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The symmetries of cubic polyhedral graphs with face size no larger than 6

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Abstract

We find the allowed point-group symmetries of the cubic polyhedra with face sizes restricted to 3, 4, 5 and 6. For each group and face signature (p_3, p_4, p_5), a polyhedron with the smallest possible number of vertices is identified.

1 Introduction

Of many scientific motivations for the study of polyhedra, one is provided by recent progress in the chemistry and physics of carbon. Research over the past two decades has

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added fullerenes,[19,21] nanotubes,[16] carbon onions,[27] peapods,[25] toroids,[22] nanocones,[20] nanohorns[17] and the graphenes[24] to the traditional repertoire of carbon allotropes. Most of the new structures are based on modified graphite networks in which each carbon centre has three directly bonded neighbours. Such trivalent networks correspond to cubic graphs. The first of the new carbons to be discovered, the fullerenes, are cubic polyhedral cages in which exactly twelve faces are pentagonal and all others are hexagonal; at least one such polyhedron exists for all $n = 20 + 2h$ where h is the number of hexagonal faces ($h \neq 1$).[15] The truncated icosahedral fullerene, C_{60}, was first to be characterised[19,21] and still has the highest availability and most extensive chemistry, but higher fullerenes including isomers of C_{70}, C_{76}, C_{84} have also been found.

Systematic theoretical treatments of the class of fullerene molecules rely on the use of models based on graph theory, both to enumerate the possible isomers and to make qualitative deductions about their electronic structure[10] and overall stability.[12] Many qualitative arguments in chemistry also rely on point-group symmetry. It turns out that the possible point-group symmetries of fullerenes are restricted: there are just 28 groups.[13] Theoretical treatments often consider a wider class of carbon cages, in which the restriction on face sizes is eased or lifted altogether.

One plausible extension of the classical fullerenes is to the set of cubic polyhedra of positive curvature, i.e., those with face sizes restricted to 3, 4, 5 and 6. Small face sizes are not favoured for carbon, as they lead to steric strain, but rings of these sizes are known in organic chemistry, and are realised in polyhedral hydrocarbon molecules such as cubane,[8] prismane,[18] and cuneane.[3] The polyhedral hydrocarbons C_nH_n also include dodecahedrane,[26] with the same carbon skeleton as the smallest mathematically possible fullerene, C_{20}.

A general polyhedron with v vertices, p faces and e edges satisfies the Euler relation

$$v + p = e + 2$$

and in the particular case of cubic polyhedra ($e = 3v/2$, $f = n/2 + 2$) this leads to a relation for the numbers of faces of each size:

$$\sum_r (6 - r) p_r = 12 \qquad (1)$$

where p_r is the number of faces of size r. The Euler formula is related to the Gauss-Bonnet formula in differential geometry, and thus $6 - r$ can be considered as the curvature of a face of size r. If a cubic polyhedron has no face of size greater than 6, then it can be said to be of positive curvature. It is known[9,14] that every triple $t = (p_3, p_4, p_5)$ that satisfies Equation (1) can be realised as a polyhedron with p_3 triangular, p_4 quadrilateral and p_5 pentagonal faces and some number of hexagonal faces, $h \equiv p_6$. There are thus 19 classes of cubic polyhedra of positive curvature, each corresponding to a unique 'face-signature' (p_3, p_4, p_5).

In the present paper we complete the work that has been done for the classical fullerenes and other bifaced cubic polyhedra, and derive the list of allowed symmetry groups for each class of cubic polyhedra of positive curvature, and for each class construct a smallest (lowest-order) polyhedron for each allowed symmetry.

General constructions for deriving infinite families of polyhedra of given face signature and point-group symmetry from a single example are already available. The Goldberg-Coxeter construction takes a cubic polyhedron and two integers k, l, and returns a cubic polyhedron with $k^2 + kl + l^2$ times as many vertices, the same rotational symmetry, and the same triple.[5,7] Another construction that preserves the triple is to split the faces in two hemispheres by a simple zigzag[6] and insert a cylindrical tube of layers of hexagons. Constructions of both types have been used to derive electron counting rules for the fullerenes.[12] Thus, given the minimal examples, it is possible to build series of polyhedral chemical graphs for exploration of their properties as functions of number of vertices, number, type and separation of non-hexagonal faces, and overall symmetry.

Enumeration of graphs was performed with the `CPF` program[2] and the results filtered by symmetry group. The Schlegel diagrams were made with `CaGe`[1] and 3D drawings were made using the 'topological coordinates'[12] derived from eigenvectors of the adjacency matrix with the `Psplot` program written by R. Batten.

2 The possible groups

Given a triple $t = (p_3, p_4, p_5)$, we denote by p_t the class of 3-valent polyhedra having p_3 triangular, p_4 quadrilateral, p_5 pentagonal and h hexagonal faces, and no other faces. The number of vertices of a polyhedron belonging to the class p_t is $n = 2p_3 + 2p_4 + 2p_5 + 2h - 4$.

In chemical applications it is often important to make the distinction between the symmetry of the polyhedron as a combinatorial object and the physical symmetry of its realisation as an affine object in 3D space. The symmetry group of a polyhedron as listed below is a combinatorial; it describes the maximum symmetry achievable by a three-dimensional embedding of the graph. If G is a 3-connected plane graph, then Mani's theorem[23] guarantees the existence of an embedding in 3D space with full symmetry. All 3-valent plane graphs with faces of size between 3 and 6 are 3-connected, with the exception of one infinite series [5, Theorem 2.0.2]. In a given chemical realisation, in the course of vibrations, in a given electronic state or with a given charge or electron configuration, or subjected to the forces of a crystalline environment, the geometric structure of a molecule whose underlying graph is that of the polyhedron may in fact have a point group that is only a subgroup of this maximum symmetry.

The list of groups for the extreme triples $(4, 0, 0)$, $(0, 6, 0)$ and $(0, 0, 12)$, i.e., the bifaced cubic polyhedra, are available in published work[4,11,13] and are summarized in

Theorem 2.1 *For the bifaced cubic polyhedra described by the triple* (p_3, p_4, p_5), *the possible point groups and vertex counts of minimal examples are* [1]:

(i) $(p_3, p_4, p_5) = (4, 0, 0)$:
$D_2(24)$, $D_{2h}(16)$, $D_{2d}(20)$, $T(28)$, $T_d(4)$.

(ii) $(p_3, p_4, p_5) = (0, 6, 0)$:
$C_1(40)$, $C_s(34)$, $C_2(26)$, $C_i(140)$, $C_{2v}(22)$, $C_{2h}(44)$, $D_2(24)$, $D_3(20)$, $D_{2d}(16)$, $D_{2h}(20)$, $D_{3d}(20)$, $D_{3h}(14)$, $D_6(84)$, $D_{6h}(12)$, $O(56)$, $O_h(8)$.

(iii) $(p_3, p_4, p_5) = (0, 0, 12)$:
$C_1(36)$, $C_2(32)$, $C_i(56)$, $C_s(34)$, $C_3(40)$, $D_2(28)$, $S_4(44)$, $C_{2v}(30)$, $C_{2h}(48)$, $D_3(32)$, $S_6(68)$, $C_{3v}(34)$, $C_{3h}(62)$, $D_{2h}(40)$, $D_{2d}(36)$, $D_5(60)$, $D_6(72)$, $D_{3h}(26)$, $D_{3d}(32)$, $T(44)$, $D_{5h}(30)$, $D_{5d}(40)$, $D_{6h}(36)$, $D_{6d}(24)$, $T_d(28)$, $T_h(92)$, $I(140)$, $I_h(20)$.

The results of the present investigations on the remaining 16 triples are summarized in

Theorem 2.2 *For the cubic polyhedra with at least two face sizes chosen from* $\{3, 4, 5\}$ *and no face of size greater than* 6, *described by the triple* (p_3, p_4, p_5), *the possible point groups and vertex counts of minimal examples are*:

[1] See `http://www.liga.ens.fr/~dutour/PointGroup/Classification.html` for Schlegel diagrams of minimal examples. For 3D drawings of the minimal fullerenes, see.[12]

(i) $(p_3, p_4, p_5) = (3, 1, 1)$:

$C_1(20)$, $C_s(12)$.

(ii) $(p_3, p_4, p_5) = (3, 0, 3)$:

$C_1(18)$, $C_s(14)$, $C_3(22)$, $C_{3v}(10)$, $C_{3h}(20)$.

(iii) $(p_3, p_4, p_5) = (2, 3, 0)$:

$C_1(22)$, $C_s(26)$, $C_2(18)$, $C_{2v}(10)$, $D_3(42)$, $D_{3h}(6)$.

(iv) $(p_3, p_4, p_5) = (2, 2, 2)$:

$C_1(16)$, $C_s(14)$, $C_i(56)$, $C_2(10)$, $C_{2v}(8)$, $C_{2h}(16)$.

(v) $(p_3, p_4, p_5) = (2, 1, 4)$:

$C_1(16)$, $C_s(14)$, $C_2(14)$, $C_{2v}(12)$.

(vi) $(p_3, p_4, p_5) = (2, 0, 6)$:

$C_1(24)$, $C_s(22)$, $C_i(40)$, $C_2(16)$, $C_{2v}(18)$, $C_{2h}(20)$, $D_3(36)$, $D_{3d}(12)$, $D_{3h}(18)$.

(vii) $(p_3, p_4, p_5) = (1, 4, 1)$:

$C_1(18)$, $C_s(12)$.

(viii) $(p_3, p_4, p_5) = (1, 3, 3)$:

$C_1(14)$, $C_s(12)$, $C_3(28)$, $C_{3v}(10)$.

(ix) $(p_3, p_4, p_5) = (1, 2, 5)$:

$C_1(18)$, $C_s(14)$.

(x) $(p_3, p_4, p_5) = (1, 1, 7)$:

$C_1(20)$, $C_s(18)$.

(xi) $(p_3, p_4, p_5) = (1, 0, 9)$:

$C_1(30)$, $C_s(26)$, $C_3(34)$, $C_{3v}(22)$.

(xii) $(p_3, p_4, p_5) = (0, 5, 2)$:

$C_1(20)$, $C_s(20)$, $C_2(18)$, $C_{2v}(14)$, $D_5(70)$, $D_{5h}(10)$.

(xiii) $(p_3, p_4, p_5) = (0, 4, 4)$:

$C_1(18)$, $C_s(18)$, $C_i(48)$, $C_2(16)$, $C_{2v}(14)$, $C_{2h}(32)$, $D_2(20)$, $D_{2h}(16)$, $D_{2d}(12)$, $S_4(36)$.

(xiv) $(p_3, p_4, p_5) = (0, 3, 6)$:

$C_1(20)$, $C_s(20)$, $C_2(18)$, $C_{2v}(18)$, $C_3(26)$, $C_{3v}(16)$, $C_{3h}(44)$, $D_3(26)$, $D_{3h}(14)$.

(xv) $(p_3, p_4, p_5) = (0, 2, 8)$:

$C_1(24)$, $C_s(22)$, $C_i(40)$, $C_2(20)$, $C_{2v}(18)$, $C_{2h}(28)$, $D_4(48)$, $D_{4h}(24)$, $D_{4d}(16)$, $D_2(28)$, $D_{2h}(24)$, $D_{2d}(40)$, $S_4(136)$.

(xvi) $(p_3, p_4, p_5) = (0, 1, 10)$:

$C_1(28)$, $C_s(24)$, $C_2(26)$, $C_{2v}(22)$.

Proof.

Size and number of faces restrict the possibilities for the rotation of the polyhedron. If Δ is a k-fold axis of (proper) rotation of a graph with triple (p_3, p_4, p_5), then $k = 1$, 2, 3 or 6, and if $p_r \neq 0$, then k could be equal to r. When considering a candidate group G for a triple (p_3, p_4, p_5), we will denote by k_{max} the largest value of k of the rotations of G. Further restrictions arise from orbit sizes: the group generated by a rotation of order k splits those faces not on the axis into orbits of size k; the presence of an inversion requires that all orbits of faces are of even size.

If $(p_3, p_4, p_5) = (3, 1, 1)$, $(1, 4, 1)$, $(1, 1, 7)$, $(1, 2, 5)$, then a priori k could be 1, 2, 3, 4, 5, or 6. But, by orbit sizes, the only possibility is $k = 1$. C_i is incompatible with odd values of p_r so the possible groups are C_1 and C_s. Both are realised.

If $(p_3, p_4, p_5) = (2, 1, 4)$, then $k = 1$ or 2. For $k_{max} = 1$, C_i is ruled out by odd p_4, but C_1 and C_s are possible. If $k_{max} = 2$, then the unique 2-fold axis passes through the single 4-gonal face. Of the three groups with a single 2-fold axis, C_{2h} is ruled out because it contains C_i, but C_2 and C_{2v} are possible. The same analysis applies to $(p_3, p_4, p_5) = (0, 1, 10)$.

If $(p_3, p_4, p_5) = (1, 3, 3)$, then $k = 1$ or 3. For $k_{max} = 1$, C_i is ruled out by odd p_3, but C_1 and C_s are possible. If $k_{max} = 3$, the unique 3-fold axis passes through the single 3-gonal face. Of the three groups with a single 3-fold axis, C_{3h} is ruled out because its mirror plane demands even p_3. The same analysis applies to $(p_3, p_4, p_5) = (1, 0, 9)$.

If $(p_3, p_4, p_5) = (3, 0, 3)$, then $k = 1$ or 3. For $k_{max} = 1$, and odd p_3, only C_1 or C_s are possible. If $k_{max} = 3$ the 3-gons fall into an orbit of size 3 and the 3-fold axis is unique. Of the groups with a single 3-fold axis, S_6 is ruled out as it contains no orbit of size 3, but C_3, C_{3v} and C_{3h} are possible.

If $(p_3, p_4, p_5) = (2, 3, 0)$, then $k = 1$, 2 or 3. If $k_{max} = 1$, the possibilities are C_1 or C_s. If $k_{max} = 2$, then there is a unique 2-fold axis since the presence of multiple 2-fold axes in the absence of a 3-fold axis implies D_2 as a subgroup and an orbit of size 4 or more for the 3-gons, which is ruled out by $p_3 = 2$. C_{2h} is ruled out because it contains C_i, but C_2 and C_{2v} are possible. If $k_{max} = 3$, then the unique 3-fold axis, passes through the centres of the two 3-gons. In fact, the 3-fold axis also implies the presence of an orthogonal 2-fold axis. To see this, take one 3-gon, say T_1, and add rings of hexagons around it until one reaches a 4-gon and so, by symmetry, three 4-gons. Continue to add hexagons until forced to add the remaining 3-gon T_2. The structure around T_1 is identical to that around T_2

and hence the symmetry is D_3, D_{3h} or D_{3d}, but D_{3d} would imply six 4-gons. D_3 and D_{3h} are both realised.

If $(p_3, p_4, p_5) = (2, 2, 2)$, then $k = 1$ or 2. If $k_{max} = 1$, then C_1, C_s and C_i are all possible. If $k_{max} = 2$, then the candidates are C_2, C_{2v}, C_{2h}, D_2, D_{2d}, D_{2h} and S_4. However, S_4 and groups of which D_2 is a subgroup are ruled out as 3- and 5-gons would have to occur in orbits of size 4 or more. The other possibilities are all realised.

If $(p_3, p_4, p_5) = (2, 0, 6)$, then $k = 1$, 2 or 3. If $k_{max} = 1$, then C_1, C_s and C_i are all possible. If $k_{max} = 2$, then D_2 and S_4 are ruled out by orbit size, but C_2, C_{2v} and C_{2h} are all possible. If $k_{max} = 3$, the unique 3-fold axis must pass through the two 3-gons. Take a 3-gon and add hexagons around it, until one reaches one pentagon and so, by symmetry a set of three pentagons, then continue until the three remaining pentagons are reached. Continue to add hexagons in a unique way to complete the graph. The graph has a symmetry that exchanges the 3-gons and also the two groups of pentagons. Hence its symmetry group is D_3, D_{3d} or D_{3h}. All are realised.

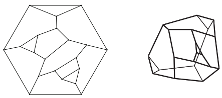
If $(p_3, p_4, p_5) = (0, 5, 2)$, then $k = 1$, 2, or 5. If $k_{max} = 1$, then C_1 and C_s are the only possibilities. If $k_{max} = 2$, then C_2, C_{2v} are possible, whereas C_{2h} and also groups containing D_2 are ruled out by odd p_4. If $k_{max} = 5$, then by analogy with the case $(2, 3, 0)$, the symmetry group is D_5 or D_{5h}.

If $(p_3, p_4, p_5) = (0, 4, 4)$, then $k = 1$ or 2. This yields the possibilities C_1, C_s, C_i, C_2, C_{2v}, C_{2h}, D_2, D_{2d}, D_{2h} or S_4, which are all realised.

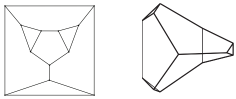
If $(p_3, p_4, p_5) = (0, 3, 6)$, then $k = 1$, 2 or 3. $p_4 = 3$ implies that there is at most one 3-fold axis and no inversion symmetry. This yields as possibilities C_1, C_s, C_2, C_{2v}, C_3, C_{3v}, C_{3h}, D_3 and D_{3h}.

If $(p_3, p_4, p_5) = (0, 2, 8)$, then $k = 1$, 2 or 4. If $k_{max} \leq 2$, then the possibilities are C_1, C_s, C_i, C_2, C_{2h}, C_{2v}, D_2, D_{2d}, D_{2h} and S_4, all realised. If $k_{max} = 4$, $p_4 = 2$ implies that the 4-fold axis is unique and by analogy with the $(2, 0, 6)$ case the symmetry is D_4, D_{4d} or D_{4h}. $\square$

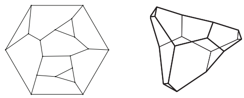
The pictures below give a catalogue of minimal examples for the realisable point groups of the 16 triples treated in Theorem 2.2.



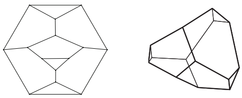
$(3, 1, 1)$, C_1, 20



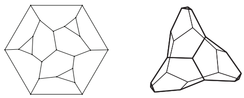
$(3, 1, 1)$, C_s, 12



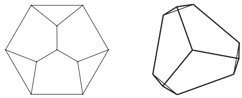
$(3, 0, 3)$, C_1, 18



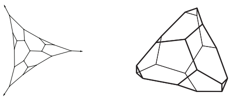
$(3, 0, 3)$, C_s, 14



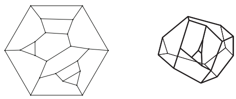
$(3, 0, 3)$, C_3, 22



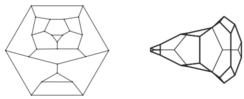
$(3, 0, 3)$, C_{3v}, 10



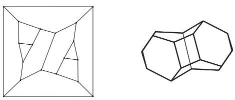
$(3, 0, 3)$, C_{3h}, 20



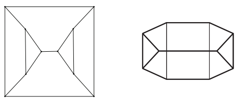
$(2, 3, 0)$, C_1, 22



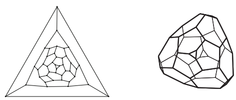
$(2, 3, 0)$, C_s, 26



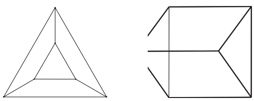
$(2, 3, 0)$, C_2, 18



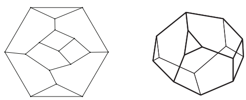
$(2, 3, 0)$, C_{2v}, 10



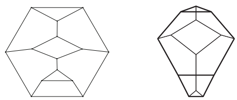
$(2, 3, 0)$, D_3, 42



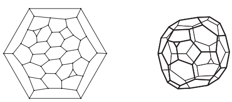
$(2, 3, 0)$, D_{3h}, 6



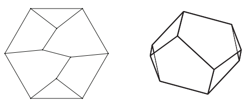
$(2, 2, 2)$, C_1, 16



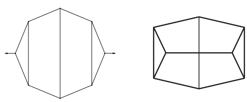
$(2, 2, 2)$, C_s, 14



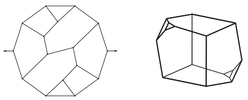
$(2, 2, 2)$, C_i, 56



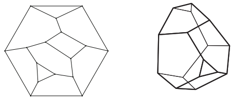
$(2, 2, 2)$, C_2, 10



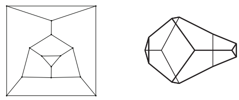
$(2, 2, 2)$, C_{2v}, 8



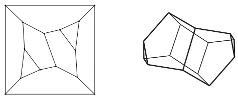
$(2,2,2)$, C_{2h}, 16



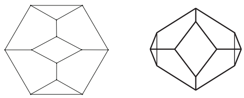
$(2,1,4)$, C_1, 16



$(2,1,4)$, C_s, 14



$(2,1,4)$, C_2, 14



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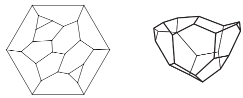

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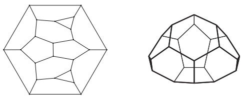

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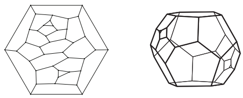

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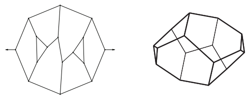

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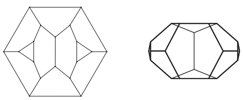
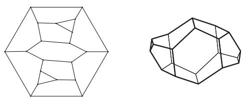


$(2,0,6)$, C_{2v}, 18



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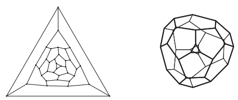

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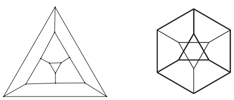

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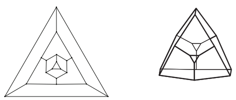

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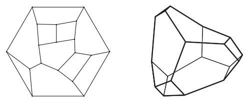
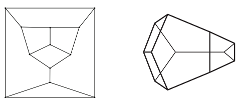


$(1,4,1)$, C_1, 18



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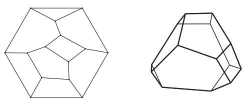

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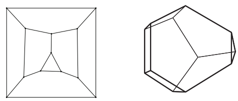

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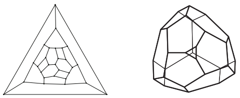

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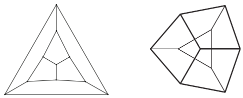

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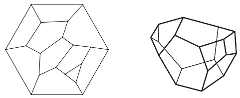

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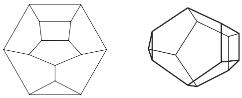

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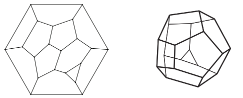

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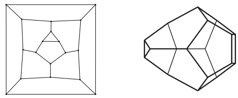

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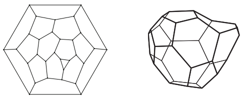

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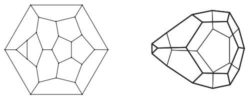

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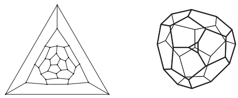

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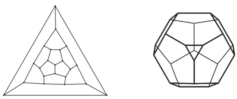

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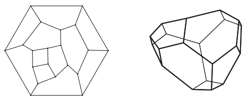

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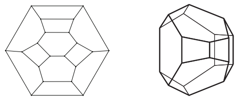

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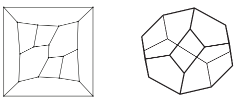

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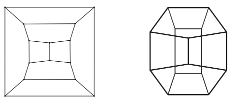

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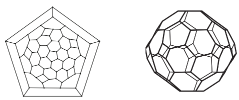

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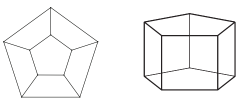

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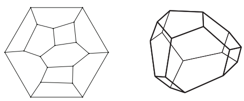

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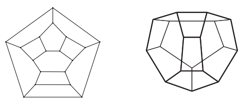

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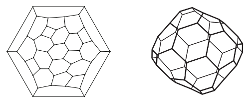
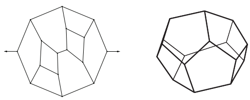


$(0,4,4)$, C_i, 48



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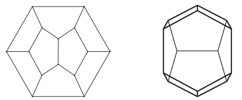

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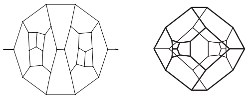

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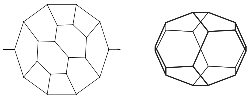

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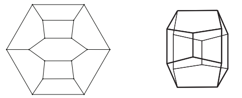

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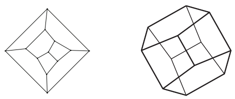
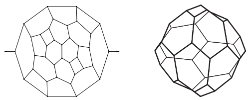


$(0,4,4)$, D_{2d}, 12



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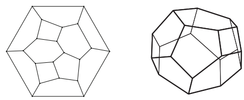

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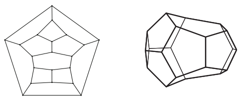

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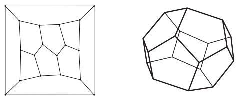

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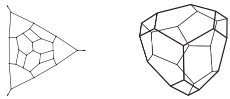

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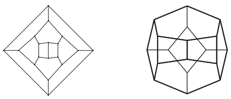

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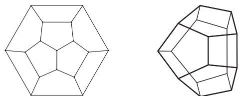

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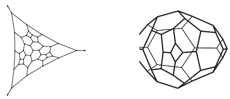

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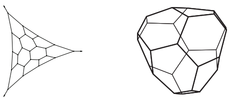

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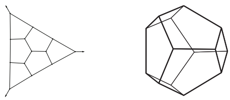

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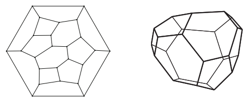

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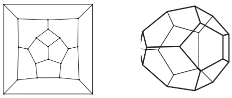

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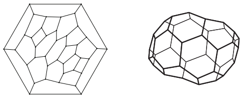
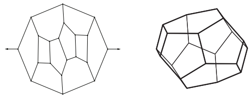


$(0,2,8)$, C_i, 40



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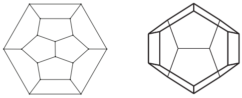
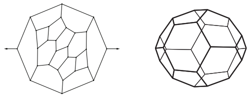


$(0,2,8)$, C_{2v}, 18



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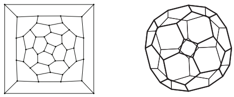
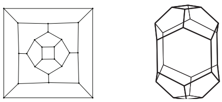


$(0,2,8)$, D_4, 48



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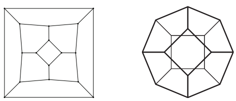
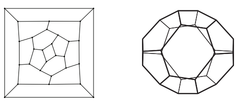


$(0,2,8)$, D_{4d}, 16



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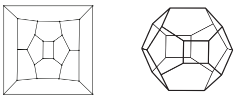

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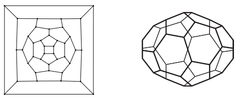
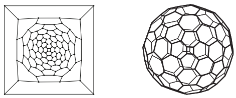


$(0,2,8)$, D_{2d}, 40



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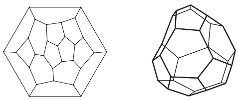

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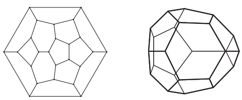

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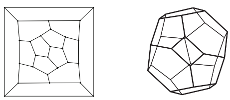

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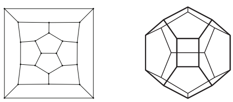

$(0,1,10)$, C_{2v}, 22

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[2] G. Brinkmann, T. Harmuth, O. Heidemeier, The construction of cubic and quartic planar maps with prescribed face degrees, *Discr. Appl. Math.* **128** (2003) 541–554.

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