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Zigzag Structures of Simple Two-Faced Polyhedra

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A *zigzag* in a plane graph is a circuit of edges, such that any two, but not three, consecutive edges belong to the same face. A *railroad* in a plane graph is a circuit of hexagonal faces, such that any hexagon is adjacent to its neighbours on opposite edges. A graph without a railroad is called *tight*. We consider the zigzag and railroad structures of general 3-valent plane graph and, especially, of simple two-faced polyhedra, *i.e.*, 3-valent 3-polytopes with only a-gonal and b-gonal faces, where $3 \leqslant a < b \leqslant 6$; the main cases are $(a,b) = (3,6)$, $(4,6)$ and $(5,6)$ (the *fullerenes*).

We completely describe the zigzag structure for the case $(a,b) = (3,6)$. For the case $(a,b) = (4,6)$ we describe symmetry groups, classify all tight graphs with simple zigzags and give the upper bound 9 for the number of zigzags in general tight graphs. For the remaining case $(a,b) = (5,6)$ we give a construction realizing a prescribed zigzag structure.

1. Introduction: main notions

A *graph* G consists of a vertex-set $V(G)$ and an edge-set $E(G)$, such that either one or two vertices are assigned to each edge as its ends. A graph is said to be *simple* if no edge has only one end-vertex and no two edges have identical end-vertices. A *plane* graph is a particular drawing of a graph in the Euclidean plane using smooth curves that cross each other only at the vertices of the graph. A graph that has at least one such drawing is called *planar*. We only deal with simple connected plane graphs whose vertex-sets and edge-sets are finite.

By a *polyhedron* we mean a convex 3-dimensional polytope. The vertices and the edges of a polyhedron form a simple planar 3-connected graph called a *skeleton*. Such a graph

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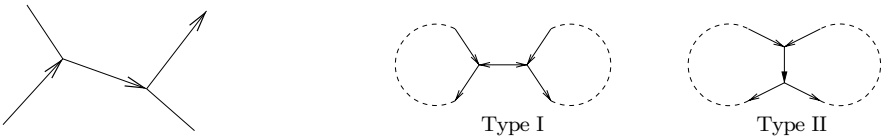


Figure 1. A fragment of a zigzag and the two types of self-intersection.

has a unique drawing (up to diffeomorphisms of the Euclidean plane), but there exist many distinct polyhedra having this graph as their skeleton; all such polyhedra are of the same *combinatorial type*. The group of isometries of a polyhedron (the so-called *point group*) is a subgroup of the algebraic symmetry group of the graph. By a theorem of Mani [26], there is, for each combinatorial type, at least one polyhedron for which this inclusion becomes equality. So we can identify the polyhedron and its graph, as well as the algebraic symmetry group and the point group.

The *v-vector* $v(G) = (\ldots, v_i, \ldots)$ of a polyhedron G enumerates the numbers v_i of vertices of degree i. A polyhedron is *simple* if $v_i = 0$ for $i \neq 3$. The *p-vector* $p(G) = (\ldots, p_i, \ldots)$ of a polyhedron G counts the numbers p_i of faces having i sides. For a connected plane graph G, we denote its *plane dual graph* by G^* and define it on the set of faces of G with two faces being adjacent if they share an edge. Clearly, $v(G^*) = p(G)$ and $p(G^*) = v(G)$.

Let G be a plane graph, such that every of its vertices has at least degree 3. Then all edges, incident to a vertex x, can be labelled in anti-clockwise order as $e_1, e_2, \ldots, e_k$, where k is the degree of x in G. For any edge e_i, $1 \leqslant i \leqslant k$, the edges e_{i+1}, and e_{i-1} (with $i+1$ and $i-1$ being addition modulo k) are called, respectively, the *left* and the *right*. A circuit of edges of G is called a *zigzag* (or a *Petrie path* [4], *geodesic* [21], *left–right path* [29]), if, in tracing the circuit, we alternately select, as the next edge, the left neighbour and the right neighbour (see Figure 1). In a 3-valent plane graph, any pair of edges sharing a vertex defines a zigzag.

Given an edge, there are two possible directions for extending it to a zigzag. Hence, each edge is covered exactly twice by zigzags. A zigzag Z is called *simple* if it has no self-intersection. Otherwise, it has at least one edge, say e, in which it self-intersects. Let us choose an orientation on Z; call the edge e of *type I* or *type II* [21] if Z traverses it twice in the opposite or in the same direction, respectively (see Figure 1). Clearly, the type of edge does not depend on the choice of orientation. Edges of type I and type II correspond to edges of *cocycle* and *cycle character* in [29]. The *signature* of a zigzag is the pair (α_1, α_2), where α_1 and α_2 are the numbers of its edges of type I and type II, respectively.

The *z-vector* of a graph G is the vector enumerating the lengths of all its zigzags with their signature as subscript. The simple zigzags are put in the beginning, in increasing order of length, without their signature $(0,0)$, and separated by a semicolon from others. Self-intersecting zigzags are also ordered by increasing lengths. If there are $m > 1$ zigzags of the same length l and the same signature $(\alpha_1, \alpha_2) \neq (0,0)$, then we write $l^m_{\alpha_1,\alpha_2}$. For a zigzag Z, its *intersection vector* $Int(Z) = (\ldots, c_k^{m_k}, \ldots)$ is such that $(\ldots, c_k, \ldots)$ is an

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increasing sequence of sizes c_k of its intersection with all others zigzags, and m_k denote respective multiplicities.

The length of each zigzag is even, because we consecutively take left and right turns. But the length of intersection of two simple zigzags can be odd (see Klein and Dyck maps on the Table 1; they both have oriented genus 3 and come as quotients of regular triangulations of the hyperbolic plane having valency 7 and 8, respectively). Returning to our plane case, the number of intersections can only be even.

A graph is called *z-uniform* if all zigzags have the same length and signature, *z-transitive* if its group acts transitively on zigzags. Clearly, z-transitivity implies z-uniformity. A graph is called *z-knotted* if it has only one zigzag, *z-balanced* if all its zigzags of the same length and same signature have identical intersection vectors. Clearly, z-transitivity implies z-balancedness.

Let $Z_1, \ldots, Z_p$ all be zigzags of G. On every zigzag choose an orientation; there are 2^p possibilities. Every edge, being covered twice by zigzags (one or two), can be, with respect to the chosen orientation of all zigzags, oriented in the opposite or same direction. We call such an edge of *type I* or *type II with respect to the fixed orientation*. If an edge is a self-intersection edge of some zigzag, then the notion of type is independent of the fixed orientation and coincides with the notion of type I and II, which was introduced above.

While for dual graphs v- and p-vectors are interchanged, the z-vector remains the same, except that type I and type II in the signature are interchanged. Other kinds of dualities (for example, interchanging z- and p-vector, but preserving v-vector) are considered in [25].

The *medial* graph $\mathrm{Med}(G)$ of G is defined on the set of edges of G with two edges being adjacent if they share a common vertex and if they belong to a common face. The medial graph is 4-valent and $\mathrm{Med}(G) = \mathrm{Med}(G^*)$. Zigzags of G and G^* correspond to central circuits (see below) of $\mathrm{Med}(G)$. Any 4-valent plane graph H is the medial graph for a pair of mutually dual plane graphs: one can assign two colours to the faces of H in the 'chess way', such that no two adjacent faces of H have the same colour. Two faces of the same colour are said to be adjacent if they share a vertex.

In general, a *central circuit* of an *Eulerian* (*i.e.*, having only vertices of even degree) plane graph is a circuit, which is obtained by starting with an edge and continuing at each vertex by the edge opposite to the entering one. A *link* is one or more circles (components of a link) embedded into the space $\mathbb{R}^3$; a link with one component is called a *knot*. A *projection* of a link is a drawing of it on the plane with gaps representing underpasses and solid lines representing overpasses. If a drawing of a link has alternating underpasses and overpasses, then it is called *alternating*; so we can see it just as a 4-valent plane graph. We will consider only *minimal* projections, *i.e.*, those without 1-gons (loops). Clearly, each edge belongs to exactly one central circuit and any 4-valent graph without 1-gons can be seen as a minimal projection of an alternating link with components corresponding to its central circuits. Since zigzags in G correspond to central circuits in $\mathrm{Med}(G)$, each zigzag corresponds to a component of the corresponding alternating link. The bipartition of edges of a z-knotted graph into type I and type II corresponds to a bipartition of the vertices of its medial graph (which is a projection of an alternating knot).

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Call a polyhedron *two-faced* if it has only a- and b-gonal faces with $3 \leqslant a < b \leqslant 6$. In particular, denote 3-valent two-faced n-vertex polyhedron by 3_n, 4_n, 5_n if $(a,b) = (3,6)$, $(4,6)$, $(5,6)$, respectively. Given two circuits $u_1, \ldots, u_m$ and $v_1, \ldots, v_m$, an *m-sided prism* Prism_m is formed when every u_i is joined to v_i by an edge. Now, an *m-sided antiprism* APrism_m is formed by adding the cycle $u_1, v_2, u_2, v_3, \ldots, v_m, u_m, v_1, u_1$.

A *point group* is a finite subgroup of the group $O(3)$ of isometries of the space $\mathbb{R}^3$, fixing the origin. The connection with plane graphs come from representing them on the sphere centred at the origin. The list of point groups is split into two classes: the infinite families and the sporadic cases. Every point group G contains a normal subgroup formed by the rotations of G. The group, denoted C_m, is the cyclic group of rotations by angle $\frac{2\pi}{m}k$ with $0 \leqslant k \leqslant m-1$ around a fixed axis Δ. Both groups C_{mv} and C_{mh} contain C_m as normal subgroups of rotations. The group C_{mh} (respectively, C_{mv}) is the group, generated by C_m and a symmetry of plane P, with P being orthogonal to Δ (respectively, containing Δ). The group D_m is the group, generated by C_m and a rotation by angle π, whose axis is orthogonal to Δ. The point group D_{mh} (respectively, D_{md}) is generated by C_{mv} and a rotation by angle π, whose axis is orthogonal to Δ and contained in a plane of symmetry (respectively, going between two planes of symmetry). Both D_{mh} and D_{md} contain D_m as a normal subgroup. If N is even, we define the point group S_N to be the cyclic group generated by the composition of a rotation by angle $\frac{2\pi}{N}$ with axis Δ and a symmetry of plane P with P being orthogonal to Δ. The particular cases C_1, C_s and C_i correspond to the trivial group, the plane symmetry group and the central symmetry inversion group. The point groups T_d, O_h and I_h are the symmetry group of the Tetrahedron, Cube and Icosahedron; the point groups T, O and I are their normal subgroup of rotations. The point group T_h is formed by all f and $-f$ with $f \in T$. More detailed descriptions of point groups are available, for example, from [15] and [13].

In Table 1, zigzag notions are illustrated by the regular and *semiregular* polyhedra (*i.e.*, such that their symmetry group is transitive on vertices). This table is a slightly more precise version (indicating types of self-intersection of zigzags) of Table 1 of [12]. It is easy to see that for self-intersecting zigzags of prisms and antiprisms, the self-intersections of type I, if any, occur on the edges of the two m-gons, while those of type II occur on other edges.

The notion of a zigzag was generalized to locally finite *infinite* planar 3-connected graphs. All such *edge-transitive* graphs without self-intersecting zigzags (*i.e.*, simple circuits and doubly infinite rays are the only zigzags) were classified in [22]: these are the three regular partitions (6^3), (3^6), (4^4) of the Euclidean plane, the Archimedean partition (3.6.3.6), its dual and several infinities of partitions of the hyperbolic plane. Also the notion of a zigzag (Petrie polygon) was extended in [4, p. 223] to n-dimensional polytopes and honeycombs.

This paper is based on extensive computation, particularly the following.

(i) All computations used the GAP computer algebra system [18] and the package PlanGraph [14] by the second author.

(ii) The program CPF [23] by Harmuth was used to generate the graphs of type 3_n and 4_n. In fact, the name n_x for a graph indicates that a graph appears at xth position in the output of CPF. Also, CaGe [2] was used for graph drawings.

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Table 1. Zigzag structure of Platonic and semiregular polyhedra; also, of Klein and Dyck maps.

# edges	Polyhedron	z-vector	Int. vector
6	Tetrahedron	4^3	2^2
12	Cube	6^4	2^3
12	Octahedron	6^4	2^3
30	Dodecahedron	10^6	2^5
30	Icosahedron	10^6	2^5
24	Cuboctahedron	8^6	$2^4, 0$
60	Icosidodecahedron	10^{12}	$2^5, 0^6$
48	Rhombicuboctahedron	12^8	$2^6, 0$
120	Rhombicosidodecahedron	20^{12}	$2^{10}, 0$
72	Truncated Cuboctahedron	18^8	$6, 2^6$
180	Truncated Icosidodecahedron	30^{12}	$10, 2^{10}$
18	Truncated Tetrahedron	12^3	6^2
36	Truncated Octahedron	12^6	$4, 2^4$
36	Truncated Cube	18^4	6^3
90	Truncated Icosahedron	18^{10}	2^9
90	Truncated Dodecahedron	30^6	6^5
60	Snub Cube	$30^4_{3,0}$	8^3
150	Snub Dodecahedron	$50^6_{5,0}$	8^5
3m	Prism_m, $m \equiv 0 \pmod 4$	$(\frac{3m}{2})^4$	$(\frac{m}{2})^3$
3m	Prism_m, $m \equiv 2 \pmod 4$	$(3m_{\frac{m}{2},0})^2$	$2m$
3m	Prism_m, $m \equiv 1, 3 \pmod 4$	$6m_{m,2m}$	
4m	APrism_m, $m \equiv 0 \pmod 3$	$(2m)^4$	$(\frac{2m}{3})^3$
4m	APrism_m, $m \equiv 1, 2 \pmod 3$	$2m; 6m_{0,2m}$	
84	Klein map	8^{21}	$1^8, 0^{12}$
48	Dyck map	6^{16}	$1^6, 0^9$

(iii) For graphs of type 5_n, we also used the face-spiral algorithm notation given in [15]; a computation by Brinkmann [1] was used in Table 7.

2. General results for plane graphs

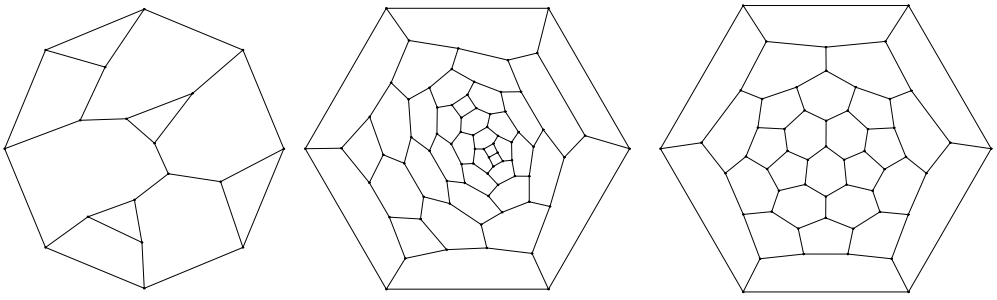
Theorem 2.1. *For any planar bipartite graph G there exist an orientation of zigzags, with respect to which each edge has type I.*

Proof. We represent the graph G on the sphere. The list of vertices, adjacent to a given vertex, can be organized in anti-clockwise order.

Let the vertex-set V be partitioned into the two subsets V_1 and V_2 of the bipartition. Fix a zigzag Z; it will turn left at vertices, say $v \in V_1$, and right at vertices $v \in V_2$. It is easy to see that the edges of self-intersection of Z can only be of type I.

Take another zigzag Z', having a common edge e with Z. We choose an orientation on Z', such that e is an edge of type I. Then Z' will turn left at vertices $v \in V_1$ and right at vertices $v \in V_2$. Iterating this construction, all zigzags will be oriented and all edges will have type I with respect to this orientation of zigzags. □

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18-vertices graph ($C2$),
$z = 8^3; 30_{2,5}$

Graph $4_{72}(C_1)$,
$z = 30_{1,0}, 54^2_{4,0}, 78_{13,0}$

Graph $5_{52}(D_{2d})$,
$z = 16^4; 92_{12,12}$

Figure 2. Smallest z-unbalanced 3-valent graphs.

In the case of one zigzag, this result was already known [29]. This theorem is also valid for any bipartite graph, which is embedded in an oriented surface, in view of the well-known topological fact that any two-dimensional orientable manifold admits coherent orientation of its faces.

Proposition 2.2. ([10]) *Let G be a plane graph; for any orientation of all zigzags of G, we have:*

(i) *the number of edges of type II, which are incident to any fixed* vertex*, is even,*
(ii) *the number of edges of type I, which are incident to any fixed* face*, is even.*

Proof. **(i)** For each vertex, the number of times that a zigzag enters it should be equal to the number of times that a zigzag leaves it.

(ii) Passing to the dual graph, the types of edges are interchanged. □

A consequence of the above proposition for any 3-valent plane graph G (see [10]) is that the set of vertices can be partitioned into two classes, say, class I and class II, where class I stands for vertices, which are incident to three edges of type I, and class II stands for vertices, which are incident to one edge of type I and two edges of type II. If n denotes the number of vertices of G and n_1 denotes the number of its vertices of class I, then the number of edges of type I is $n_1 + \frac{n}{2}$. Clearly, the number of edges of type II is equal to the number of vertices of class II, *i.e.*, to $n - n_1$.

It was conjectured in [10] that any 3-valent plane graph, which is z-knotted, has an odd number of edges of type I. The condition of 3-valency is necessary: for example, the 3-bipyramid (*i.e.*, Prism_3^*) has z-vector $18_{6,3}$.

Clearly, any graph with 1, 2 or 3 zigzags is z-balanced. See the smallest z-unbalanced 3-valent graph and graphs of type 4_n, 5_n in Figure 2. We did computations trying to find an example of a z-unbalanced and *z-uniform* 3-valent polyhedron (for $n \leqslant 22$), and graphs of type 4_n (for $n \leqslant 250$) and 5_n (for $n \leqslant 80$); surprisingly, we did not find any such example.

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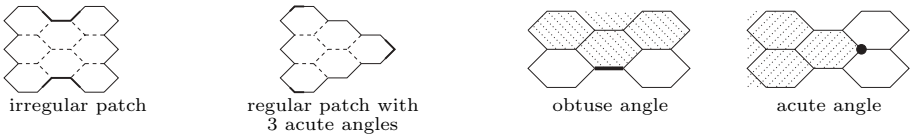


Figure 3. Example of patches and their angles.

In the rest of this section, we give a local Euler formula for zigzags. Let G be a plane 3-valent graph. Consider a patch A in G which is bounded by t arcs (*i.e.*, paths of edges) belonging to zigzags (different or coinciding).

We also admit 0-gonal patch A, *i.e.*, just the interior of a simple zigzag. Suppose that the patch A is *regular*, *i.e.*, the continuation of any of its bounding arcs (on the zigzag to which it belongs) lies outside the patch (see Figure 3). Let $p'(A) = (\ldots, p'_i, \ldots)$ be the p-vector enumerating the faces of G which are contained in the patch A.

There are two types of intersections of arcs on the boundary of a regular patch: either intersection in an edge of the boundary, or intersection in a vertex of the boundary. Let us call these types of intersections *obtuse* and *acute*, respectively (see Figure 3); denote by t_{ob} and t_{ac} the respective number of obtuse and acute intersections. Clearly, $t_{\mathrm{ob}} + t_{\mathrm{ac}} = t$, where t is the number of arcs forming the patch.

Theorem 2.3. *Let G be a 3-valent plane graph (1-gonal and 2-gonal faces are permitted). If A is a regular patch, then the following equality holds:*

$$6 - t_{\mathrm{ob}} - 2t_{\mathrm{ac}} = \sum_{i \geqslant 1} (6 - i) p'_i.$$

Proof. Let $P(A)$ be the induced plane subgraph of G formed by the patch A. The vertices of $P(A)$ have degree 2 or 3; we denote their respective number by v_2 and v_3. The exterior face is l-gonal, where l is the length of the boundary of the patch. Direct enumeration gives the following expressions for the number $|E|$ of edges of $P(A)$:

$$|E| = \frac{1}{2}(3v_3 + 2v_2) = \frac{1}{2}\left(l + \sum_{i \geqslant 1} i p'_i\right).$$

Euler's formula, applied to the plane graph $P(A)$, yields

$$2 = (v_2 + v_3) - |E| + \left(1 + \sum_{i \geqslant 1} p'_i\right).$$

The above two expressions of $|E|$ give

$$1 = -\frac{v_3}{2} + \sum_{i \geqslant 1} p'_i = (v_2 + v_3) - \frac{l}{2} + \sum_{i \geqslant 1} \left(1 - \frac{i}{2}\right) p'_i.$$

Eliminating v_3 yields $3 = v_2 - \frac{l}{2} + \sum_{i \geqslant 1} (3 - \frac{i}{2}) p'_i$.

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For example, if the patch A is a 0-gon (*i.e.*, if it is bounded by a simple zigzag), then $l = 2v_2$ and we get

$$3 = \sum_{i \geqslant 1} \left(3 - \frac{i}{2}\right) p'_i.$$

Denote by v'_2 and v'_3 the numbers of vertices on the boundary of A having degree 2 and 3, respectively. Clearly, $l = v'_2 + v'_3$ and $v'_2 = v_2$.

Now we use the fact that A is a regular patch. Specifying acute and obtuse types of arc intersections on the boundary of A, we get $v'_2 = v'_3 + t_{\text{ob}} + 2t_{\text{ac}}$, which gives $6 - t_{\text{ob}} - 2t_{\text{ac}} = \sum_{i \geqslant 1}(6 - i)p'_i$. □

Corollary 2.4. *Let G be a 3-valent plane graph. Let A be a t-gonal regular patch with p-vector $(\dots, p'_i, \dots)$ in G. Then we have:*

(i) *if G has no q-gonal faces with $q > 6$, then $t \leqslant 6$.*

(ii) *if G is a two-faced graph w_n, $w \in \{3, 4, 5\}$, then*

$$6 - t_{\text{ob}} - 2t_{\text{ac}} = (6 - w)p'_w.$$

Proof. **(i)** By the above theorem

$$6 - t_{\text{ob}} - 2t_{\text{ac}} = \sum_{1 \leqslant i \leqslant 6} (6 - i)p'_i \geqslant 0,$$

which gives the result.

(ii) This also follows, by direct application of Theorem 2.3. □

3. Railroads and pseudo-roads

Let G be a plane graph. Call a *railroad* of G a circuit of hexagonal faces in G, such that each hexagon is adjacent to its neighbours on opposite edges (in [21], a *simple* railroad, *i.e.*, without self-intersections, is called a *belt*). Clearly, a railroad is bounded by two 'parallel' (concentric if the railroad is simple) zigzags. The graph G is called *tight* if it has no railroads. A railroad in G corresponds to a central circuit in G^*, which goes only through 6-valent vertices.

We associate to each railroad a *representing* plane curve in the following way: in each of its hexagons we connect, by an arc, the midpoints of opposite edges, on which it is adjacent to its two neighbours. The sequence of those arcs can be seen as a Jordan curve in the plane and self-intersections of railroad correspond to self-intersections of the curve.

Those self-intersections can only be double or triple, because a railroad consists of hexagons. If the railroad has no triple self-intersection points, then this curve can be seen as a projection (not minimal, if there are 1-gons) of an alternating knot (see, for example, [24] and [27]) with n crossings, where n is the number of self-intersection points. If there are several railroads without triple intersections and triple self-intersections, then the set of plane curves, representing them, can be seen as a projection of an alternating link. See Figure 4 for examples.

A set of railroads can be seen as a plane graph H with valency 4 or 6 of its vertices, accordingly to double or triple points of intersection or self-intersection of the curves.

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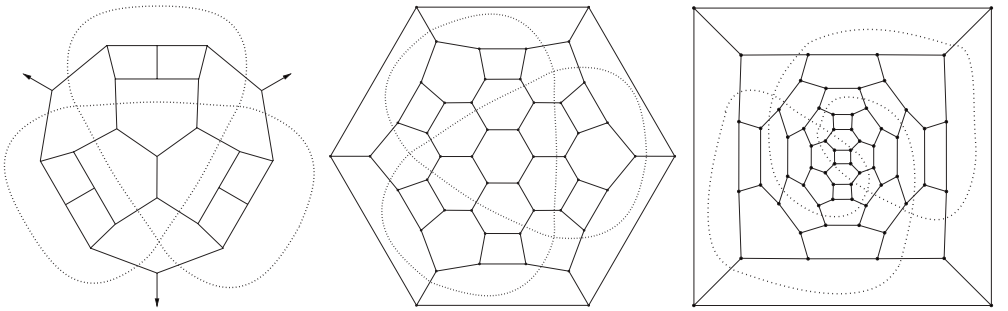


Figure 4. Three graphs of type 4_n with self-intersecting railroads.

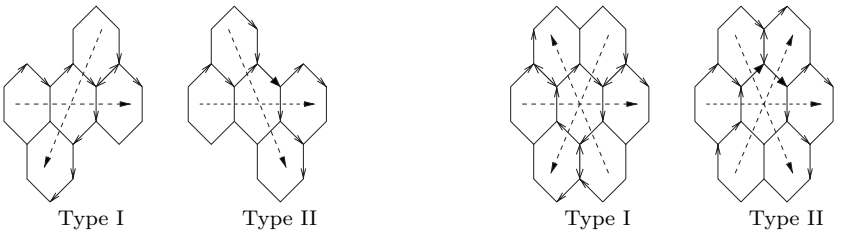


Figure 5. Types of self-intersection of a railroad.

Every t-gonal face F of H can be viewed as a regular patch with t intersections of arcs. In the case when G has no q-gonal faces with $q > 6$, Corollary 2.4(i) implies that $t \leqslant 6$.

A railroad R is bounded by two zigzags Z_1 and Z_2, which have the same length and signature. Each edge of self-intersection of Z_1, Z_2 corresponds to a self-intersection of R, and so to a hexagon of self-intersection of R. Since Z_1 can self-intersect in an edge of type I or type II, there are two types of double self-intersections of railroad. Simple analysis yields two types for triple self-intersections of railroad: either Z_1 self-intersects in three edges of type I or it self-intersects in one edge of type I and two edges of type II. See Figure 5 for all possibilities.

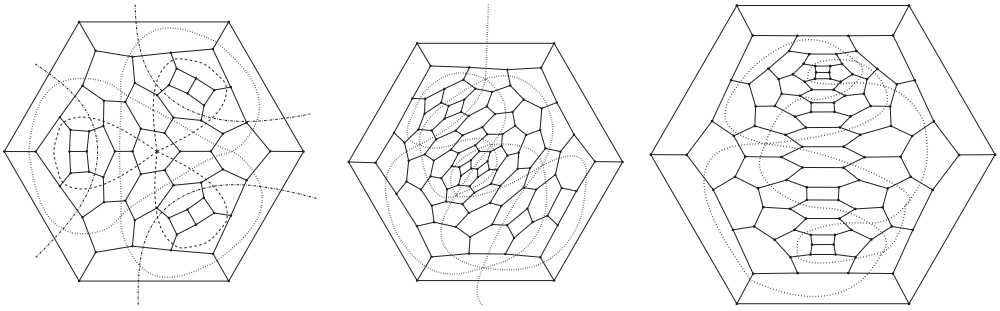
In order to illustrate the notion of railroads, we give in the remainder of this section two lists: those having or, respectively, not having triple self-intersections of the curves representing railroads in two-faced n-vertex polyhedra of type 4_n for small n. In Tables 2 and 3 and Figure 6, we present the first cases of such curves, the first column being the name of the curve. The smallest graph of type 4_n, which is denoted by n_x, x being the number of the graph in CPF output (see [23]), is listed in the second column. In some cases the curve appears twice in this graph; we mark this situation by putting 'twice' in parenthesis. The third and fourth columns give the number m of intersection points and the number p_i of i-gons, $1 \leqslant i \leqslant 6$. The fifth and sixth columns give the point group and the z-vector of the corresponding graph of type 4_n.

The computation of all railroads in the class of polyhedra 4_n, $n \leqslant 88$, with at least two self-intersections, all being double self-intersections, produced a list of projections of

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Table 2. Alternating knots in railroads of graphs of type 4_n, $n \leqslant 88$.

Knot	First appearance	m	$p_1, \ldots, p_6$	Group	z-vector
0_1	20_3	0		D_{3d}	$6^3; 42_{12,0}$
3_1	26_2	3	0, 3, 2, 0, 0, 0	D_{3h}	$24^2_{3,0}, 30_{3,0}$
4_1	64_{17} (twice)	4	0, 2, 4, 0, 0, 0	D_{2d}	$48^4_{4,0}$
5_2	74_{24}	5	0, 3, 2, 2, 0, 0	C_{2v}	$18^4; 48^2_{5,0}, 54_{3,0}$
6_3	74_{21}	6	0, 2, 4, 2, 0, 0	C_2	$54^2_{6,0}, 114_{27,0}$
7_4	80_{30} (twice)	7	0, 4, 2, 2, 0, 1	D_{2h}	$60^4_{7,0}$
9_{23}	62_{16}	9	0, 2, 6, 2, 0, 1	C_{2v}	$60^2_{9,0}, 66_{9,0}$
9_{40}	56_{19}	9	0, 8, 3, 0, 0, 0	D_{3h}	$12^4; 60^2_{9,0}$
11_{332}	88_{44}	11	0, 2, 4, 7, 0, 0	C_{2v}	$24^4; 84^2_{11,0}$
15_y	80_{29}	15	0, 0, 8, 6, 0, 0	D_{3d}	$12^6; 84^2_{12,0}$
18_y	80_{28}	18	0, 0, 14, 0, 6, 0	D_3	$24^2; 96^2_{18,0}$



Graph 66_{11},1 – 1 Graph 108_{18},6 – 1 Graph 108_{48}, 1 – 6

Figure 6. Three graphs of type 4_n with triple self-intersecting railroads.

alternating knots, as presented in Table 2. We use Rolfsen's notation (see [27]) for knots with at most 10 crossings and those of Thistlethwaite [30], for other knots. We denote by 15_y and 18_y the 15- and 18-crossing alternating knots, appearing in a graph of type 4_{80}, which are 80_{29} and 80_{28}, respectively. (The knot 15_y comes from APrism_3 or from knot 9_{40} by inscribing consecutively 3 or 2 triangles, respectively.) All curves representing railroads with triple self-intersections in the graphs 4_n, with $n \leqslant 142$, are given in Figure 6 and Table 3. The notation $i - j$, given in the first column, means that i is the number of triple points of the curve and j is the order of appearance (amongst curves with i triple points) in this table.

Remark. Let Z be a zigzag of signature (α_1, α_2) bounding a railroad R with m_2 double and m_3 triple self-intersections. Then we have $m_2 + 3m_3 = \alpha_1 + \alpha_2$.

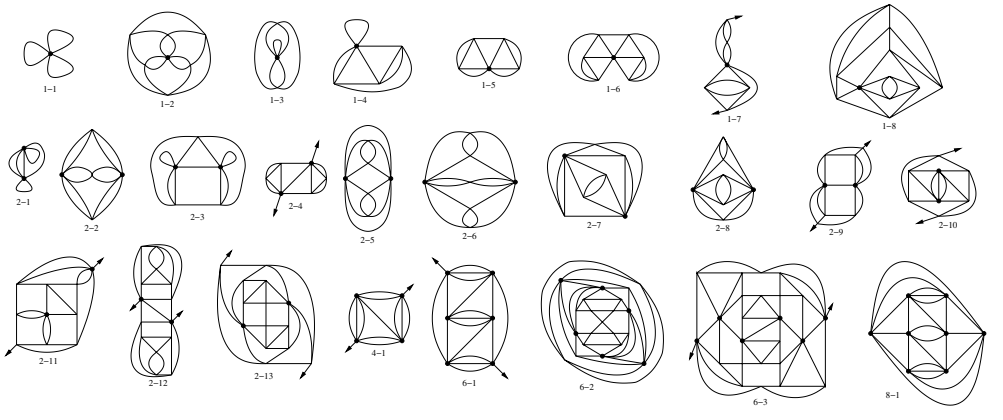
Proposition 3.1. *Let G be a simple polyhedron with p-vector $p = (\ldots, p_i, \ldots)$ and let G be tight. Then the number of zigzags of G is at most*

$$\sum_{i \neq 6} ip_i/2.$$

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Table 3. Curves with triple self-intersections in railroads of graphs of type 4_n, $n \leqslant 142$.

Curve	First appearance	m	$p_1, \ldots, p_6$	Group	z-vector
1–1	66_{11} (twice)	1	3, 0, 1, 0, 0, 0	D_{3h}	$36^4_{3,0}, 54_{3,0}$
1–2	126_{76}	7	0, 3, 4, 3, 0, 0	D_{3h}	$18^6; 90^3_{9,0}$
1–3	106_{53}	3	1, 2, 3, 0, 0, 0	C_s	$18^4; 30_{1,0}, 42_{1,0}, 54_{1,0}, 60^2_{5,0}$
1–4	86_{39}	4	1, 2, 3, 1, 0, 0	C_1	$60^2_{6,0}, 138_{33,0}$
1–5	114_{36} (twice)	5	0, 4, 3, 0, 1, 0	C_{2v}	$54_{3,0}, 72^4_{7,0}$
1–6	108_{48} (twice)	7	0, 2, 7, 0, 1, 0	C_{2v}	$78^3_{9,0}, 90_{9,0}$
1–7	142_{82}	5	0, 3, 4, 2, 0, 0	C_1	$24^3; 60_{1,0}, 90^2_{8,0}, 114_{14,0}$
1–8	114_{61}	11	0, 2, 8, 5, 0, 0	C_1	$102^2_{13,0}, 138_{19,0}$
2–1	140_{68}	2	2, 2, 2, 0, 0, 0	C_2	$24^2; 72^2_{6,0}, 114^2_{13,0}$
2–2	90_{30}	5	0, 6, 0, 3, 0, 0	D_{3h}	$18^4; 54_{3,0}, 72^2_{9,0}$
2–3	122_{21}	5	2, 2, 2, 3, 0, 0	C_2	$42_{1,0}, 78^2_{5,0}, 84^2_{9,0}$
2–4	126_{39}	6	0, 4, 4, 2, 0, 0	C_2	$36^2_{1,0}, 90^2_{10,0}, 126_{21,0}$
2–5	134_{130}	6	0, 3, 6, 1, 0, 0	C_{2v}	$36^2; 42^2_{2,0}, 54_{3,0}, 96^2_{11,0}$
2–6	122_{104}	7	0, 4, 4, 3, 0, 0	C_{2v}	$30^4; 54_{3,0}, 96^2_{11,0}$
2–7	124_{100}	7	0, 3, 6, 2, 0, 0	C_2	$90^2_{9,0}, 96^2_{11,0}$
2–8	128_{64}	7	0, 2, 6, 3, 0, 0	C_s	$54_{3,0}, 96^2_{11,0}, 138_{17,0}$
2–9	110_{24}	8	0, 4, 4, 4, 0, 0	C_2	$90^2_{12,0}, 150_{33,0}$
2–10	110_{74}	8	0, 2, 8, 2, 0, 0	C_2	$90^2_{12,0}, 150_{33,0}$
2–11	134_{50}	10	0, 4, 4, 6, 0, 0	C_2	$114^2_{14,0}, 174_{29,0}$
2–12	134_{149}	14	0, 2, 8, 8, 0, 0	C_2	$126^2_{18,0}, 150_{21,0}$
2–13	126_{57}	14	0, 0, 12, 6, 0, 0	D_3	$126_{9,0}, 126^2_{18,0}$
4–1	72_{17}	4	0, 6, 4, 0, 0, 0	D_2	$24; 48_{4,0}, 72^2_{12,0}$
6–1	108_{18}	6	0, 6, 8, 0, 0, 0	D_3	$24^3, 36; 108^2_{18,0}$
6–2	138_{102}	21	0, 1, 20, 6, 2, 0	C_2	$78_{3,0}, 168^2_{33,0}$
6–3	158_{150}	24	0, 0, 24, 6, 0, 2	D_3	$102_{9,0}, 186^2_{36,0}$
8–1	144_{151}	8	0, 6, 12, 0, 0, 0	D_2	$36; 108_{12,0}, 144^2_{24,0}$



Proof. In fact, each zigzag has a non 6-gonal face on each of its sides, since otherwise it would have a railroad on this side; so the total number of incidences between zigzags and non 6-gons is at least twice the number of zigzags. On the other hand, the number of those incidences is exactly $\sum_{i \neq 6} ip_i$. □

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Proposition 3.2. *Let G be a graph of type 4_n having railroads $R_1, \ldots, R_p$; let H be a plane graph formed by the curves representing those railroads. Then:*

(i) *every t-gonal face of H with $t = 0, 1$ contains exactly 3-t 4-gons of G, and every 2-gonal face of H contains one or two 4-gons of G,*

(ii) *if q_t is the number of t-gonal faces of H, then we have the inequality*

$$3q_0 + 2q_1 + q_2 \leqslant 6.$$

Proof. Every t-gonal face F of H can be viewed as a regular patch with $t = t_{\mathrm{ob}} + t_{\mathrm{ac}}$ (obtuse and acute) intersections of arcs. Let p'_4 be the number of 4-gons inside F. We will apply Theorem 2.3.

(i) If $t = 0$ then $2p'_4 = 6$, and we are done. If $t = 1$ then

$$2p'_4 = 6 - t_{\mathrm{ob}} - 2t_{\mathrm{ac}} \geqslant 4 \quad \text{and} \quad 2p'_4 = 6 - t_{\mathrm{ob}} - 2t_{\mathrm{ac}} < 6.$$

Since $2p'_4$ is even, we get that $2p'_4 = 4$, *i.e.*, every 1-gon contains exactly two 4-gons. If $t = 2$, then

$$2p'_4 = 6 - t_{\mathrm{ob}} - 2t_{\mathrm{ac}} \geqslant 2 \quad \text{and} \quad 2p'_4 = 6 - t_{\mathrm{ob}} - 2t_{\mathrm{ac}} < 6.$$

This yields $p'_4 = 1$ or $p'_4 = 2$.

(ii) Any graph of type 4_n has six 4-gons, so the result follows. □

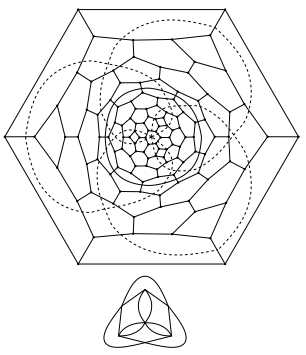
The Euler formula for the p-vector of a 3-valent polyhedron, $12 = \sum_t (6 - t)p_t$, is a discrete analogue of the Gauss–Bonnet formula, $2\pi(1 - g) = \int_S K(x)dx$, for the Gaussian curvature K of a surface S of genus g. So, the q-gons can be seen as *positively curved*, *flat*, or *negatively curved*, if $q < 6$, $q = 6$, or $q > 6$, respectively.

Consider a two-faced graph G, which is a 3_n, 4_n or 5_n; it has four 3-gons, six 4-gons, or twelve 5-gons, respectively. Let us call the *graph of curvatures* of G the following graph (possibly, with loops and multiple edges) having as vertex-set all non-6-gonal faces of G. Two vertices, say, non-6-gonal faces b and c of G, are called adjacent if there exist a pseudo-road connecting faces b and c. A *pseudo-road* is a sequence of hexagons, say $a_1, \ldots, a_l$, such that putting $a_0 = b$ and $a_{l+1} = c$, we have that any a_i, $1 \leqslant i \leqslant l$, is adjacent to a_{i-1} and a_{i+1} on opposite edges. Clearly, the graph of curvatures of a graph w_n, $w \in \{3, 4, 5\}$, is regular of degree w.

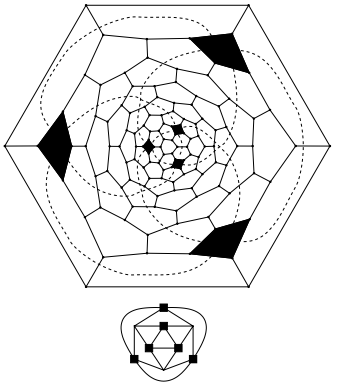
Given a hexagon in a graph of type 3_n, 4_n, or 5_n, any pair of opposite edges belongs to a railroad or a pseudo-road; so, we have exactly a triple covering of the set of all hexagons by the set of all railroads and pseudo-roads. Every non-6-gonal face, *i.e.*, t-gonal face with $t < 6$, has t adjacencies with the system of pseudo-roads.

For the special case when our graph is of type 4_n, any pseudo-road arriving on a 4-gonal face can be extended on the opposite edge. So the set of such extended pseudo-roads, together with the set of railroads, can be identified with the set of central circuits of the dual of our graph. Hence, extended pseudo-roads can be seen (in the same way as for railroads) as projections of a Jordan curve on the plane with double and, eventually, triple points of self-intersection. Those notions are illustrated in Figure 7. This graph $4_{126}(D_{3h})$

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One of two self-intersecting railroads and the equatorial simple railroad



All twelve pseudo-roads

Figure 7. Road-decomposition of a graph $4_{126}(D_{3h})$.

Table 4. All simple polyhedra with only a-gonal and b-gonal faces, $3 \leqslant a < b \leqslant 6$.

(a,b)	Polyhedra	Exist if and only if	p_a	n
$(5,6)$	5_n (fullerenes)	$p_6 \in N - \{1\}$	$p_5 = 12$	$n = 20 + 2p_6$
$(4,6)$	4_n	$p_6 \in N - \{1\}$	$p_4 = 6$	$n = 8 + 2p_6$
$(3,6)$	3_n	$p_6/2 \in N - \{1\}$	$p_3 = 4$	$4 + 2p_6$
$(4,5)$	4 dual deltahedra	$p_5 = 2,3,4,5$	$p_4 = 5,4,3,2$	$n = 10,12,14,16$
$(3,5)$	Dürer's Octahedron	$p_5 = 6$	$p_3 = 2$	$n = 12$
$(3,4)$	Prism_3	$p_4 = 3$	$p_3 = 2$	$n = 6$

has the following *road decomposition*: five concentric simple railroads (we indicate only the central, *equatorial* one), two self-intersecting railroads (they differ only by their opposite position on the sphere, and we present only one of them) and all 12 pseudo-roads.

4. Two-faced polyhedra

Recall that *two-faced* polyhedra have only a- and b-gonal faces with $3 \leqslant a < b \leqslant 6$ (see [7]). Denote by $p_a > 0$ and $p_b \geqslant 0$ the number of a-gonal and b-gonal faces.

Any 3-valent n-vertex two-faced polyhedron has $3n/2 = (ap_a + bp_b)/2$ edges and satisfies the Euler relation $n - 3\frac{n}{2} + (p_a + p_b) = 2$, *i.e.*, $n = 2(p_a + p_b - 2)$ and $p_a(6-a) + p_b(6-b) = 12$. So $b < 6$ is possible only for 6 simple polyhedra with $(a,b) = (3,4)(\text{Prism}_3)$, $(3,5)$(Dürer's Octahedron), $(4,5)$(four dual deltahedra). The other cases, namely $(a,b) = (3,6),(4,6),(5,6)$, are denoted by 3_n, 4_n, 5_n, where n is the number of vertices. The polyhedra 5_n are the well-known *fullerenes* (of Organic Chemistry). See Table 4 for all the possibilities. The criterion for the existence of the polyhedra of type 3_n, 4_n and 5_n is due to [21].

For the types 3_n, 4_n and 5_n in Table 4 the case $p_6 = 0$ yields the Tetrahedron, the Cube and the Dodecahedron. Those three polyhedra, together with 4 dual deltahedra and Prism_3, are the duals of the eight *convex deltahedra*. *Dürer's Octahedron* is the Cube

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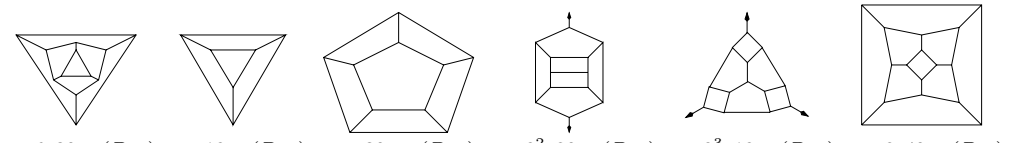


Figure 8. Dürer's Octahedron, Prism_3 and four dual deltahedra.

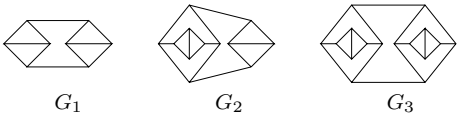
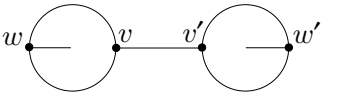


Figure 9. First graphs $(G_n)_{n\geqslant 1}$.

truncated at two opposite vertices. The four dual deltahedra from the fourth line of Table 4 are: Prism_5 (dual 5-bipyramid), dual *bisdisphenoid*, dual 3-*augmented* Prism_3, dual 2-*capped* APrism_4. Those four dual deltahedra, preceded by the Dürer's Octahedron and Prism_3, are given in Figure 8 with their z-vectors and groups.

Lemma 4.1. *Any connected* 3*-valent plane graph having only* q*-gonal faces with* $3 \leqslant q \leqslant 6$ *is* 2*-connected.*

Proof. Let G be one such graph and assume that there is one vertex v, such that $G-\{v\}$ is disconnected. $G-\{v\}$ has two or three components; clearly, it cannot have three components, since $q \leqslant 6$. Denote by C_1 and C_2 the two components and by $e=\{v,v'\}$ the edge linking C_1 to C_2. Then two edges from v will connect to another vertex w and two edges from v' will connect to another vertex w', since we assume that the faces are incident to at most 6 edges. See below the corresponding drawing:



But the vertex w will disconnect the graph and so, iterating the construction, we obtain an infinite sequence $v_1,\ldots,v_n$ of vertices that disconnect G. This contradicts the initial assumption and proves that G is 2-connected. □

Denote by $(G_n)_{n\geqslant 1}$ the 3-valent plane $4(n+1)$-vertex graph whose faces are (organized in pairs of adjacent ones) triangles and hexagons. The graph G_n is 2-connected but not 3-connected; its z-vector is $4^{n+1},(4n+4)^2$; its symmetry group is D_{2d} or D_{2h}, if n is even or odd, respectively. The first occurrences are depicted in Figure 9.

Proposition 4.2. *Any* 3*-valent plane graph having only* q*-gonal faces with* $3 \leqslant q \leqslant 6$ *is* 3*-connected, except the graphs of the family* $(G_n)_{n\geqslant 1}$.

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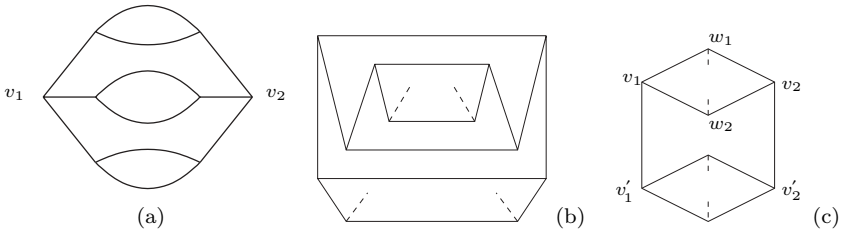


Figure 10. Some 2-connected graphs

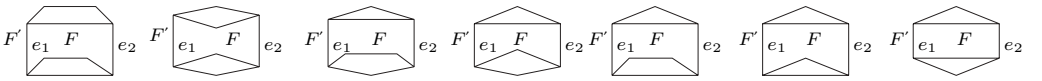


Figure 11.

Proof. Let G be a 3-valent plane graph with k-gonal faces, $3 \leqslant k \leqslant 6$ and assume that it is not 3-connected. Then there are two vertices, say v_1 and v_2, such that $G - \{v_1, v_2\}$ is disconnected. If $G - \{v_1, v_2\}$ has three components, then since $q \leqslant 6$, it is of the form depicted in Figure 10(a), which is impossible by the condition $q \geqslant 3$; so $G - \{v_1, v_2\}$ has two components, say C_1 and C_2.

There are two edges, say $e_1 = \{v_1, v_1'\}$ and $e_2 = \{v_2, v_2'\}$, that connect C_1 to C_2. Since $G - \{v_1, v_2\}$ is disconnected, e_1 and e_2 are both incident to faces F and F'. Then, by our assumption on size of faces, we get the possibilities shown in Figure 11. Only the first two cases are possible, since otherwise we would have a non-2-connected plane graph. Figure 10(b), (c) shows the possible continuation of those graphs.

In case (b) we obtain an infinite structure; so we again get a contradiction.

Let us now consider the case (c). The two points w_1 and w_2 can either be connected by an edge and we are done, or be non-connected, in which case w_1 and w_2 disconnect the graph. In the latter case, we can iterate the construction. Since the graph is finite, the construction eventually finish and we get a graph G_{n_0}, $n_0 \geqslant 1$. □

All graphs of type 3_n, 4_n, 5_n with maximal pair of symmetry (T or T_d, O or O_h, I or I_h, respectively) are known; in fact, the Goldberg–Coxeter construction, denoted $GC_{k,l}$ [3, 19, 6], implies that any graph of this type 3_n, 4_n, 5_n and that symmetry is of the form $GC_{k,l}(G_0)$ with $0 \leqslant l \leqslant k$ and G_0 being Tetrahedron, Cube or Dodecahedron, respectively. These graphs have $n_0(k^2 + kl + l^2)$ vertices with $n_0 = 4$, 8 or 20, respectively, and are tight if and only if $\gcd(k, l) = 1$; they are of symmetry T_d, O_h or I_h if and only if $l = 0$ or $k = l$.

The polyhedra dual to the 3-valent polyhedra without q-gonal faces, $q > 6$, are studied in [31], where they are called *nonnegatively curved triangulations* (in fact, the reference [28] is an application of a preliminary version of [31]). Theorem 3.4 in [28] implies that $N_3(n) = O(n)$, $N_4(n) = O(n^3)$ and $N_5(n) = O(n^9)$, where $N_w(n)$ denotes the number of polyhedra w_n for $w = 3, 4, 5$, respectively.

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Table 5. Numbers $N_3(n)$ of graphs 3_n and $N_3^t(n)$ of tight 3_n for $n \leqslant 512$.

n	N_3	N_3^t	n	N_3	N_3^t	n	N_3	N_3^t	n	N_3	N_3^t	n	N_3	N_3^t	n	N_3	N_3^t
12	1	1	96	14	0	180	15	2	264	25	0	348	21	5	432	52	0
16	2	0	100	6	3	184	12	0	268	12	12	352	34	0	436	19	19
20	1	1	104	7	0	188	8	8	272	23	0	356	15	15	440	37	0
24	2	0	108	8	2	192	27	0	276	17	4	360	41	0	444	27	7
28	2	2	112	12	0	196	11	7	280	25	0	364	21	11	448	48	0
32	4	0	116	5	5	200	16	0	284	12	12	368	30	0	452	19	19
36	3	1	120	13	0	204	13	3	288	39	0	372	23	6	456	41	0
40	3	0	124	6	6	208	19	0	292	13	13	376	24	0	460	25	11
44	2	2	128	14	0	212	9	9	296	19	0	380	21	9	464	37	0
48	7	0	132	9	2	216	21	0	300	23	3	384	50	0	468	33	6
52	3	3	136	9	0	220	13	5	304	26	0	388	17	17	472	30	0
56	4	0	140	9	3	224	24	0	308	17	8	392	29	0	476	25	13
60	5	1	144	19	0	228	15	4	312	29	0	396	28	5	480	69	0
64	8	0	148	7	7	232	15	0	316	14	14	400	40	0	484	23	17
68	3	3	152	10	0	236	10	10	320	37	0	404	17	17	488	31	0
72	7	0	156	11	3	240	33	0	324	22	5	408	37	0	492	29	7
76	4	4	160	19	0	244	11	11	328	21	0	412	18	18	496	40	0
80	9	0	164	7	7	248	16	0	332	14	14	416	39	0	500	27	13
84	7	2	168	17	0	252	20	3	336	43	0	420	35	3	504	54	0
88	6	0	172	8	8	256	26	0	340	19	8	424	27	0	508	22	22
92	4	4	176	16	0	260	15	6	344	22	0	428	18	18	512	48	0

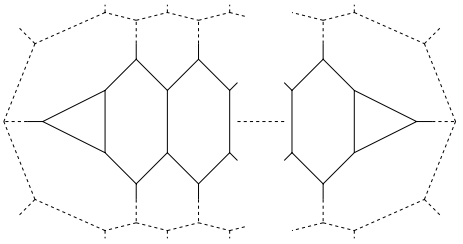


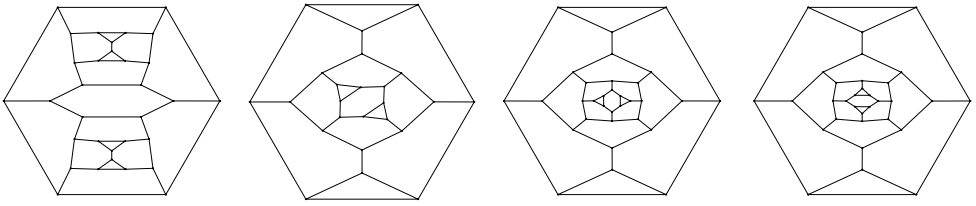
Figure 12. A pseudo-road in a graph of type 3_n and a circular railroad.

5. Polyhedra 3_n

We present in Table 5 the numbers $N_3(n)$ of 3_n and the numbers $N_3^t(n)$ of tight 3_n for $n \leqslant 512$.

In [21] it was shown that each zigzag in a graph of type 3_n is simple and a general construction of all 3_n was given; we sketch this construction with slightly different notation. If a zigzag contains two edges, say e_1 and e_2, of a triangle, then its third edge, say e_3, defines a pseudo-road PR that finish on another triangle. Denote by s one quarter of the length of the zigzag; then $s-1$ is the number of hexagons of PR. Consider the sequence of concentric simple railroads which, possibly, goes around the patch depicted in Figure 12; let m denote the number of zigzags and let $m-1$ be the number of corresponding railroads. The same patch (with the same number $s-1$ of hexagons between the other two triangles and with the same number $m-1$ of concentric simple railroads going around it) occurs on the other side of the sphere. As in [21], we get

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(a) 32 vertices, case (iii), D_{2h} (b) 24 vertices, case (ii), D_2 (c) 32 vertices, case (ii), D_{2d} (d) 32 vertices, case (ii), D_{2h}

Figure 13. Graphs with hexagons adjacent to two triangles.

by direct computation the equality $p_6 = 2(sm - 1)$ and $n = 4sm$, where p_6 is the number of hexagons. See Figure 13(c), (d) for two examples with $s = 2$ and $m = 4$.

Take a triangle T and an edge e of this triangle; e belongs to a sequence of adjacent 6-gons, which is concluded by another triangle T'. If we consider the three edges e_1, e_2, e_3, then we obtain three triangles T_1, T_2, T_3, respectively, that may or may not be distinct.

Theorem 5.1. *Any graph* 3_n *has exactly one of the following forms.*

(i) *The Tetrahedron or the Truncated Tetrahedron* (*the only case when a hexagon is adjacent to more than two triangles*).

(ii) *There are two hexagons, every of which is adjacent to two triangles on opposite edges; there are one or two such graphs of type* 3_n *depending on* $n \equiv 8 \pmod{16}$ *or* $n \equiv 0 \pmod{16}$, *respectively. Their symmetry groups are, respectively,* D_2 *if* $n \equiv 8 \pmod{16}$ *and* D_{2h}, D_{2d} *if* $n \equiv 0 \pmod{16}$.

(iii) *There are four hexagons* (*in two adjacent pairs*), *every one of which is adjacent to two triangles on non-opposite and non-adjacent edges; there is exactly one such graph* 3_n *for every* $n \geqslant 16$, $n \equiv 0 \pmod{4}$.[1] *The symmetry group is* D_{2h} *or* D_{2d} *if* $\frac{n}{4}$ *is even or odd, respectively.*

(iv) *Each hexagon is adjacent to at most one triangle; there is a one-to-one correspondence between such graphs* 3_n *having isolated triangles and IPT fullerenes* 5_n (*i.e., those having their* 12 *pentagons organized in* 4 *triples of mutually adjacent ones*).

Proof. For given graph G of type 3_n, denote by $t(G)$ the maximal number of triangles that are adjacent to a hexagon. The only graph of type 3_n without hexagons is the Tetrahedron. The case $t(G) = 4$ corresponds to the 2-connected but not 3-connected 6-vertex plane graph G_1 (see Figure 9). The only graph of type 3_n with $t(G) = 3$ is the Truncated Tetrahedron. If $t(G) = 2$ then two cases occur: either two triangles are adjacent to a hexagon on opposite edges or they are adjacent to a hexagon on non-opposite and non-adjacent edges.

[1] In the exceptional case $n = 16$, there are only two polyhedra 3_{16}: the Cube truncated at four non-adjacent vertices and the Cube truncated at four vertices of two opposite edges. The second polyhedron is the unique and only example which is of types (ii) and (iii).

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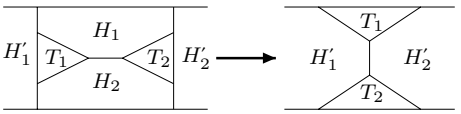
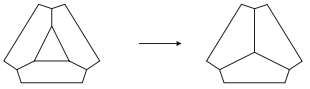


Figure 14.

The first case corresponds to the case $s = 2$ of the Grünbaum–Motzkin construction. The divisibility of n by 8 follows from the formula $n = 4sm$. At the last step of the Grünbaum–Motzkin construction, namely, after adding railroads, we add a pair of triangles in one of two possible ways. If $n \equiv 8 \pmod{16}$, then both ways give isomorphic graphs, both of symmetry D_2, for $n \geqslant 8$ (see Figure 13(b) for this possibility). If $n \equiv 0 \pmod{16}$, then we get two non-isomorphic graphs, one of symmetry D_{2h}, the other of symmetry D_{2d} (see Figure 13(c), (d) for those two possibilities).

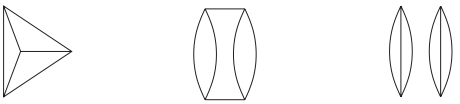
Let our graph be of type (iii), *i.e.*, two hexagons H_1, H_2 are adjacent to two triangles T_1, T_2 on non-opposite and non-adjacent edges, as in Figure 14. The two hexagons H_1, H_2 are adjacent, respectively, to two hexagons H'_1, H'_2. By replacing the patch H_1, H_2, T_1, T_2 by two triangles, we get a graph 3_{n-4}, which is also of type (iii). By induction, we get for any $n \equiv 0 \pmod{4}$ with $n \geqslant 16$ a unique graph. A graph of type (iii) has two pairs of hexagons, each pair being adjacent to two triangles; if one does this operation to the two pairs, then the symmetry group remains the same. So we have a periodicity of order 8 for the symmetry groups and the result on groups follows.

If the graph has $t(G) = 1$, then the operation depicted in the picture below on all triangles establishes a one-to-one correspondence: □



See Figure 13(a), (c), (d) for all graphs 3_{32} having hexagons adjacent to two triangles.

Proposition 5.2. *The graph of curvatures of a* 3_n *is one of the three following* 4*-vertex graphs:*



Proof. Take a triangle, say T_1, and an edge e_1 of T_1. The pseudo-road, which is defined by T_1 and e_1, establishes an edge between T_1 and, say, T_2; this pseudo-road is bounded by one zigzag Z_1. This zigzag belongs to a sequence of m concentric zigzags $Z_1, Z_2, \ldots, Z_m$. The zigzag Z_m defines a pseudo-road between the remaining triangles T_3 and T_4, *i.e.*, an edge connecting T_3 to T_4 in the graph of curvatures. Since any vertex of the graph of curvatures has degree 3, we are done. □

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Conjecture 5.3. *The graph of curvatures of any tight graph of type* 3_n *is as in the first case of Theorem* 5.2.

Fix a graph G of type 3_n. Denote by T_i, $1 \leqslant i \leqslant 4$, the triangles in G, by $(e_i)_{1 \leqslant i \leqslant 3}$ the edges of T_1, by PR_i the pseudo-road defined by T_1, e_i and by $(4s_i)_{1 \leqslant i \leqslant 3}$ the lengths of corresponding zigzags. Without loss of generality, we can suppose that $s_1 \leqslant s_2 \leqslant s_3$. Denote by $m_1 - 1$, $m_2 - 1$, $m_3 - 1$, respectively, the corresponding number of concentric railroads around each of three patches. Denote by $Z_{i,k}$, where $1 \leqslant i \leqslant 3$ and $1 \leqslant k \leqslant m_i$, the zigzags of G.

Theorem 5.4. *For a graph* G *of type* 3_n*, the following properties hold:*

(i) *its z-vector is* $(4s_1)^{m_1}, (4s_2)^{m_2}, (4s_3)^{m_3}$*; the number of railroads is* $m_1 + m_2 + m_3 - 3$,
(ii) G *has at least three zigzags with equality if and only if it is tight,*
(iii) *if* G *is tight, then* $z(G) = n^3$ *(so each zigzag is a Hamiltonian circuit),*
(iv) G *is z-balanced and*

$$|Z_{i,k} \cap Z_{j,l}| = \begin{cases} 0 & \text{if } i = j, \\ \frac{n}{2m_i m_j} & \text{if } i \neq j. \end{cases}$$

Proof. If Z is a fixed zigzag of G, then it belongs to a sequence of m_i concentric zigzags of a patch defined by two triangles and a pseudo-road. Property (i) follows immediately; (ii) is a corollary of (i), since G is tight if and only if all m_i are equal to 1.

Let G be a tight 3_n; the formula $n = 4sm$ becomes $n = 4s_1 = 4s_2 = 4s_3$. So, $z = n^3$.

Clearly, any two zigzags $Z_{i,k}$ and $Z_{j,l}$ are disjoint if $i = j$. Moreover, the size of the intersection $Z_{i,k} \cap Z_{j,l}$ depends only on i and j. Denote by β_{ij} the size of the pairwise intersections $|Z_{i,1} \cap Z_{j,1}|$. We obtain the linear system

$$\begin{cases} 4s_1 = \beta_{13} m_3 + \beta_{12} m_2, \\ 4s_2 = \beta_{23} m_3 + \beta_{12} m_1, \\ 4s_3 = \beta_{23} m_2 + \beta_{13} m_1, \end{cases}$$

which has the unique solution $\beta_{ij} = \frac{n}{2m_i m_j}$. If we write this intersection size as $8s_i s_j / n$, then it is easy to see that G is z-balanced. □

Theorem 5.5. *All graphs of type* 3_n *are tight if and only if* $\frac{n}{4}$ *is prime.*

Proof. Assume that $\frac{n}{4}$ is prime; let G be a graph 3_n with parameters s_i, m_i defined before Theorem 5.4. If $\frac{n}{4} = s_i m_i$, then either $s_i = 1$, or $m_i = 1$. The first case corresponds to a 2-connected but not 3-connected plane graph; so, $m_1 = m_2 = m_3 = 1$ and G has no railroad. The second case $m_i = 1$ also means the absence of a railroad.

Assume that $\frac{n}{4}$ is not prime; if $n = 4pq$ for $q > 1$, then, using the Grünbaum–Motzkin construction, we can construct a graph of type 3_n with a system of $q > 1$ concentric zigzags of length $4p$, and so with at least $q - 1 \geqslant 1$ railroads. □

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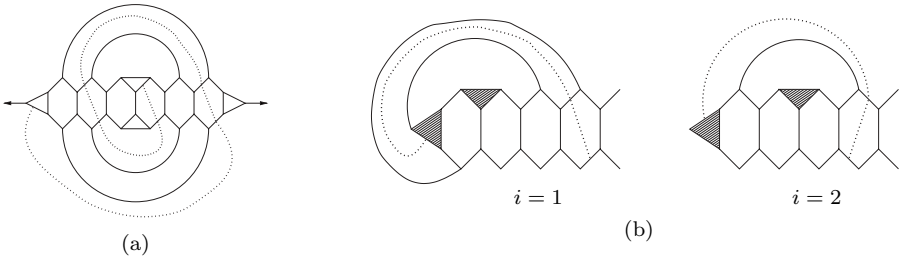


Figure 15. The pseudo-road construction.

Remark. In Table 5, the number of graphs of type 3_n for prime $\frac{n}{4}$ is a non-decreasing function.

Theorem 5.6. *There exists a tight graph G of type 3_n if and only if $\frac{n}{4}$ is odd.*

Proof. The unique (for every integer $\frac{n}{4} \geqslant 4$) graph, defined in Theorem 5.1(iii), is tight if $\frac{n}{4}$ is odd; we represent this graph in Figure 15(a) for $n = 28$.

Suppose now that $\frac{n}{4}$ is even and that G is tight. We will use the necessary conditions of Theorem 5.4 to get a contradiction.

Consider the patch formed by a pseudo-road PR between two triangles, say T_1 and T_2. Since G is assumed to be tight, there are $\frac{n}{4} - 1$ hexagons in PR. Moreover, since there are no railroads, any of the remaining two triangles T_3 and T_4 will be adjacent to the hexagons of PR. Let i be the position of T_3 in PR. The choice of position for T_3 and T_4 determines our graph of type 3_n; so we need to show that every choice of i leads to a non-tight graph 3_n. If we find a shorter pseudo-road, then we are done.

Define a pseudo-road PR$'$ by starting with T_1 and taking the upper edge if i is even and the lower edge if i is odd (see Figure 15(b)). PR$'$ intersects with PR. From the choice of PR$'$, the position p of the first hexagon of intersection, of PR$'$ with PR, satisfies $p \equiv 0 \pmod 4$. Moreover, all positions of hexagons of intersection satisfy this condition. So, PR$'$ is shorter than $\frac{n}{4} - 1$ and the graph is *not* tight. □

The list of all symmetry groups of graphs 3_n is known (see [16]); they are (with their first appearance): $D_2(24_2)$, $D_{2h}(16_1)$, $D_{2d}(20_1)$, $T(28_2)$, $T_d(4_1)$ (see [13] for the corresponding drawings).

For the point groups D_2, D_{2d} and D_{2h}, we have the following conjecture, which we checked for $n \leqslant 500$.

Conjecture 5.7.

(i) *$3_n(D_{2h})$ exists if and only if $\frac{n}{4}$ is even and $n \geqslant 16$; there are no tight $3_n(D_{2h})$.*
(ii) *$3_n(D_{2d})$ exists if and only if either $\frac{n}{4}$ is odd and $n \geqslant 20$, or $\frac{n}{8}$ is even and $n \geqslant 24$; the graph defined in Theorem* 5.1(iii) *is a unique $3_n(D_{2d})$ tight graph if $\frac{n}{4}$ is odd and $n \geqslant 20$.*

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Table 6. Numbers $N_4(n)$ of graphs 4_n and $N_4^t(n)$ of tight 4_n for $n \leqslant 260$.

n	N_4	N_4^t	n	N_4	N_4^t	n	N_4	N_4^t	n	N_4	N_4^t	n	N_4	N_4^t	n	N_4	N_4^t
8	1	1	52	13	10	94	46	27	136	165	104	178	291	176	220	646	403
12	1	1	54	10	6	96	59	45	138	110	89	180	298	215	222	426	276
14	1	0	56	23	16	98	65	38	140	220	134	182	356	190	224	776	469
16	1	1	58	12	8	100	70	50	142	150	96	184	388	246	226	584	361
18	1	1	60	19	15	102	48	34	144	164	116	186	259	174	228	567	413
20	3	2	62	21	11	104	99	62	146	189	109	188	479	285	230	684	357
22	1	1	64	22	17	106	65	43	148	207	145	190	352	203	232	754	481
24	3	3	66	16	12	108	79	60	150	142	106	192	352	264	234	489	331
26	3	1	68	36	24	110	89	53	152	265	167	194	418	230	236	894	517
28	3	3	70	21	12	112	97	63	154	190	109	196	463	310	238	681	421
30	2	2	72	29	23	114	68	47	156	202	146	198	303	207	240	663	471
32	8	5	74	31	16	116	133	80	158	237	121	200	559	338	242	781	463
34	3	2	76	34	24	118	90	58	160	262	162	202	419	274	244	867	533
36	7	5	78	24	14	120	99	75	162	175	123	204	424	313	246	566	381
38	7	4	80	53	32	122	115	67	164	330	205	206	498	260	248	1016	594
40	7	5	82	32	21	124	127	81	166	239	140	208	553	355	250	790	466
42	5	4	84	42	33	126	86	58	168	249	193	210	365	251	252	751	541
44	14	7	86	47	25	128	171	103	170	288	154	212	663	400	254	902	487
46	6	5	88	50	36	130	118	79	172	319	221	214	500	309	256	1006	629
48	12	9	90	35	27	132	133	100	174	209	135	216	483	358	258	661	459
50	12	8	92	75	48	134	152	82	176	397	250	218	580	332	260	1173	675

(iii) *$3_n(D_2)$ exists if and only if $n \geqslant 24$ and $n \neq 28, 32$; tight $3_n(D_2)$ exists if and only if $\frac{n}{4}$ is odd, $n \geqslant 44$ and $n \neq 60, 84$; there are i tight $3_n(D_2)$ graphs starting with $\frac{n}{4} = 6i + 5$ for $1 \leqslant i \leqslant 9$, except the case $i = 5$ starting with $\frac{n}{4} = 37$.*

6. Polyhedra 4_n

Since any graph of type 4_n is bipartite, we can apply Theorem 2.1: all self-intersections of every zigzag are of type I. Moreover, there exists an orientation of zigzags with respect to which each edge has type I. We will always work with such orientation. Any self-intersection, double or triple, of railroads is of type I (see Figure 4).

We present in Table 6 the numbers $N_4(n)$ of 4_n and the numbers $N_4^t(n)$ of tight 4_n for $n \leqslant 260$.

Conjecture 6.1.

(i) *z-knotted 4_n exists if and only if $n \geqslant 30$, $n \equiv 2 \pmod 4$.*
(ii) *Tight 4_n exists if and only if $n \geqslant 8$, $n \neq 10, 14$.*
(iii) *Every tight 4_n has at most eight zigzags.*

Theorem 6.2. *All symmetry groups of 4_n (with their first appearance) are $C_1(40_4)$, $C_s(34_2)$, $C_2(26_1)$, $C_i(140_{12})$, $C_{2v}(22_1)$, $C_{2h}(44_7)$, $D_2(24_2)$, $D_3(20_1)$, $D_{2d}(16_1)$, $D_{2h}(20_2)$, $D_{3d}(20_3)$, $D_{3h}(14_1)$, $D_6(84_{42})$, $D_{6h}(12_1)$, $O(56_{17})$, $O_h(8_1)$.*

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Proof. Let G be a graph of type 4_n and let r be a rotation of G of order k. By definition of a graph 4_n, we have $k = 2$, 3, 4 or 6.

If $k = 6$, then the axis of r goes through two hexagons, say H_1 and H_2. Consider the ring of hexagons around H_1 adjacent to it; then, after adding p such concentric rings of hexagons, we will encounter a square and so, by 6-fold symmetry, all squares of G. We can then complete the graph, in a unique way, by adding the same number of rings of hexagons on the other side of the sphere. This construction implies the existence of rotations of order two passing through opposite squares and middles of consecutive squares. This implies symmetry D_6 or D_{6h}.

If $k = 4$, then the axis of r goes through two squares, say sq_1 and sq_2. After adding p rings of hexagons around sq_1, we find a square and so, by symmetry, four squares, say $sq_3, \ldots, sq_6$. We can complete the graph in a unique way; from the construction it is clear that there is a 4-fold axis through sq_3. So the group is O or O_h.

If $k = 3$, then the axis of r goes through either one vertex or one hexagon. After adding p rings of hexagons around this centre, we find three squares; then, adding q rings of hexagons, we find the three other squares. The patch formed by those six squares and the q rings of hexagons has an additional symmetry, formed by exchanging the two triples of squares. So G has this symmetry too, and the symmetry group is D_3, D_{3h}, or D_{3d}.

Assume that G has symmetry S_4. The six squares are partitioned in one orbit of two squares, say sq_1 and sq_2, and another of four squares. The 2-fold axis goes through sq_1 and sq_2; moreover, if we consider the four pseudo-roads PR_i from sq_1, then all of them stop at sq_2. Consider the patch P formed by PR_1 and PR_2. This patch has two acute angles; so by Theorem 2.3 it contains exactly one square sq. We will show that sq is in the plane, defined by sq_1 and sq_2, which will prove that there is a plane of symmetry for G. If sq is next to PR_1 and PR_2, then their length is two and the result holds; otherwise, by removing some hexagons, we find a smaller patch with the same property and we conclude by induction.

The above reasonings yield the following list of possibilities: C_1, C_s, C_2, C_i, C_{2v}, C_{2h}, D_2, D_3, D_{2d}, D_{2h}, D_{3d}, D_{3h}, D_6, D_{6h}, O, O_h. For every such group there is a graph of type 4_n with $n \leqslant 140$ having this symmetry; their pictures are available from [13]. □

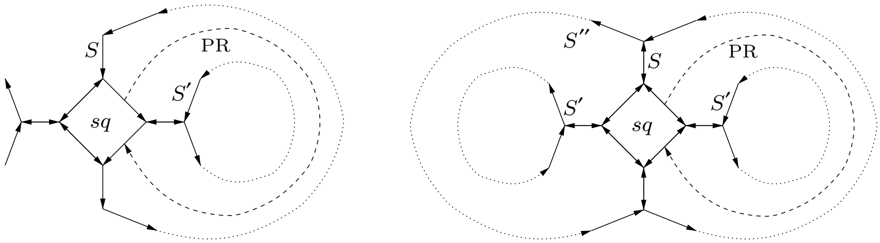
A similar study of point groups for 4-valent plane graphs was done in [11].

Theorem 6.3. *Every tight* 4_n *has at most* 9 *zigzags.*

Proof. Let G be a tight 4_n with zigzags $Z_1, \ldots, Z_l$. We obtain $2l$ sides, since every zigzag has two sides. A side S is called *lonely* if it is incident to exactly one square sq. We can define a pseudo-road PR, parallel to S, which will begin and finish on sq. On the other side of the pseudo-road there will be a side S' of a zigzag Z', which will be incident twice to sq. Moreover, if S' is incident exactly twice to sq, then it defines another lonely side S'' (see Figure 16(b)).

Call n_{1a} the number of lonely sides in the first case and n_{1b} the number of lonely sides in the second case. Also let n_2 be the number of sides incident to exactly two squares

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(a) One lonely side S (b) Two lonely sides S and S''

Figure 16. Two cases of lonely sides.

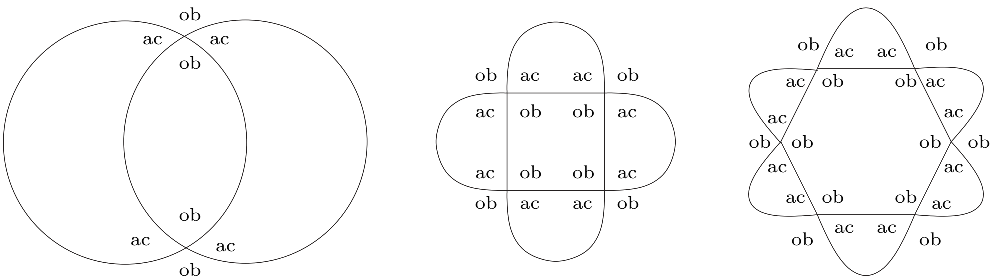


Figure 17.

(identical or not) and n_3 the number of sides incident to at least three squares (identical or not). Obviously, $l = \frac{1}{2}(n_{1a} + n_{1b} + n_2 + n_3)$.

In case (a), a lonely side, S' is incident to at least three squares, so $n_{1a} \leqslant n_3$; while in case (b) S' is incident exactly twice to sq, so $n_{1b} \leqslant n_2$. Every square sq can be incident to 0, 1 or 2 lonely sides, so we have the inequality $n_{1a} + \frac{n_{1b}}{2} \leqslant 6$. By an enumeration of incidences, we get $n_{1a} + n_{1b} + 2n_2 + 3n_3 \leqslant 4 \times 6 = 24$. The 4-dimensional polyhedron defined by the above inequalities and nonnegativity inequalities $n_{1a}, \ldots, n_3 \geqslant 0$ is denoted by $\mathscr{P}$. We can maximize the linear function $\frac{1}{2}(n_{1a} + n_{1b} + n_2 + n_3)$ over P using the cdd program (see [17]) and obtain the upper bound 9, which is attained for the unique 4-uple $(n_{1a}, n_{1b}, n_2, n_3) = (0, 12, 6, 0)$. □

The following theorem is in sharp contrast to Theorem 5.4(iv) for graphs 3_n and Theorem 7.1 for graphs 5_n.

Theorem 6.4. *The intersection of every two simple zigzags of a graph of type* 4_n*, if non-empty, has one of the forms shown in Figure* 17 (*and so its size is* 2, 4 *or* 6).

Proof. Define the graph H as the graph whose vertices are edges of intersection between simple zigzags Z and Z', with two vertices being adjacent if they are linked by a path belonging to one of Z, Z'. The graph H is a plane 4-valent graph and Z, Z' define two central circuits in H. Since Z and Z' are simple, the faces of H are t-gons with even t.

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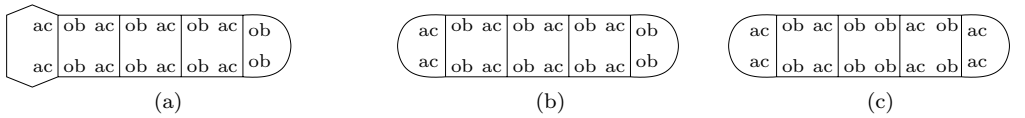


Figure 18. Three cases of sequence of 4-gons.

Applying Theorem 2.3 to a t-gonal face F of H, we obtain that the number p'_4 of 4-gons in F satisfies $6 - t_{ob} - 2t_{ac} = 2p'_4$. So the numbers t_{ob} and t_{ac} are even, since $t = t_{ob} + t_{ac}$. Also, $6 - t_{ob} - 2t_{ac} \geqslant 0$. So $t \leqslant 6$.

We obtain the following five possibilities for the faces of H: 2-gons with two acute angles, 2-gons with two obtuse angles, 4-gons with four obtuse angles, 4-gons with two acute and two obtuse angles, 6-gons with six obtuse angles.

Take an edge e of a 6-gon in H and consider the sequence (possibly empty) of adjacent 4-gons of H emanating from this edge. This sequence will stop at a 2-gon or a 6-gon; the case-by-case analysis of angles yields that this sequence has to stop at a 2-gon (see Figure 18(a)).

Take an edge of a 2-gon in H and consider the same construction. If the angles are both obtuse, then the construction is identical and the sequence will terminate at a 2-gon or a 6-gon. If the angles are both acute, then cases (b), (c) of Figure 18 are possible.

In the first case, all 4-gons contain two obtuse angles and two acute angles, so the pseudo-road finishes with an edge of two obtuse angles. In the second case, there is a 4-gon whose angles are all obtuse; this 4-gon is unique in the sequence and its position is arbitrary. Every pair of opposite edges of a 4-gon belongs to a sequence of 4-gons considered above. So all angles of a 4-gon are the same, *i.e.*, obtuse. This fact restricts the possibilities of intersections to the three cases of the theorem. □

Corollary 6.5. *The only tight 4_n having only simple zigzags are the Cube and the Truncated Octahedron.*

Proof. By Theorem 6.4, every two simple zigzags intersect in at most six edges. Since, by Theorem 6.3, there are at most 9 zigzags, we obtain the upper bound $(9-1)6 = 48$ on the length of every zigzag. This yields the upper bounds $\frac{9}{2}48 = 216$ on the number of edges of G and $\frac{2}{3}216 = 144$ on the number of its vertices. However, our exhaustive computation in this range of values gave the Cube and the Truncated Octahedron as the only solutions. □

7. Polyhedra 5_n

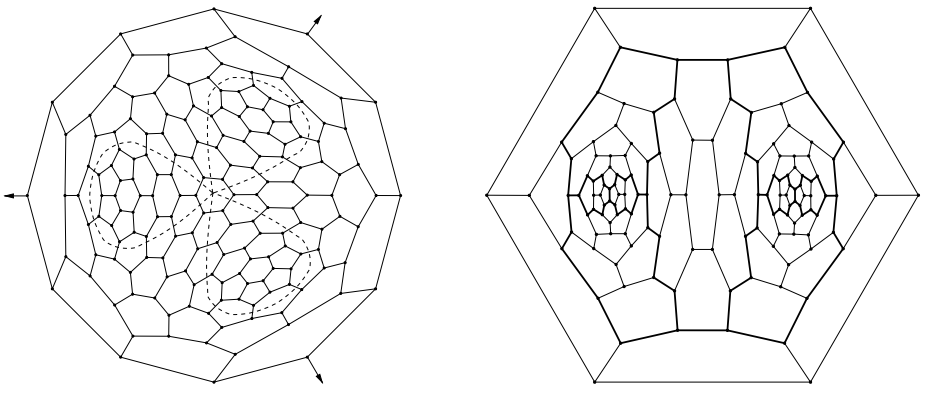
Zigzag structure of fullerenes was studied in [10], to which the present paper is a follow-up. Here we merely add a few observations.

The smallest z-unbalanced fullerenes 5_n with only simple zigzags are $5_{108}(D_{2d})$ and $5_{144}(D_3)$ with z-vectors 24^8, 26^4, 28 and 28^{12}, 32^3, respectively. Any z-uniform or tight 5_n having only simple zigzags with $n \leqslant 200$ is z-balanced.

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Table 7. All tight fullerenes 5_n with $n \leqslant 200$ having only simple zigzags.

n	Group	z-vector	Orb. sizes	Int. vector
20	I_h	10^6	6	2^5
28	T_d	12^7	3,4	2^6
48	D_3	16^9	3,3,3	2^8
60	I_h	18^{10}	10	2^9
60	D_3	18^{10}	1,3,6	2^9
76	D_{2d}	$22^4, 20^7$	1,2,4,4	$4, 2^9$ and 2^{10}
88	T	22^{12}	12	2^{11}
92	T_h	$24^4, 20^9$	3,4,6	2^{12} and $2^{10}, 0^2$
140	I	28^{15}	15	2^{14}



(a) $5_{172}(C_{3v})$ with triple self-intersecting railroad

(b) Two zigzags in $5_{136}(D_{2h})$ with $|Z \cap Z'| = 8$

Figure 19. Two particular fullerenes.

Table 7 gives all tight 5_n, $n \leqslant 200$ with simple zigzags; we conjecture that this list is complete. Apropos, amongst the 9 fullerenes of Table 7 only $5_{60}(I_h)$, $5_{88}(T)$, $5_{140}(I)$ have 12 isolated pentagons, and only $5_{76}(D_{2d})$ has 6 isolated pairs of adjacent pentagons.

It was conjectured in [10] that, for any even $n \geqslant 20$, $n \neq 22$, there exists a tight 5_n. Moreover, we could not find a tight graph 5_n with more than 15 zigzags.

The list of all symmetry groups of fullerenes 5_n is known (see [15]); they are (with their first appearance): $C_1(36_3)$, $C_2(32_1)$, $C_i(56_{314})$, $C_s(34_2)$, $C_3(40_{30})$, $D_2(28_1)$, $S_4(44_{82})$, $C_{2v}(30_2)$, $C_{2h}(48_{80})$, $D_3(32_6)$, $S_6(68_{6263})$, $C_{3v}(34_6)$, $C_{3h}(62_{2334})$, $D_{2h}(40_{33})$, $D_{2d}(36_6)$, $D_5(60_{1794})$, $D_6(72_{11144})$, $D_{3h}(26_1)$, $D_{3d}(32_3)$, $T(44_{73})$, $D_{5h}(30_1)$, $D_{5d}(40_1)$, $D_{6h}(36_{15})$, $D_{6d}(24_1)$, $T_d(28_2)$, $T_h(92_{126311})$, $I(140_x)$, $I_h(20_1)$.

There exist fullerenes admitting railroads with *triple* self-intersection; see, for example, Figure 19(a). More generally, we believe that any curve which represents a railroad in a graph of type 4_n also appears as a curve representing a railroad in some $5_{n'}$.

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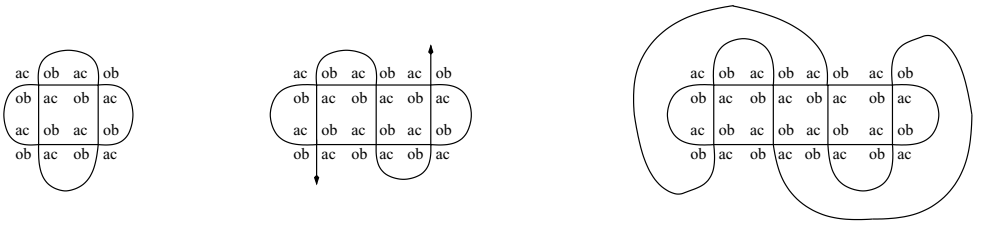


Figure 20.

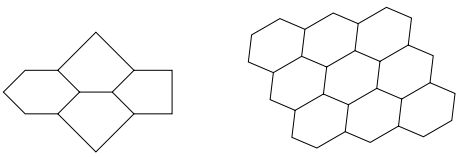


Figure 21.

Theorem 7.1. *For any even number $h \geqslant 2$, there exists a fullerene 5_n, with $n = 18h - 8$, having two simple zigzags intersecting in exactly h edges. It has symmetry T_d if $h = 2$ and D_{2h}, D_{2d} if $\frac{h}{2}$ is even, odd respectively.*

Proof. For any even $h \geqslant 2$ there exist a unique h-vertex 4-valent plane graph H whose faces are four 2-gons (in two pairs of adjacent ones) and $\frac{h}{2} - 2$ 4-gons only, and having two simple central circuits (see [9]). This graph has symmetry D_{4h} for $h = 2, 4$ and, for larger values, symmetry D_{2h}, D_{2d} if $\frac{h}{2}$ is even, odd respectively.

We will identify each of the two central circuits of H with simple zigzags, Z_1 and Z_2, and each vertex with an edge of intersection between them. Every face of H can be seen as a patch in the graph 5_n which we will construct, and so the local Euler formula (2.3) can be applied. Fix a face F of H; we can assign to every angle of F an angle (obtuse or acute), so that every 2-gon has one acute and one obtuse angle, while every 4-gon has two obtuse and two acute angles. See in Figure 20 the graph for the first values of h.

So, 2-gonal patches will contain three pentagons, while 4-gonal patches will contain only hexagons. We replace 2- and 4-gonal faces of H by patches depicted in Figure 21.

The obtained graph has $9(h-2)+4$ hexagonal faces, and so $n = 18h - 8$ vertices. The symmetry group is the same as that of H, except for the first values $h = 2, 4$. See Figure 19(b) for the corresponding graph with $h = 8$. □

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