14–3**	12
24–1 (*30*)	*30*	38	60	Snub cube ($\mathscr{A}$), $\mathscr{D}$ = **38–1**	12
24–2	*32*	14	36	Truncated cube ($\mathscr{A}$), $\mathscr{D}$ = **14–3′**	14
24–2′	*32*	26	48	Rhombicuboctahedron† ($\mathscr{A}$), $\mathscr{D}$ = **26–1**	14
24–3	*89*	14	36	Dodecagonal prism	45
24–4	*64*	26	48	Antirhombicuboctahedron	45
26–1	*32*	24	48	Trapezohedron (trapezoidal icositetrahedron, $\mathscr{A}$*), $\mathscr{D}$ = **24–2′**	17
26–1 (*29*)	*29*	24	48	Diploid	17
26–1′	*32*	48	72	Hexoctahedron ($\mathscr{A}$*), $\mathscr{D}$ = **48–1**	17
30–1	*46*	32	60	Icosidodecahedron ($\mathscr{A}$), $\mathscr{D}$ = **32–1**	7
32–1	*46*	30	60	Rhombic triacontahedron ($\mathscr{A}$*), $\mathscr{D}$ = **30–1**	7
32–2	*46*	60	90	Trisicosahedron ($\mathscr{A}$*), $\mathscr{D}$ = **60–1**	7
32–3	*46*	60	90	Pentakisdodecahedron ($\mathscr{A}$*), $\mathscr{D}$ = **60–2**	7

Table 5 (*cont.*)

No.	P.g.	F	E	Polyhedron	Table
38–1	*30*	24	60	Gyroid (pentagonal icositetrahedron, $\mathscr{A}$*), $\mathscr{D}$=**24–6**	18
48–1	*32*	26	72	Truncated cuboctahedron ($\mathscr{A}$), $\mathscr{D}$=**26–2**	18
60–1	*46*	32	90	Truncated dodecahedron ($\mathscr{A}$), $\mathscr{D}$=**32–2**	7
60–1 (*45*)	*45*	92	150	Snub dodecahedron ($\mathscr{A}$), $\mathscr{D}$=**92–1**	7
60–2	*46*	32	90	Truncated icosahedron ($\mathscr{A}$), $\mathscr{D}$=**32–3**	7
60–3	*46*	62	120	Rhombicosidodecahedron ($\mathscr{A}$), $\mathscr{D}$=**62–1**	7
62–1	*46*	60	120	Trapezoidal hexecontahedron ($\mathscr{A}$*), $\mathscr{D}$=**60–3**	7
62–2	*46*	120	180	Hecatonicosahedron (hexicosahedron, $\mathscr{A}$*) $\mathscr{D}$=**120–1**	7
92–1	*45*	60	150	Pentagonal (pentagonoidal) hexecontahedron ($\mathscr{A}$*), $\mathscr{D}$=**60–1** (*45*)	7
120–1	*46*	62	180	Truncated icosidodecahedron ($\mathscr{A}$), $\mathscr{D}$=**62–2**	7

† Rotate projection in Fig. 2 by 45° to bring **24–2′** in Z-coincidence with **24–2**.

Table 7. I_h *and subgroups* ($V>20$)

Partition	*46*	*45*	*29*	*28*
		30-1 Icosidodecahedron		
$29^1 1^1$	1	1	2	3
$28^1 2^1$	8	11	23	40
$27^1 3^1$	46	78	183	352
$26^1 4^1$	262	483	1 179	2 310
$25^1 5^1$	1 257	2 423	6 006	11 921
$24^1 6^1$	5 113	10 025	24 929	49 625
$23^1 7^1$	17 238	34 112	85 098	169 832
$22^1 8^1$	49 270	97 890	244 413	488 085
$21^1 9^1$	119 997	238 993	596 922	1 192 843
$20^1 10^1$	251 512	501 507	1 253 109	2 504 502
$19^1 11^1$	456 729	911 456	2 277 639	4 553 276
$18^1 12^1$	722 750	1 442 875	3 606 061	7 209 160
	32-1 (= 32-2, 32-3) Rhombic triacontahedron			
$31^1 1^1$	2	2	3	4
$30^1 2^1$	12	13	29	46
$29^1 3^1$	62	86	229	420
$28^1 4^1$	378	636	1 584	3 040
$27^1 5^1$	1 838	3 362	8 551	16 788
$26^1 6^1$	8 004	15 263	38 235	75 686
$25^1 7^1$	28 832	56 130	141 041	280 548
$24^1 8^1$	89 355	175 775	440 034	877 010
$23^1 9^1$	236 269	467 520	1 171 249	2 337 480
$22^1 10^1$	546 217	1 076 382	2 692 807	5 377 272
	60-1 (= 60-2, 60-3) Truncated dodecahedron			
$59^1 1^1$	1	1	3	5
$58^1 2^1$	23	37	83	155
$57^1 3^1$	303	577	1 447	2 865
$56^1 4^1$	4 190	8 236	20 459	40 745
$55^1 5^1$	45 718	91 030	227 766	455 126
$54^1 6^1$	418 470	835 476	2 087 434	4 173 130
$53^1 7^1$	3 220 218	6 436 782	16 093 782	32 183 910
$52^1 8^1$	21 330 558	42 650 532	106 618 833	213 225 255
	62-1 (= 62-2) Hexecontahedron			
$61^1 1^1$	3	3	5	7
$60^1 2^1$	32	40	96	166
$59^1 3^1$	391	652	1 655	3 180
$58^1 4^1$	5 023	9 427	23 640	46 630
$57^1 5^1$	55 276	108 079	270 977	539 481
$56^1 6^1$	517 350	1 025 772	2 566 679	5 124 127
$55^1 7^1$	4 113 656	8 198 764	20 506 922	40 985 296
	92-1 Pentagonoidal hexecontahedron			
$91^1 1^1$	-	3	-	9
$90^1 2^1$	-	82	-	361
$89^1 3^1$	-	2 103	-	10 485
$88^1 4^1$	-	46 848	-	233 145
$87^1 5^1$	-	819 636	-	4 098 114
$86^1 6^1$	-	11 888 427	-	59 426 448
	120-1 Truncated icosidodecahedron			
$119^1 1^1$	1	2	5	10
$118^1 2^1$	75	134	315	610
$117^1 3^1$	2 347	4 694	11 715	23 430
$116^1 4^1$	68 912	137 352	342 790	684 990
$115^1 5^1$	1 588 155	3 176 310	7 940 751	15 881 502
$114^1 6^1$	30 448 389	60 887 906	152 209 015	304 406 610

Table 15. *Cuboctahedron* +6 **18–3**

Partition	*32*	*31*	*30*	*29*	*28*	*20*	*19*	*15*	*14a*	*14d*	*13*	*12*	*11*	*10*	*9*	*8mha*	*8mhd*	*7maa*	*7mdd*	*7mad*	*6va*	*5a*	*5d*	*4ma*	*4md*
$17^1 1^1$	2	2	2	2	2	4	7	4	4	5	6	4	4	5	6	4	6	7	9	8	6	6	7	12	13
$16^1 2^1$	9	11	10	12	15	24	42	21	26	31	32	25	26	41	41	31	36	47	57	52	45	46	51	83	93
$15^1 3^1$	31	46	42	50	76	97	186	78	116	132	136	112	116	208	208	128	144	224	256	240	216	216	232	424	456
$14^1 4^1$	94	149	142	161	264	322	620	255	413	452	459	406	420	776	776	444	483	806	884	845	792	799	838	1562	1640
$13^1 5^1$	230	392	380	416	728	832	1636	646	1120	1196	1212	1108	1132	2156	2160	1172	1248	2212	2364	2288	2184	2184	2260	4340	4492
$12^1 6^1$	471	832	811	877	1578	1745	3433	1339	2395	2520	2541	2374	2427	4664	4664	2488	2613	4746	4996	4871	4704	4725	4850	9366	9616
$11^1 7^1$	770	1396	1368	1456	2680	2912	5768	2226	4076	4252	4280	4048	4108	7984	7984	4192	4368	8096	8448	8272	8040	8040	8216	16024	16376
$10^1 8^1$	1043	1907	1872	1985	3678	3970	7856	3028	5585	5800	5835	5550	5645	10974	10974	5740	5955	11104	11534	11319	11034	11069	11284	22012	22442
9^2	1154	2120	2088	2200	4100	4390	8710	3344	6200	6430	6468	6168	6248	12190	12196	6350	6580	12330	12790	12560	12260	12260	12490	24450	24910

18 = 18-1(*26a*). - *17* = 18-1(*23*). - *16* = 18-1(*22*). - *6vd* = *6va*. - *3a*, *3d* = 18-1(*7mha*). - *2* = 18-1(*7mhd*).

partitions. Tabulation is then restricted to the first few binary partitions and to the cubic or icosahedral point groups (Tables 7 and 18).

When the p.g. symmetry of a polyhedron is C_1, $N[\Pi(V)]$ for a partition $\Pi(V)=a^\alpha b^\beta c^\gamma \ldots$, $\alpha a+\beta b+\gamma c+\ldots=V\ (a>b>c\ldots)$, is equal to the multinomial coefficient $C(V;\Pi)=C(V;a^\alpha,b^\beta,c^\gamma\ldots)=V!/a!^\alpha b!^\beta c!^\gamma\ldots$ and is not listed.

Evaluation of *N* by computer

Initially only binary partitions and a small number of polyhedra were considered, and the N were obtained essentially by hand calculation using Miller's (1954) extensive tables of binomial coefficients. However, as the enumeration assumed a more systematic character, the labour involved in hand computation became prohibitive and the evaluation of N was adapted to machine computation. Special programming methods had to be employed (White, 1972), for the evaluation is essentially an algebraic rather than numerical task involving expansion of products and powers of polynomials with integral coefficients and exponents. The computations were performed on an IBM 360/50 installation at the Dalhousie Computer Centre.

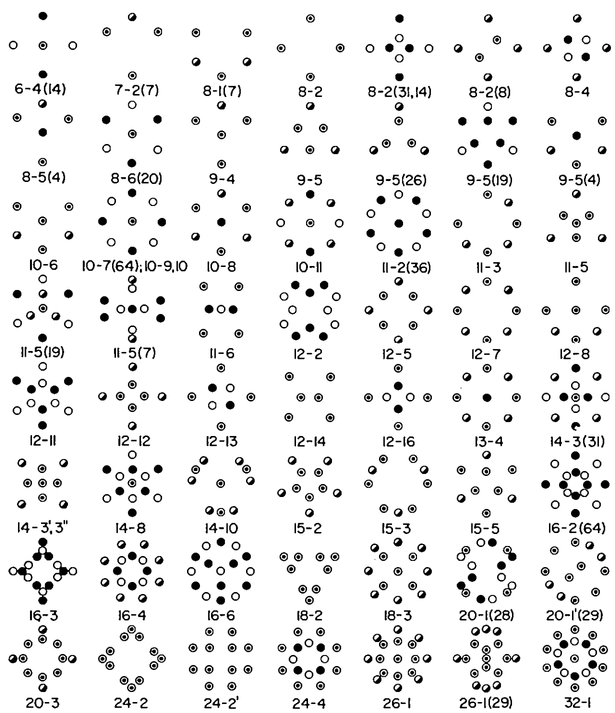

Fig. 2. Schematic parallel projections of the vertices of some of the less common polyhedra of Table 5. Full circles, vertices above the equatorial plane; half-filled circles, vertices in the equatorial plane; open circles, vertices below the equatorial plane. Double circles indicate coincidence, in projection, of a vertex above the equatorial plane and one below the equatorial plane.

Presentation of the results

The values of N for the polyhedra of Table 5 are listed in Tables 6 to 45.* The following conventions are observed.

All the point groups required are listed in Table 3. They are identified by running numbers *1* to *116*. The crystallographic point groups follow the order in which they appear in the space-group sequence in *International Tables for X-ray Crystallography* (1952).

Progressive reduction of the p.g. symmetry of a polyhedron sometimes results in two or more distinct orientations of the vertices relative to the symmetry elements of the reduced p.g., each orientation corresponding to a different Z and thus to a different set of values of N. To specify the position of a twofold axis, the letters v (vertical), a (axial), or d (diagonal) are associated with the running p.g. number. A *vertical* digyre coincides with the principal rotation axis of order $2n$, or an inversion axis of order $4n$, in the parent polyhedron of maximum p.g. symmetry. An *axial* digyre passes through a vertex, or a pair of opposing vertices, situated in the equatorial plane of the poly-

* Most of these voluminous tables have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 30962 (41 pp., 1 microfiche). Tables 7, 15 and 31 are reproduced in full, as examples of the type of information contained. Copies of the deposited tables may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 31. *Decagonal bipyramid* **12–10**

Partition	*44*	*43a*	*43d*	*42*	*41*	*39*	*38*	*37a*	*36md*	*8*	*7mha*	*7mhd*	*4mh*
$11^1 1^1$	2	3	2	3	2	3	3	2	3	4	7	6	11
$10^1 2^1$	7	10	9	8	7	12	8	7	10	19	32	31	56
$10^1 1^2$	8	15	12	11	8	23	15	8	15	30	59	56	111
$9^1 3^1$	14	25	20	19	14	35	23	16	27	50	95	90	175
$8^1 4^1$	29	49	45	37	33	75	51	33	57	107	199	195	375
$9^1 2^1 1^1$	32	61	54	43	36	103	67	38	71	136	267	260	515
$7^1 5^1$	40	74	64	56	46	118	82	50	90	158	306	296	582
6^2	48	84	78	64	58	136	96	58	104	186	352	346	672
$9^1 1^3$	54	108	102	72	66	204	132	66	132	258	516	510	1020
$8^1 3^1 1^1$	82	161	148	115	102	291	199	104	203	374	743	730	1455
$8^1 2^2$	129	240	231	174	165	432	300	165	312	567	1104	1095	2160
$7^1 4^1 1^1$	154	302	284	222	204	558	398	208	406	714	1418	1400	2790
$6^1 5^1 1^1$	208	410	388	306	284	766	558	288	566	974	1938	1916	3822
$8^1 2^1 1^2$	224	445	430	315	300	855	595	302	599	1080	2155	2140	4275
$7^1 3^1 2^1$	298	584	556	436	408	1092	796	416	812	1394	2768	2740	5460
$6^1 4^1 2^1$	506	976	954	748	726	1848	1392	726	1416	2366	4672	4650	9240
$7^1 3^1 1^2$	552	1104	1080	816	792	2160	1584	792	1584	2712	5424	5400	10800
$5^2 2^1$	586	1154	1112	892	850	2194	1670	862	1694	2784	5538	5496	10962
$6^1 3^2$	642	1272	1228	980	936	2436	1852	944	1868	3082	6144	6100	12180
$7^1 2^2 1^1$	830	1648	1612	1236	1200	3204	2380	1208	2396	4038	8056	8020	16020
$6^1 4^1 1^2$	934	1862	1832	1422	1392	3654	2774	1396	2782	4590	9170	9140	18270
$5^1 4^1 3^1$	936	1854	1800	1458	1404	3570	2778	1416	2802	4512	8994	8940	17850
$5^2 1^2$	1102	2204	2168	1700	1664	4336	3328	1664	3328	5436	10872	10836	21672
4^3	1170	2286	2250	1818	1782	4410	3474	1782	3510	5598	11106	11070	22050
$6^1 3^1 2^1 1^1$	1822	3632	3580	2836	2784	7140	5548	2792	5564	8966	17912	17860	35700
$5^1 4^1 2^1 1^1$	2664	5310	5244	4242	4176	10458	8322	4188	8346	13128	26226	26160	52290
$6^1 2^3$	2736	5400	5352	4272	4224	10584	8328	4224	8376	13344	26568	26520	52920
$5^1 3^2 1^1$	3480	6960	6888	5616	5544	13776	11088	5544	11088	17256	34512	34440	68880
$4^2 3^1 1^1$	4308	8598	8520	7026	6948	17010	13866	6960	13890	21324	42618	42540	85050
$5^1 3^1 2^2$	5190	10344	10236	8460	8352	20412	16644	8376	16692	25614	51168	51060	102060
$4^2 2^2$	6438	12768	12690	10572	10494	25200	20808	10494	20880	31674	63168	63090	126000
$4^1 3^2 2^1$	8394	16752	16620	14028	13896	33180	27732	13920	27780	41586	83112	82980	165900
3^4	10992	21984	21840	18624	18480	43680	36960	18480	36960	54672	109344	109200	218400

40 = 12-9(*40*). – *37d* = 12-9(*37*). – *36ma* = 12-9(*36*). – *35a* = *36md*. – *35d* = 12-9(*35*). – *34* = 12-9(*34*). – *33* = 12-9(*33*). – *7mad* = 12-5(*7mad*). – *6*, *5a* = 12-5(*7maa*). – *5d* = 12-9(*5*). – *4ma* = 12-9(*4*). – *4md*, *3d*, *2* = 12-9(*3*). – *3v*, *3a* = 12-5(*4ma*).

hedron (⊥ principal axis); if the polyhedron has no vertices in the equatorial plane, the axial digyre is an intersection of the equatorial plane and an axial mirror plane (see below). A *diagonal* digyre corresponds to the remaining, third type of position. Similarly, the position of a mirror plane is specified by the letters *h* (horizontal), *a* (axial), *d* (diagonal), which follow *m* after the running p.g. number. A *horizontal* mirror plane is perpendicular to the principal axis of the parent polyhedron of maximum p.g. symmetry. An *axial* mirror plane contains a vertex, or a pair of opposing vertices, in the equatorial plane; alternatively it contains a vertical edge, or a pair of opposing vertical edges, of the parent polyhedron. In polyhedra belonging to the tetragonal and hexagonal systems it corresponds to the axial plane *xz* or *yz* with the polyhedron in the 'first-order' setting. A *diagonal* mirror plane corresponds to the remaining, third type of position. In C_{2v} two nonequivalent mirror planes, mutually orthogonal but containing different numbers of vertices, are distinguished by v' and v''.

For the polyhedra represented in Fig. 2 the axial digyre or mirror plane (*ma* or v') is always vertical in the plane of paper. It is important to note that the cube does not have the standard crystallographic orientation: it is oriented like a 'first-order' tetragonal prism, to facilitate comparison with its derivative polyhedra of subgroup symmetries. Where no letters in italics are associated with the running p.g. number even though multiple choice of orientation is possible, the alternatives are all *Z*-isomorphic.

The entries for $(V-1)^1 1^1$, which give the numbers of nonequivalent sets of vertices of the unsubstituted polyhedron, can serve to check orientation of the vertices relative to the symmetry elements.

In Tables 6 to 45 the polyhedra are grouped so as to effect a maximum economy of space. Duplication due to *Z*-isomorphism has been eliminated by suitable entries and footnotes in the tables, and by listing additional *Z*-isomorphisms in Table 46. In Table 12 the entries *31* and *19* for **24–1** signify that the *N* values for **24–1** (*29*) and **24–1** (*18*) are the same as for **24–1** (*31*) and **24–1** (*19*) respectively.

Table 46. *Z-equivalences for polyhedra of Table* 5

4–1 (15, 14a, 14d, 13, 12) = **4–2** (14). – **4–1** (11, 10, 9) = **4–2** (10). – **4–1** (8mha, 7maa, 6va, 5a) = **4–2** (7). – **4–1** (8mhd, 7mdd, 6vd, 5d) = **4–2** (6). – **4–1** (7mha, 4ma, 3a) = **4–2** (4). – **4–1** (7mhd, 5v, 4md, 3v, 3d, 2) = **4–2** (3). – **4–1** (4mh) = **4–2** (1).

6–1 (27, 25, 24, 20a, 20d) = **6–2** (26) = **6–4** (20). – **6–1** (26a, 19ma, 18a) = **6–2** (19) = **6–4** (19). – **6–1** (26d, 19md, 18d) = **6–2** (18) = **6–4** (18). – **6–1** (23, 21, 17) = **6–2** (22) = **6–4** (17). – **6–1** (22, 16) = **6–2** (16) = **6–4** (16). – **6–1** (8, 7mad, 6, 5a, 5d) = **6–2** (7) = **6–4** (6vd). – **6–1** (7mha, 4ma, 3a) = **6–2** (4ma) = **6–4** (4md). – **6–1** (7mhd, 5v, 4md, 3v, 3d, 2) = **6–2** (4mh, 3) = **6–4** (3d). – **6–1** (4mh) = **6–4** (1).
Subgroups. **6–4** (20): 19, 18, 17, 16, 5d, 4ma, 3d = 2. – **6–4** (15): 14a, 14d, 13, 12, 11, 10, 9, 8ma, 8md, 7maa, 7mdd = 6va, 7mad = 5a, 6vd = 5d, 4ma, 4md = 3a, 3d = 2. – **6–4** (14d): 10, 7maa, 6vd, 4ma, 3a, 3d.

Subgroups. **7–2** (19ma): 16, 4ma. – **7–2** (7mad): 4ma, 4md = 3v.

Table 46 (*cont.*)

8–4 (14) = **8–1** (15ma). – **8–4** (10) = **8–1** (11). – **8–4** (7, 6) = **8–1** (8mha). – **8–4** (4, 3a) = **8–1** (7mha). – **8–4** (3v) = **8–1** (7mhd). – **8–5** = **8–2** for 19, 18, 16. – **8–5** (26) = **8–2** (20). – **8–5** (22) = **8–2** (17). – **8–5** (7) = **8–2** (7mad). – **8–5** (4ma) = **8–2** (4ma). – **8–5** (4mh, 3) = **8–2** (4md).
Subgroups. **8–1** (64a): 60, 13ma, 12d, 9, 7maa, 6vd, 4ma, 3v = 3d. – **8–1** (7maa): 4ma, 3v. – **8–2** (31): 28, 19, 16, 14d, 10, 7maa, 6vd, 4ma, 3a. – **8–2** (20): 19, 18, 17, 16, 5a, 4ma, 3a = 2. – **8–2** (15): 14a = 12, 14d = 13, 11, 10 = 9, 8mha, 8mhd, 7maa, 7mdd = 6va = 6vd = 5d, 7mad = 5a, 4ma, 4md = 3a = 3d = 2. – **8–2** (14d): 10, 7maa, 6vd, 4ma, 3a = 3d. – **8–2** (8mha): 7maa, 7mad = 5a, 6va = 5d, 4ma, 4md = 3a = 2.

Subgroups. **9–2** (13ma): 9, 7maa, 4ma, 3. – **9–5** (19): 16, 4ma.

10–2 = **10–4** for 36, 35, 33, 4mh, 4ma, 3. – **10–2** (43) = **10–4** (37) = **10–1** (44). – **10–2** (39) = **10–4** (34) = **10–1** (40). – **10–4** (36) = **10–1** (43a). – **10–4** (35) = **10–1** (43d). – **10–4** (33) = **10–1** (39). – **10–2** (7) = **10–4** (5) = **10–9** (6) = **10–1** (8). – **10–4** (4mh, 3, 2) = **10–6** (3) = **10–1** (7mhd). – **10–4** (4ma) = **10–6** (4mh) = **10–1** (7mha). – **10–6** (7) = **10–7** (5a). – **10–6** (4ma) = **10–8** (4) = **10–9** (4) = **10–7** (4ma). – **10–8** (19) = **10–11** (19). – **10–8** (16) = **10–3** (16). – **10–9** (64) = **10–7** (64d). – **10–9** = **10–7** for 60, 9, 3v, 3d. – **10–9** (13) = **10–7** (13ma). – **10–9** (12) = **10–7** (12d). – **10–9** (7) = **10–7** (7maa).
Subgroups. **10–7** (64d): 60, 13ma, 12d, 9, 7maa, 6vd, 4ma, 3v, 3d.

11–3 (7) = **11–6** (7) = **11–2** (7mad). – **11–3** (4mh) = **11–6** (4mv″) = **11–2** (4ma). – **11–3** (4md, 3) = **11–6** (4mv′, 3) = **11–1** (7mha).
Subgroups. **11–2** (36): 33, 4ma. – **11–5** (19): 16, 4ma.
Setting. **11–6**: v', $m_1^1 m_2^5$; v'', $m_1^3 m_2^4$.

12–2 = **12–5** for 31, 28, 19, 16, 10. – **12–2** (14) = **12–6** (14d) = **12–13** (14a) = **12–5** (14d). – **12–2** (7) = **12–6** (7maa) = **12–7** (7mdd, 6vd, 5d) = **12–13** (7mdd) = **12–5** (7maa). – **12–2** (6) = **12–6** (6vd) = **12–7** (6va) = **12–13** (6va) = **12–14** (7mhv′, 6, 5v, 5mv′) = **12–16** (6vd) = **12–9** (6). – **12–2** (4) = **12–6** (4ma, 4md, 3v, 3d) = **12–7** (4md, 3d) = **12–8** (4md) = **12–13** (4md) = **12–5** (4ma). – **12–2** (3) = **12–7** (3v, 3a, 2) = **12–8** (3a) = **12–13** (3v, 3a) = **12–14** (4mh, 4mv′, 3, 2) = **12–15** (4mh, 3) = **12–16** (3v, 3d) = **12–9** (3). – **12–6** = **12–9** for 18, 16. – **12–6** (88) = **12–1** (89). – **12–6** (84) = **12–1** (85). – **12–6** (25ma) = **12–5** (20). – **12–6** (24d) = **12–1** (27md). – **12–6** (21) = **12–9** (17). – **12–6** (19) = **12–5** (19). – **12–6** (10) = **12–7** (9) = **12–13** (10) = **12–16** (10) = **12–5** (10). – **12–7** = **12–5** for 15, 14a, 14d, 13, 12, 11, 10. – **12–7** (8mha) = **12–9** (8). – **12–7** (8mhd) = **12–5** (8mha). – **12–7** (7mha, 7maa) = **12–9** (7). – **12–7** (7mhd) = **12–5** (7mad). – **12–7** (5v, 5a) = **12–14** (7mhv″, 7mv′v″, 5mv″) = **12–15** (7) = **12–9** (5). – **12–7** (4mh, 4ma) = **12–14** (4mv″) = **12–15** (4ma) = **12–9** (4). – **12–8** (7mad) = **12–12** (5a). – **12–8** (4ma) = **12–12** (4ma). – **12–10** (5v) = **12–10** (7mhd). – **12–14** (8) = **12–3** (8). – **12–15** = **12–9** for 36, 35, 33. – **12–15** (43) = **12–9** (37). – **12–15** (39) = **12–9** (34). – **12–16** (14) = **12–12** (14d). – **12–16** (7) = **12–12** (7maa).
Subgroups. **12–9** (37): 36, 35, 34, 33, 5, 4, 3, 2.
Setting. **12–14**: v', m_2^6; v'', $m_1^4 m_2^4$.

14–2 = **14–9** for 50, 49, 47, 3. – **14–2** (57) = **14–9** (51) = **14–1** (58). – **14–2** (53) = **14–9** (48) = **14–1** (54). – **14–9** (50) = **14–1** (57a). – **14–9** (49) = **14–1** (57d). – **14–9** (47) = **14–1** (53). – **14–2** (7) = **14–7** (6vd) = **14–9** (5) = **14–3** (6va). – **14–2** (4mh) = **14–7** (3d) = **14–8** (3, 2) = **14–9** (3, 2) = **14–3** (3a). – **14–2** (4ma) = **14–7** (3v) = **14–9** (4) = **14–3** (3d). – **14–7** = **14–3** for 16, 10. – **14–7** = **14–6** for 84, 25ma, 24d, 21. – **14–7** (88) = **14–6** (88d). – **14–7** (19) = **14–6** (19ma). – **14–7** (18) = **14–8** (18) = **14–6** (18d). – **14–7** (14d) = **14–3** (14a). – **14–7** (7mad) = **14–3** (7mdd). – **14–7** (4ma, 4md) = **14–3** (4md). – **14–8** = **14–3** for 20, 19, 17, 16. – **14–8** (5) = **14–3** (5a). – **14–8** (4) = **14–3** (4ma).
Subgroups. **14–3** (31): 28, 19, 16, 14d, 10, 7maa, 6vd, 4ma, 3d.

16–6 = **16–3** for 19, 16. – **16–6** (4ma) = **16–2** (4ma).
Subgroups. **16–1** (105d): 101, 63ma, 62d, 59, 13ma, 12d, 9, 7maa, 6vd, 4ma, 3v = 3d. – **16–1** (64d): 60, 13ma, 9, 7maa, 4ma, 3v. – **16–2** (64d): 60, 13ma, 12d, 9, 7maa, 6vd, 4ma, 3d = 3v.

Table 46. (*cont*)

18–2 (*26*) = **18–1** (*27ma*). – **18–2** (*22*) = **18–1** (*23*). – **18–2** (*19*) = **18–1** (*19ma*). – **18–2** (*18*) = **18–1** (*18d*). – **18–2** (*16*) = **18–1** (*16*). – **18–2** (*7mha*) = **18–1** (*8mha*). – **18–2** (*4mh, 3*) = **18–1** (*7mhd*). – **18–2** (*4ma*) = **18–1** (*7mha*).

Note: For **12–14** the p.g. symbols *5mv′* and *5mv″* specify the positions of the two nonequivalent mirror planes.

The partitions are arranged in the ascending order of $C(V;\Pi)$. Where one value of the multinomial coefficient corresponds to several partitions, a partition with larger component numbers preceeds one with smaller component numbers, *e.g.* the partition $4^1 1^3$ preceeds $3^1 2^2$, $C(7;\,4^1 1^3) = 7!/4!1!1!1! = 210$, $C(7;\,3^1 2^2) = 7!/3!2!2! = 210$.

Enumeration of pairs of enantiomorphs

Consider the complete set of isomeric configurations on a polyhedron that belong to a particular $\Pi(V)$. The total number N of these configurations will be the sum of the number of configurations $N^{\pm}$ containing an m or i and the number of configurations N° not containing m or i. The configurations not containing m or i will occur in pairs, hence N° is an even number.

When the p.g. $\mathbf{G_m}$ assumed for the symmetry of the polyhedron contains a reflexion operation, $N(\mathbf{G_m}) = N^{\pm} + \frac{1}{2}N^{\circ}$, *i.e.* no distinction is made between enantiomorphs (relative to m) and each pair of enantiomorphs is counted as one configuration. When instead of $\mathbf{G_m}$ one assumes the highest *purely rotational* subgroup $\mathbf{G_r} \subset \mathbf{G_m}$, then $N(\mathbf{G_r}) = N^{\pm} + N^{\circ}$. The number of pairs of enantiomorphs $\frac{1}{2}N^{\circ}$ is then equal to $N(\mathbf{G_r})$–$N(\mathbf{G_m})$ and is obtained directly by subtracting the appropriate tabulated values. For example, the $\mathbf{G_m}|\mathbf{G_r}$ and $N(\mathbf{G_m})|N(\mathbf{G_r})$ pairs for the four polyhedra with $V=8$ for which the values of $N^{\pm}$ and $\frac{1}{2}N^{\circ}$ have been listed by Marchi *et al.* (1943), are:

Cube **8–2**: $O_h|O$, N[**8–2**(*32*)]|N[**8–2**(*30*)]
Square antiprism **8–1**(*64*): $D_{4d}|D_4$,
N[**8–1**(*64a*)]|N[**8–1**(*12d*)] = N[**8–2**(*14a*)]
Dodecadeltahedron **8–2**(*14*): $D_{2d}|D_2$,
N[**8–2**(*14d*)]|N[**8–2**(*6*)] = N[**8–2**(*7mdd*)]
Bicapped trigonal prism **8–5**: $D_{3h}|D_3$,
N[**8–5**(*26*)] = N[**8–2**(*20*)]|N[**8–5**(*18*)] = N[**8–2**(*18*)].

Seven of the eight N values required are tabulated under only one polyhedron, the cube. The advantage of using the cycle-index method is thus apparent.

In a completely analogous way one can determine the number of pairs related by other elements of symmetry, *e.g.* in $\bar{3}$ and 3 (enantiomorphism relative to i) or in 422 and 222 (discrimination against 4).

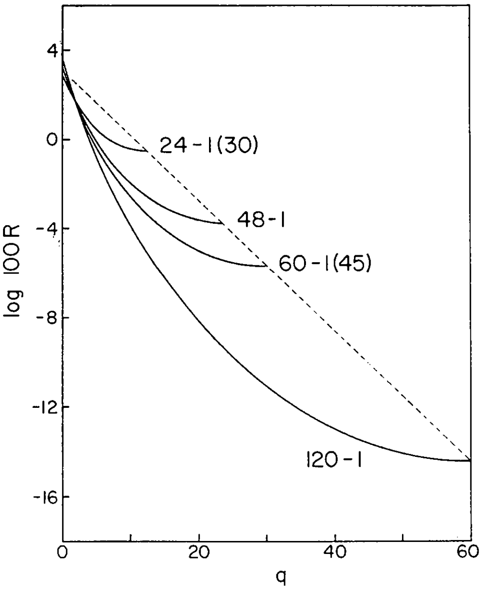

Fig. 3. Variation of log 100*R* (see text) with *q* for configurations $A_{V-q}B_q$ of large *V*.

Polyhedra with large values of *V*

Polyhedra of cubic or icosahedral symmetry exist in which no vertices are located on symmetry elements, hence no binary or higher *s*-products occur in the *Z*-polynomials. Examples among the semiregular solids are the snub cube, the truncated cuboctahedron, the snub dodecahedron, and the truncated icosidodecahedron:

24–1(*30*): 432 $Z = (\frac{1}{24})\,(s_1^{24} + 9s_2^{12} + 8s_3^{8} + 6s_4^{6})$
48–1: $m3m$ $Z = (\frac{1}{48})\,(s_1^{48} + 19s_2^{24} + 8s_3^{16} + 12s_4^{12} + 8s_6^{8})$
60–1(*45*): 532 $Z = (\frac{1}{60})\,(s_1^{60} + 15s_2^{30} + 20s_3^{20} + 24s_5^{12})$
120–1: $53m$ $Z = (\frac{1}{120})\,(s_1^{120} + 31s_2^{60} + 20s_3^{40} + 24s_5^{24} + 20s_6^{20} + 24s_{10}^{12})$.

Such polyhedra are well suited for demonstrating the rapidly diminishing effect of symmetry with increasing $C(V;\Pi)$, *i.e.* with increasing complexity of the 'chemical composition'. In the simplest case, that of the binary compositions $A_{V-q}B_q$, the generating functions are $f_n = (x_1^n + x_2^n)^{i_n}$, $i_n = V/n$. The values of $N[(V-q)^1q^1]$ are given by the coefficients of the terms $x_1^{V-q}x_2^q$ in the Z expansions. These coefficients in turn are integral multiples of the binomial coefficients $C(V,q)$. Since the values of $C(V,q)$ increase steeply with V/q, the Z are dominated by the f_1^V and $f_2^{V/2}$ terms. Because of this an idea of how much the terms arising from symmetry contribute to $N[(V-q)^1q^1]$ can be obtained by plotting $\log 100R = \log 100kf_2^{V/2}/f_1^V$ against q (Fig. 3). The R ratios are, respectively, $9C(12,q)/C(24,2q)$, $19C(24,q)/C(48,2q)$, $15C(30,q)/C(60,2q)$, and $31C(60,q)/C(120,2q)$. It is seen that for the snub cube the relative contribution of the $f_2^{V/2}$ term varies over more than three, for the truncated cuboctahedron over about seven, for the snub dodecahedron over almost nine, and for the truncated icosidodecahedron over about 18 orders of magnitude. The contribution of this term, which is greater than 1% of f_1^V up to $q \sim 7$ and which completely overwhelms f_1^V for $q=0$ and 1, thus falls off very rapidly with q. If the cubic or icosahedral p.g. is purely rotational, 432 or 532, then at $q=V/2$ for any polyhedron (or assembly of points) of this symmetry with no vertex (point) on a rotation axis $\frac{1}{2}(1-V)\log 2-(3\log e)/4V+\log k\le\log R<\frac{1}{2}(1-V)\log 2+\log k$, where $k=9$ for 432 and 15 for 532. The linearity of $\log R$ improves asymptotically as V increases. This expression shows that the effect of symmetry on N tends to vanish even in point groups of high symmetry if V is sufficiently large. For $V=240$ and p.g. 532, for example, $\log R\sim -34{\cdot}80$, which means that $N(A_{120}B_{120})\sim C(240,120)\sim 10^{72}$, so that the effect of symmetry relative to N is completely negligible.

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Use of Negative Quartet Cosine Invariants as a Phasing Figure of Merit: NQEST

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Recent theoretical advances in the identification of those cosine invariants $\cos(\varphi_h+\varphi_k+\varphi_l+\varphi_m)$ which are probably negative suggest algorithms for the calculation of a figure of merit which is sensitive to the integrity of a phase set. The negative quartet figure of merit, NQEST, defined here is of particular utility in conjunction with fast multi-solution tangent formula techniques. Development of the methods and applications to both known and unknown crystal structures are presented.

Introduction

A general methodology of crystal structure determination which has found wide application in one form or another is the multi-solution tangent refinement technique. Although the actual procedures employed within the general framework of the method may vary widely, the use of the tangent formula (Karle & Hauptman, 1956) to extend and refine a number of plausible basis sets of phases is a common feature to all. On one end of the spectrum are those procedures which introduce

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