Chapter 6
4-Regular and Self-Dual Analogs of Fullerenes

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Abstract An *i-hedrite* is a 4-regular plane graph with faces of size 2, 3 and 4. We do a short survey of their known properties (Deza et al. Proceedings of ICM Satellite Conference On Algebra and Combinatorics, 2003b; Deza et al. J Math Res Expo 22:49,2002; Deza and Shtogrin, Polyhedra in Science and Art 11:27, 2003a) and explain some new algorithms that allow their efficient enumeration. Using this we give the symmetry groups of all i-hedrites and the minimal representative for each. We also review the link of 4-hedrites with knot theory and the classification of 4-hedrites with simple central circuits. An *i-self-hedrite* is a self-dual plane graph with faces and vertices of size/degree 2, 3 and 4. We give a new efficient algorithm for enumerating them based on i-hedrites. We give a classification of their possible symmetry groups and a classification of 4-self-hedrites of symmetry T, T_d in terms of the *Goldberg-Coxeter construction*. Then we give a method for enumerating 4-self-hedrites with simple zigzags.

6.1 Introduction

A *fullerene* is a 3-regular plane graph whose faces have size 5 or 6. As a consequence of Euler's formula any fullerene has exactly 12 5-gonal faces. For a 3-regular plane graph G and a r-gonal face F of G, the quantity $6-r$ is called *curvature* and Euler's formula is then a statement about the curvature on the sphere. A natural generalization of fullerene is the class of 3-regular plane graphs with faces of size between 3 and 6 (see, for example, Deza et al. (2009)).

Here we consider another generalization, that is a suitable k-regular plane graph. The Euler formula $V-E+F=2$ becomes then

$$\sum_{j=2}^{\infty} p_j(s-j) = \frac{4k}{k-2} \text{ with } s = \frac{2k}{k-2}; \tag{6.1}$$

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we will permit 2-gons (doubled edges) but not 1-gons. The only integral pairs (s, k) are $(6, 3)$, $(4, 4)$ and $(3, 6)$. We will permit only s- and $(s-1)$-gonal faces. So, $p_{s-1} = \frac{4k}{k-2}$ and p_s is not bounded. The number n of vertices is

$$n = \frac{4(k+2)}{(k-2)^2} + p_s \frac{2}{k-2}. \tag{6.2}$$

For $k = 3, 4$ and 6 we get spherical analogs of the regular partition of the Euclidean plane E^2: $\{6^3\}$, $\{4^4\}$ and $\{3^6\}$, respectively, where 12 pentagons, 8 triangles and 6 doubled edges play role of "defects", disclinations needed to increase the curvature to the one of sphere S^2. The graphs with smallest number n of vertices have only $(s-1)$-gons; they are Dodecahedron, Octahedron and *Bundle*$_6$ (2 vertices connected by 6 edges) for $k = 3, 4, 6$, respectively. The case $k = 3$ gives fullerenes. The case $k = 4$, i.e., of 4-regular plane graphs with faces of size 3 or 4, gives *octahedrites* treated in the foundational paper Deza et al. (2003b). Let us call graphs in the remaining case $k = 6$ (6-regular plane graphs with faces of size 2 or 3) *bundelites*. Thurston's work (Thurston 1998) implies that fullerenes can be parametrized by 10 Eisenstein integers and the number of fullerenes with n vertices grows as n^9; those results can be generalized to octahedrites and bundelites. The ring of definition for octahedrites, respectively bundelites, is the Gaussian, respectively Eisenstein integers. Those cases belong to two of 94 cases enumerated in Thurston (1998).

We present here a short review of known facts about octahedrites as established in Deza et al. (2002, 2003b) and Deza and Shtogrin (2003a) and present a few new facts and applications. We give the possible symmetry groups of octahedrites and the graphs of minimal vertex-sets realizing them. Then we show how octahedrites can be used for the enumeration of all *i-hedrites*, i.e. 4-regular plane graphs with faces of size 2, 3 or 4 and $p_2 + p_3 = i$.

Then we consider *central circuit partition* of the edge-sets of octahedrites and the corresponding knot-theoretic notions, that is *alternating knot*, *Borromean link*, and *equivalence*.

A *i-self-hedrite* is a plane graph with vertices and faces of size 2, 3 or 4 that is isomorphic to its dual with $p_2 + p_3 = i$. Such graphs have $2p_2 + p_3 = 4$ and i-self-hedrites can be enumerated effectively by using $2i$-hedrites with a method detailed below. We determine their possible symmetry groups and we list the minimal representatives for each of them. We characterize the 4-self-hedrites of symmetry T or T_d in terms of the *Goldberg-Coxeter construction* for octahedrites. Then we give a method based on $2i$-hedrites for determining the i-self-hedrites with *simple zigzags*.

The computations of this paper were done using the GAP computer algebra system and the computer packages `polyhedral`, `plangraph` of the first author. The enumeration of octahedrites was done using the `ENU` program by O. Heidemeier (Heidemeier 1998; Brinkmann et al. 2003) and the program `CaGe` (Brinkmann et al. 1997) was used for making the drawings.

6.2 Structural Properties

A *plane graph* is a graph drawn on the plane with edges intersecting only at vertices. A graph G is *3-connected* if after removing any 2 vertices of G the resulting graph is connected. A *3-polyhedron* is a 3-dimensional polytope, its skeleton defines a 3-connected plane graph and it is known that this characterizes the skeleton of 3-polytopes. Furthermore (Mani, 1971), a 3-connected plane graph G can be represented as a skeleton of a 3-polytope P such that any symmetry of G is realized as a isometry of the polytope P. We refer to Deza et al. (2008) for more details on such questions.

It is proved in Deza et al. (2003b) that any octahedrite is 3-connected which implies that its symmetry groups is realized as isometry of 3-space. Since those group have been classified long ago and are much used in chemistry, we can use the chemical nomenclature here (see, for a possible presentation, Dutour (2004)).

An octahedrite exists for any $n \geq 6$ except $n = 7$ (see Grünbaum 1967, p. 282). For a 4-regular graph with p_j denoting the number of faces of size j, the classical Euler formula $V - E + F = 2$ can be rewritten (see Deza and Dutour-Sikirić 2008, Chapter 1, for the details) as

$$\sum_{j=2}^{\infty}(4-j)p_j = 8. \tag{6.3}$$

For octahedrites this directly implies $p_3 = 8$. Octahedron is the unique octahedrite with $n = 6$.

Theorem 1 *The only symmetry groups of octahedrites are:* C_1, C_s, C_2, C_{2v}, C_i, C_{2h}, S_4, D_2, D_{2d}, D_{2h}, D_3, D_{3d}, D_{3h}, D_4, D_{4d}, D_{4h}, O, O_h. *The minimal possible representative are given in Fig. 6.1.*

The proof that the list of groups is complete is given in Deza et al. (2003b), but the minimal possible representatives were not determined at the time. The method is first to go through the restrictions that vertex degree and face size impose. An m-fold axis of rotation has necessarily $m = 4$ (passing though a face of size 4 or a vertex), $m = 3$ (axis passing through a face of size 3), or $m = 2$ (axis passing though an edge, a vertex of degree 4 or a face of size 4). Then the classification of point groups gives a list of possible candidates. Some candidates are excluded for reason of orbit size and other similar simple arguments. But some groups are excluded for a subtler reason: the existence of a symmetry implies another symmetry. For example a 3-, 4-fold axis of symmetry, i.e. C_3, C_4 implies actually at least D_3, D_4 for possible symmetry groups. See Deza et al. (2003b) for details.

On the other hand, finding the minimal possible representative is done in a very non-clever way: we look at all the generated octahedrites and select the representatives with minimal vertex-sets. The enumeration of octahedrites was done by using

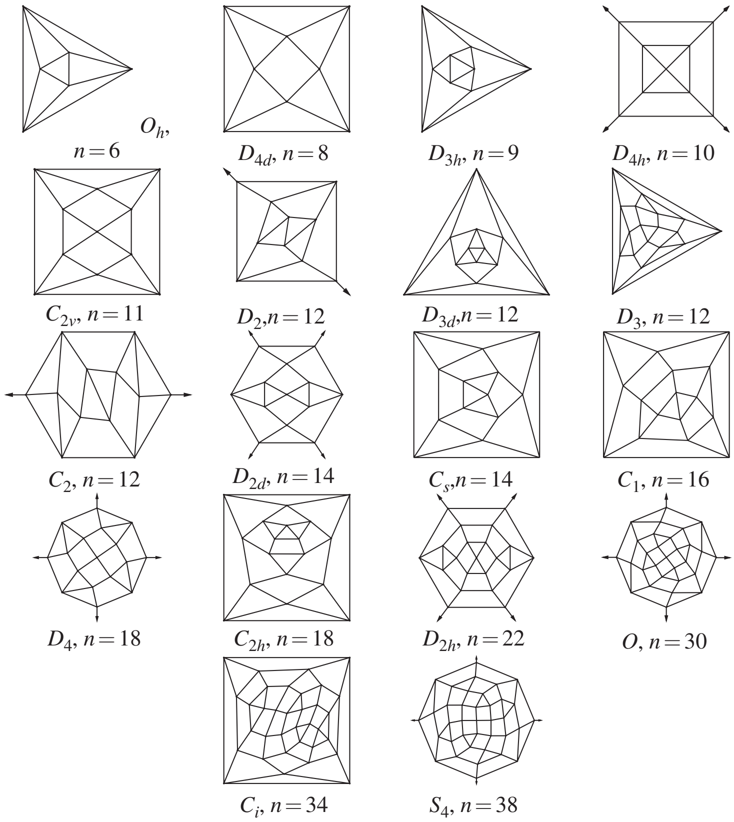


Fig. 6.1 Minimal representatives for each possible symmetry group of an octahedrite

the program ENU (see Heidemeier 1998; Brinkmann et al. 2003) by O. Heidemeier, that enumerates classes of 4-regular graphs with constraint on the size of their faces, fairly efficiently.

6.3 Generation of *i*-Hedrites

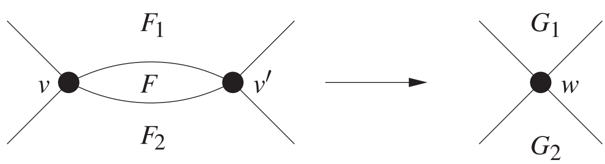
Define an *i-hedrite* to be a 4-regular n-vertex plane graph, whose faces have size 2, 3 and 4 only and $p_2 + p_3 = i$ (see, for more details, Deza et al. (2003)). Using Formula 3, we get for an i-hedrite $2p_2 + p_3 = 8$ and the only solutions are $i = 4, 5, 6, 7, 8$, which have, respectively, (p_2, p_3)=$(4, 0)$, $(3, 2)$, $(2, 4)$, $(1, 6)$ and $(0, 8)$. So, 8-hedrites are octahedrites. We will be concerned here only about the generation of i-hedrites. Actually, 4-hedrites admit a reasonably simple explicit description, see Deza et al. (2003b, 2008), Chapter 2. So, it remains to find efficient methods for the enumeration of 5-, 6- and 7-hedrites. The program ENU cannot deal with faces of size 2; so, we sought a method that allows for reasonable enumeration of such graphs. See Table 6.1 for the number of i-hedrites with at most 70 vertices.

Table 6.1 Number of i-hedrites, $4 \le i \le 8$, with $2 \le n \le 70$

n	4	5	6	7	8	n	4	5	6	7	8	n	4	5	6	7	8
2	1	0	0	0	0	25	0	12	85	107	51	48	21	45	613	1574	2045
3	0	1	0	0	0	26	5	16	119	126	109	49	0	40	614	1751	1554
4	2	0	1	0	0	27	0	21	105	142	78	50	10	54	771	1874	2505
5	0	1	1	0	0	28	8	18	134	179	144	51	0	66	704	1963	1946
6	2	2	2	0	1	29	0	16	135	198	106	52	13	58	771	2247	3008
7	0	3	1	1	0	30	8	24	187	216	218	53	0	48	788	2419	2322
8	4	1	5	1	1	31	0	32	149	257	150	54	12	66	989	2511	3713
9	0	2	5	1	1	32	12	24	189	304	274	55	0	92	849	2735	2829
10	3	3	9	3	2	33	0	18	197	329	212	56	18	68	938	3041	4354
11	0	5	7	4	1	34	6	26	251	382	382	57	0	49	1005	3187	3418
12	5	3	14	5	5	35	0	37	218	431	279	58	9	71	1175	3453	5233
13	0	4	14	7	2	36	13	23	278	483	499	59	0	98	1038	3659	4063
14	3	7	23	9	8	37	0	24	275	547	366	60	22	70	1215	3954	6234
15	0	10	17	12	5	38	6	38	354	601	650	61	0	63	1193	4315	4784
16	7	6	28	18	12	39	0	45	313	643	493	62	9	96	1440	4526	7301
17	0	6	27	22	8	40	15	37	361	764	815	63	0	104	1328	4674	5740
18	5	7	44	25	25	41	0	30	359	838	623	64	21	92	1378	5248	8514
19	0	12	35	36	13	42	10	33	472	889	1083	65	0	74	1440	5600	6631
20	7	9	54	46	30	43	0	52	405	998	800	66	14	80	1751	5741	10103
21	0	8	57	48	23	44	11	44	480	1134	1305	67	0	122	1531	6159	7794
22	4	15	77	62	51	45	0	34	511	1197	1020	68	16	98	1675	6730	11572
23	0	20	59	76	33	46	7	56	609	1324	1653	69	0	72	1792	7005	9097
24	11	11	87	88	76	47	0	69	519	1435	1261	70	14	120	2066	7465	13428

Easy to check that an n-vertex i-hedrite exists for even $n \ge 2$ if $i = 4$, $n \ge 5$ (and $n = 3$) if $i = 5$, $n \ge 4$ if $i = 6$, $n \ge 7$ if $i = 7$, $n \ge 8$ (and $n = 6$) if $i = 8$.

Take an i-hedrite G with $i \in \{5, 6, 7\}$. Then, if F is a face of size 2, we reduce it to a vertex by using the following reduction operation:



and get a graph denoted by $Red_F(G)$. During this operation the vertices v and v' are merged into one vertex w and the faces F_1 and F_2 are changed into G_1 and G_2 with one edge less. Thus, it is possible that G_1 and/or G_2 are themselves of size 2. We apply the reduction operation whenever, by doing it, the reduced graph is still an i-hedrite. Eventually, since every application of the technique diminish the vertex-set one obtains a graph, denoted by $Red_\infty(G)$ for which we cannot apply the reduction operation anymore.

We call a graph *unreducible* if we cannot apply to it any reduction operation. Let G' be an unreducible graph. If G' has no faces of size 2, then it is an 8-hedrite, i.e.

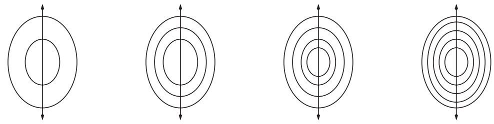


Fig. 6.2 Infinite family of unreducible 4-hedrites

an octahedrite. If G' has a face F of size 2, then denote by e_1, e_2 the two edges of F. Since G' is unreducible, F is adjacent on e_1 or e_2, say e_1, to another face of size 2.

If e_2 is incident to another face of size 2, then G' is actually 2_1, i.e. the unique graph with two vertices, and four faces of size 2, i.e. the 1st one on Fig. 6.2. It is easy to see that e_2 cannot be incident to another face of size 3, but it can be incident to another face of size 4 and in that case G' is not 3-connected and thus (see Deza et al. 2003) it belongs to the infinite family depicted in Fig. 6.2.

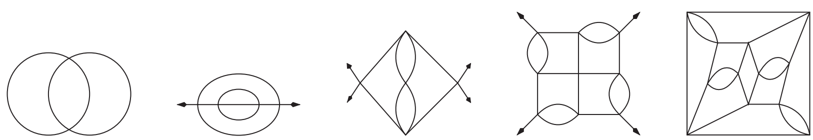
Call *expansion operation* the reverse of the reduction operation. The generation method of i-hedrite is to consider all unreducible i-hedrites and all possible ways of expanding them. For an unreducible graph G denote by $\mathcal{E}xp(G)$ the set of all possible i-hedrites that can be obtained by repeated application of the expansion operation. For the graphs of the infinite family of Fig. 6.2 no expansion operation is possible and thus no i-hedrite is obtained from them. A priori, the set $\mathcal{E}xp(G)$ can be infinite but, as far as we know, for any 8-hedrite G the set $\mathcal{E}xp(G)$ is finite although we have no proof of it. It turns out that $\mathcal{E}xp(2_1)$ is infinite but it has a simple description.

Theorem 2

(i) The only symmetry groups of 4*-hedrites are* D_{4h}, D_4, D_{2h}, D_{2d} *and* D_2.
(ii) The only symmetry groups of 5*-hedrites are:* D_{3h}, D_3, C_{2v}, C_s, C_2 *and* C_1.
(iii) The only symmetry groups of 6*-hedrites are:* D_{2d}, D_{2h}, D_2, C_{2h}, C_{2v}, C_i, C_2, C_s, C_1.
(iv) The only symmetry groups of 7*-hedrites are:* C_{2v}, C_2, C_s *and* C_1.

The theorem is proven in the same way as for octahedrites. Minimal representative for each symmetry groups are given in Figs. 6.3, 6.4, 6.5 and 6.6.

Further generalization of octahedrites are 4-regular plane graphs with 4-, 3-, 2- and 1-gonal faces only. Then, besides i-hedrites, we get graphs with (p_1, p_2, p_3)=(2, 1, 0), (2, 0, 2), (1, 2, 1), (1, 1, 3), (1, 0, 5). The enumeration method is then to use i-hedrites and to add a 1-gon when we have a pair of 2-gon and 3-gon that are adjacent in all possible ways. This is simlar to the strategy of squeezing of 2-gons used for the enumeration of i-hedrites.



D_{4h}, $n=2$ D_{2h}, $n=4$ D_{2d}, $n=6$ D_4, $n=10$ D_2, $n=12$

Fig. 6.3 Minimal representatives for each possible symmetry group of a 4-hedrite

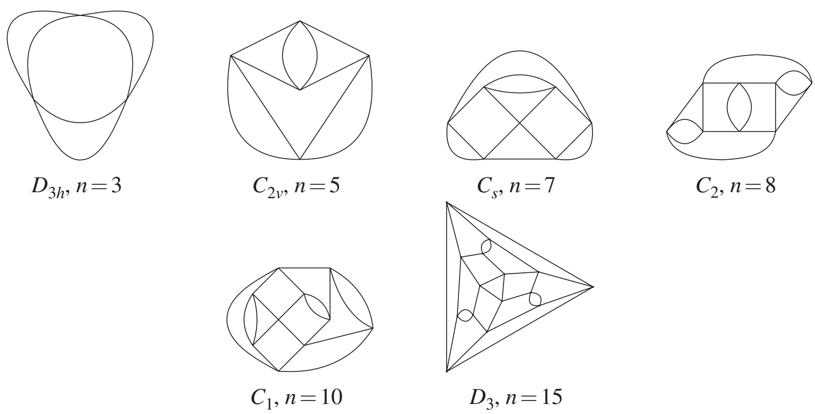


Fig. 6.4 Minimal representatives for each possible symmetry group of a 5-hedrite

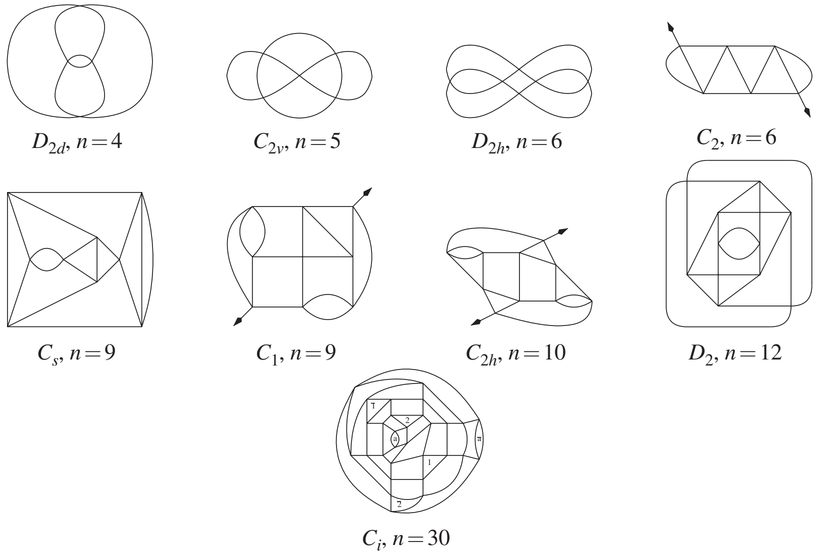


Fig. 6.5 Minimal representatives for each possible symmetry group of a 6-hedrite

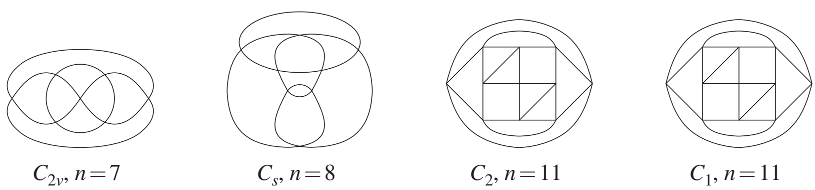


Fig. 6.6 Minimal representatives for each possible symmetry group of a 7-hedrite

6.4 Central Circuits and Alternating Knots

The edges of an octahedrite, as of any Eulerian plane graph, are partitioned by its *central circuits*, i.e. those which are obtained by starting with an edge and continuing at each vertex by the edge opposite the entering one. The central circuits of an octahedrite can define circle in the plane or have self-intersections.

If C_1, C_2 are two (possibly, self-intersecting) central circuits of an octahedrite G, then they are called *parallel* if they are separated by a sequence of faces of size 4 (such pair is called *railroad* in Deza et al. (2003a) and Deza and Shtogrin (2003)). It is possible to reduce those two central circuits into just one and thus get an octahedrite with less vertices. We call an octahedrite *irreducible* if it has no parallel central circuits. Of course, the reverse operation is possible, i.e. split a central circuit into two or more parallel central circuits. In this way every octahedrite is obtained from an irreducible octahedrite.

It is proved in Deza et al. (2003a) that an irreducible octahedrite has at most 6 central circuits and in Deza et al. (2003a) that an irreducible *i*-hedrite has at most $i-2$ central circuits. All irreducible octahedrites with non self-intersecting central circuits have been classified in Deza et al. (2003a) (see, for another presentation, Deza et al. 2003b).

Theorem 3 *There are exactly eight irreducible octahedrites with simple central circuits (see Fig. 6.7).*

A *link* is a set of circles embedded in 3-space that do not intersect; a link can be represented with its overlapping and underlapping on the plane. A link with only one component is called a *knot* and Knot Theory is concerned with characterizing different plane presentations of links (see Lickorish (1997) for a pleasant introduction). A link is called *alternating* if it admits a plane representation in which overlappings

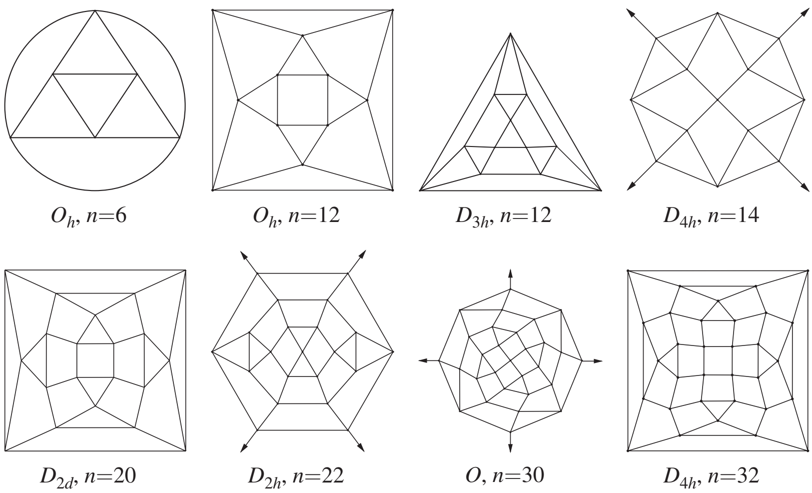


Fig. 6.7 The irreducible octahedrites with simple central circuits

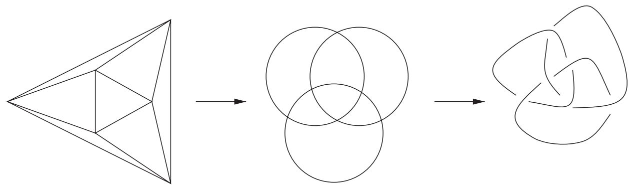


Fig. 6.8 The link corresponding to the octahedron

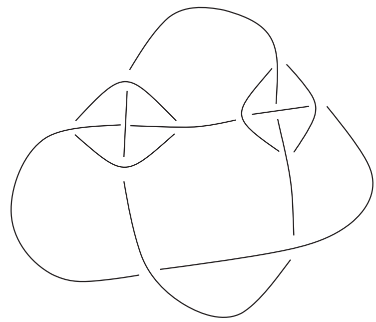


Fig. 6.9 A Borromean link

and underlappings alternate. For a 4-regular plane graph we can define a corresponding alternating link, where the central circuits correspond to the components of the link (see an example on Fig. 6.8). It is interesting that there is no known topological characterization of alternating links.

Since an octahedrite with n vertices is 3-connected, there is no disjointing vertex and thus (Lickorish 1997, Chapter 5) the corresponding alternating link cannot be represented with less than n crossings. But it can happen that two octahedrites that are not equivalent as graphs give rise to equivalent alternating links. A link with m components is called *Borromean* if after removal of any $m-2$ components the remaining two components can be separated one from the other. It is conjectured in Deza et al. (2003a) that an alternating link obtained from a 4-regular 3-connected plane graph is Borromean if and only if for any two central circuits the distance between any two of its consecutive points of its intersection is even. This condition is, of course, sufficient but there are reasons to think that it is not necessary since there exist 4-regular plane graphs (but not 3-connected) which are Borromean without satisfying the specified condition, see Fig. 6.9.

6.5 Self-Dual Graphs

A graph G is called *self-dual* if it is isomorphic to its dual G^*. The *medial graph* $Med(G)$ of a plane graph G is the plane graph obtained by putting a vertex on any edge with two edges adjacent if they share a common vertex and are contained in a common face. One has $Med(G) = Med(G^*)$. The graph $G' = Med(G)$ is always 4-regular and its dual $(Med(G))^*$ is bipartite, that is the face-set $\mathcal{F}$ of $Med(G)$ is split into two sets $\mathcal{F}_1(G')$ and $\mathcal{F}_2(G')$, which correspond to the vertices and faces of

Table 6.2 Number of i-self-hedrites with $4 \le n \le 40$ and $2 \le i \le 4$

n	2	3	4	n	2	3	4	n	2	3	4	n	2	3	4
2	1	0	0	12	4	29	24	22	10	90	191	32	9	239	584
3	1	1	0	13	6	30	33	23	7	119	198	33	9	256	631
4	2	1	1	14	5	42	40	24	7	131	234	34	14	232	748
5	2	4	1	15	5	47	48	25	10	124	276	35	10	290	760
6	3	6	2	16	8	48	69	26	10	162	304	36	14	308	857
7	3	7	4	17	5	64	73	27	8	170	332	37	16	286	956
8	3	11	6	18	6	72	92	28	12	158	407	38	11	342	1002
9	3	16	8	19	8	70	114	29	10	190	421	39	11	359	1070
10	5	16	15	20	6	89	130	30	9	210	476	40	16	332	1239
11	4	26	16	21	8	104	148	31	14	202	550				

the graph G. The bipartition $\mathcal{F}_1(G')$, $\mathcal{F}_2(G')$ can be computed easily from a given 4-regular plane graph, i.e. one can compute easily from a graph G' the two dual graphs G_1 and G_2 such that $G' = Med(G_1) = Med(G_2)$.

Call G a *i-self-hedrite* if it is a self-dual plane graph with vertices of degree 2, 3 or 4 with $v_2 + v_3 = i$ and, consequently, faces of size 2, 3 or 4. If G is a i-self-hedrite then $Med(G)$ is a $2i$-hedrite.

The Euler formula $V - E + F = 2$ for a self-dual plane graph is, clearly:

$$\sum_{j=2}^{\infty} p_j(4-j) = 4; \tag{6.4}$$

we again permit 2-gons but not 1-gons. Define an *i-self-hedrite* to be such a graph with faces of size 2, 3, 4 only and $p_2+p_3 = i$. So, $2p_2+p_3 = 4$ and p_4 is not bounded; also $n = p_4 + \frac{p_3}{2} + 2 = p_4 - p_2 + 4$. Clearly, an i-self-hedrite can have $i = 2, 3, 4$ only with $(p_2, p_3) = (2,0), (1,2), (0,4)$, respectively. The i-self-hedrites with smallest number n of vertices have no 4-gons; they are $Bundle_2$ (2 vertices connected by 2 edges), triangle with one doubled edge and Tetrahedron, respectively. Easy to check that n-vertex an i-self-hedrite exists if $n \ge i$.

Thus our enumeration method for i-self-hedrites is to consider all $2i$-hedrites G', determine for them the graphs G_1, G_2 such that $G' = Med(G_1) = Med(G_2)$ and keep the ones that have G_1 isomorphic to G_2. We denote by $Med^{-1}(G') = G_1 \simeq G_2$ the obtained plane graph if it exists. Using the enumeration of $2i$-hedrites, we can derive the i-self-hedrite, see Table 6.2. Another method would be possible with the results of Archdeacon and Richter (1992) (but it would require more hard programming work and the speed gain is uncertain).

Theorem 4

(i) *The possible symmetry groups of 2-self-hedrites graphs are C_2, C_{2v}, C_{2h}, D_2 and D_{2h}. Minimal representatives are given in Fig. 6.11.*

(ii) *The possible symmetry groups of 3-self-hedrites graphs are C_1, C_2, C_s and C_{2v}. Minimal representatives are given in Fig. 6.12.*

(iii) *The possible symmetry groups of 4-self-hedrites graphs are* C_1, C_2, C_{2h}, C_{2v}, C_3, C_{3v}, C_4, C_{4v}, C_i, C_s, D_2, D_{2d}, D_{2h}, S_4, T, T_d. *Minimal representatives are given in Fig.* 6.13.

Proof If G is a 4-self-hedrite then $G' = Med(G)$ is an octahedrite. If Γ, Γ' are the symmetry groups of G, G', then the self-duality of G becomes a symmetry in G' that exchanges $\mathcal{F}_1(G')$ and $\mathcal{F}_2(G')$. Thus Γ is identified with the subgroup of Γ' formed by the transformations preserving the bipartition. Obviously, the order of Γ is half the one of Γ'. The possible groups of G' are known (see Theorem 1). So, we set out to enumerate the index 2 subgroups of each of the 18 groups and found, besides the groups in the statement, the groups D_3, D_4, C_{4h}, C_{3h}, S_6, S_8 and T_h.

The graph G has 4 vertices of degree 3 and 4 faces of size 3; both should be partitioned in the same number of orbits and this excludes D_4, D_3, C_{3h}, S_6 and T_h. Suppose G has symmetry C_{4h}. Due to the plane of symmetry, the 4-fold axis pass through, either two vertices of degree 4, or through two faces of size 4. But self-duality requires that it passes through a vertex and a face. The same argument excludes S_8.

For 2-self hedrites, using the known groups for 4-hedrites gives candidates C_2, C_{2h}, C_{2v}, C_4, C_{4h}, C_{4v}, D_2, D_{2d}, D_{2h}, D_4, S_4. Same kind of orbit reasons exclude C_4, C_{4h}, C_{4v}, D_{2d}, D_4, S_4. A 3-self-hedrite has only one vertex of degree 2 that has to be preserved by any symmetry. So, the symmetry is a subgroup of C_{2v} and all possible subgroups do occur. □

It is known (Deza et al. 2003; Dutour and Deza 2004) that all octahedrites of symmetry O or O_h are obtained from the Goldberg-Coxeter construction, i.e. they are of the form $GC_{k,l}(Octahedron)$ for some integer $0 \le l \le k$. The pairs (k, l) correspond to the relative position of the triangles; see Fig. 6.10 for the smallest such graphs and Dutour and Deza (2004) for more details on the construction itself.

Theorem 5 *All* 4-*self-hedrites of symmetry* T *or* T_d *are obtained by the Goldberg Coxeter construction as* $Med^{-1}(GC_{k,l}(Octahedron))$ *with* $k + l$ *odd.*

Proof If G is a 4-self-hedrite of symmetry T or T_d then its medial $G' = Med(G)$ is an octahedrite of symmetry O or O_h. So, $G' = GC_{k,l}(Octahedron)$ for some (k, l). The

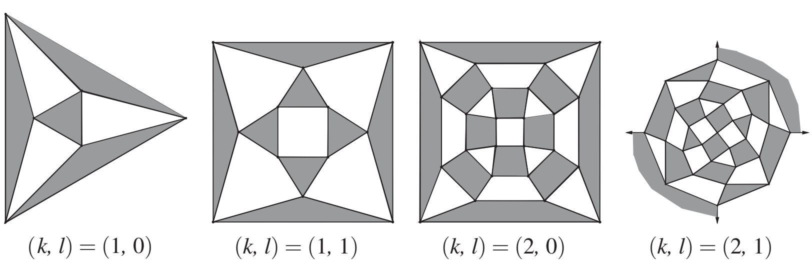


Fig. 6.10 First examples of octahedrites of symmetry O or O_h expressed as $GC_{k,l}(octahedron)$

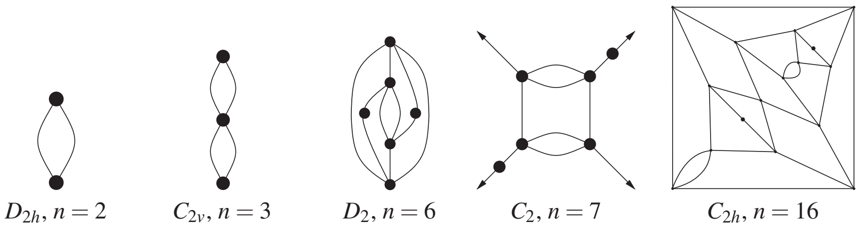


Fig. 6.11 Minimal representatives for each possible symmetry group of 2-self-hedrites

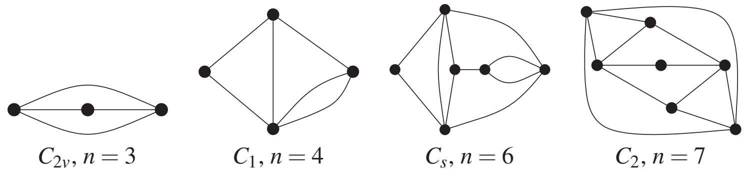


Fig. 6.12 Minimal representatives for each possible symmetry group of 3-self-hedrites

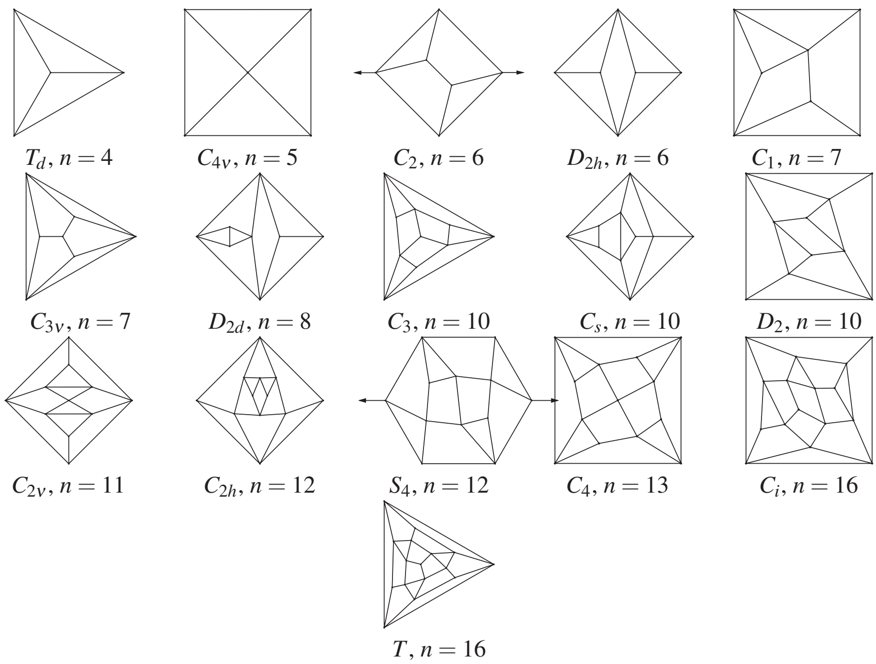


Fig. 6.13 Minimal representatives for each possible symmetry group of 4-self-hedrites

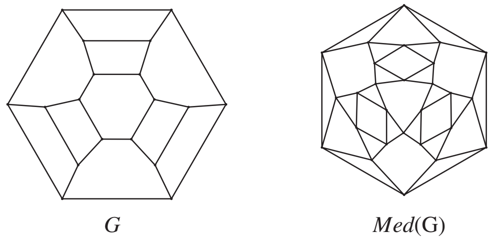


Fig. 6.14 Example of a zigzag in a plane graph G and the corresponding central circuit in $Med(G)$

automorphism group of the plane graph $GC_{k,l}(Octahedron)$ is transitive on triangles; so, we only need to determine when the triangles are not all in $\mathcal{F}_1(G')$ or $\mathcal{F}_2(G')$. Clearly, this correspond to $k + l$ odd. □

For a plane graph G a *zigzag* is a circuit of edges, such that any two but no three, consecutive edges belong to the same face. Zigzags of G correspond to central circuits of $Med(G)$, see an example on Fig. 6.14. So, if G is a 4-self-hedrite with simple zigzags, then $Med(G)$ is an octahedrite with simple central circuits. By Section 6.4, octahedrites G' with simple central circuits are obtained by taking the ones of Fig. 6.7 and splitting each central circuit C_i into m_i parallel central circuits. Then we have to determine for which $m = (m_i)$ the triangles are in two parts $\mathcal{F}_1(G')$ and $\mathcal{F}_2(G')$ which are equivalent under an automorphism of G'. This requires a detailed analysis of the automorphism and a search of the necessary relations between m_i and parity conditions. The details are very cumbersome but in principle we can get a classification of the 4-self-hedrites with simple zigzags.

In particular, 1, 3, 4, 5, 6, 7th irreducible octahedrites in Fig. 6.7 are the medial graphs of 1, 6, 7, 11, 13, 16th 4-self-hedrites in Fig. 6.13, respectively; they are all *irreducible* 4-self-hedrites with simple zigzags.

6.6 Going on Surfaces

In Deza et al. (2000) was considered a generalization of plane fullerenes on any irreducible surface. Similarly, it is easy to see that any *generalized octahedrite*, i.e., a 4-regular map on an irreducible surface, having only 3- and 4-gonal faces, is either an octahedrite on sphere S^2, or a partition of torus T^2 (or Klein bottle K^2) into 4-gons, or the antipodal quotient of a centrally symmetric octahedrite on the projective plane P^2 (having 4 3-gonal faces). Maps on surfaces of high genus can be very complicated. Actually, there are examples with the genus being about half the number of vertices. Here, for the sake of simplicity and the search of more complex examples, we limit ourselves to graphs with no loops or multiple edges. The *minimal*, i.e. with minimal number of vertices, generalized octahedrite on S^2 is Octahedron $K_{2,2,2}$; on P^2 it is the antipodal quotient of Cube with two opposite faces triangulated in their center, that is K_5. On T^2 it is K_5, and on K^2 it is again $K_{2,2,2}$ (but embedded as a quadrangulation); see Fig. 6 in Nakamoto (2001).

Finally, it is easy to check that any *generalized 4-self-hedrite*, i.e., self-dual map on an irreducible surface, having only 3- and 4-gonal faces, is either a 4-self-hedrite on sphere S^2, or a 4-regular partition of torus T^2 (or Klein bottle K^2) into 4-gons, or the antipodal quotient of a centrally symmetric 4-self-hedrite on the projective plane P^2 (having 2 3-gonal faces). The minimal generalized 4-self-hedrite graph on S^2 is Tetrahedron; on P^2 it is the antipodal quotient of the 12th graph on Fig. 6.13, that is complete graph K_6 with disjoint 2- and 4-vertex paths deleted. On T^2 it is K_5, and on K^2 it is again $K_{2,2,2}$ (see Fig. 6 in Nakamoto (2001)) embedded as a quadrangulation.

Similar results hold for generalization of i-hedrites and i-self-hedrites from sphere on any irreducible surface. On T^2 and K^2 it gives the 4-regular quadrangulations. On P^2 they are the antipodal quotients of such centrally symmetric graphs on S^2. So, $2p_2 + p_3$ becomes 4 for i-hedrites and 2 for i-self-hedrites on P^2.

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