Chapter 2
Zigzags of Fullerenes and *c*-Disk-Fullerenes

The *fullerenes*, i.e., the maps $(\{5, 6\}, 3)$-$\mathbb{S}^2$, are of particular interest in Carbon Chemistry. Denote by $F_v(G)$ any v-vertex fullerene of symmetry G. Denote by C_v and call *IP fullerene* any F_v with *isolated* (i.e., no two of them are adjacent) 5-gons. A number of C_v's with $60 \le v < 100$, including $C_{60}(I_h)$, $C_{70}(D_{5h})$, $C_{76}(D_2)$, and some with $v = 78, 82, 84$ have been characterized as all-carbon molecular cages.

When v is of moderate size, a useful notation taken up in IUPAC nomenclature, is to label $F_v(G)$ as $v : m$ or $v : m(G)$ where m is the place of the fullerene in the *spiral lexicographical order* of general, or IP fullerenes [FoMa95].

In fact, Goldberg introduced the notion of fullerenes (as putative best approximations of $\mathbb{S}^2$) already in [Gold34]; he mentioned there that Kirkman, in 1882, found over 80 out of the 89 44-vertex fullerenes. Goldberg defined a *medial polyhedron* as a simple v-vertex ($4 \le v \ne 18, 22$) polyhedron with only $\lfloor 6 - \frac{24}{v+4} \rfloor$- and $\lfloor 7 - \frac{24}{v+4} \rfloor$-gonal faces. Clearly, the first eight, i.e., ones with $v \le 20$, medial polyhedra are the 8 dual convex deltahedra (3 simple Platonic solids and all, but the 1-st one, on Fig. 1.12) and the medial polyhedra with $v \ge 20$ are exactly the fullerenes.

We first give statistical information on the zigzags of fullerenes. Then we consider the Kekulé structure, that one can obtain from zigzags, and the z-knotted fullerenes. Later we consider railroads structure, that one can define on fullerenes, and prove that a fullerene without railroads has at most 15 zigzags. Our emphasis then shifts to c-disk-fullerenes, i.e., $(\{5, 6, c\}, 3)$-spheres with $p_c = 1$ for which we consider existence, symmetries, and zigzags structure.

2.1 Zigzags Statistics for Small Fullerenes

Table 2.1 lists all z-vectors for the set of fullerenes with $v \le 38$ vertices. Table 2.2 lists z-vectors for the IP fullerenes with $v \le 82$ vertices and 4 of 24 C_{84} including the experimentally observed ones. So, $C_{78} : 1$ and $C_{84} : 23$ are all experimental fullerenes sharing their zigzag structure with a less stable IP *isomer*, i.e., C_v with the same v.

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Table 2.1 Zigzag structure of the fullerenes F_v with $v \leq 38$ vertices

v	z-vectors					
20	10^6					
24	$12; 60_{12,12}$					
26	$12^3; 42_{0,9}$					
28	$12; 32_{0,4}, 40_{0,8}$	12^7				
30	$10^2; 70_{15,10}$	$22_{0,1}, 68_{6,18}$	$12^3; 54_{2,13}$			
32	$14; 82_{10,24}$	$14^2; 34^2_{0,4}$	$14^3; 54_{0,12}$	$12, 14; 70_{10,14}$	$12^3; 30_{0,3}, 30_{3,0}$	$12; 84_{18,18}$
34	$102_{17,34}$	$12, 14^3; 48_{1,8}$	$12; 30_{0,3}, 60_{7,9}$	$14^2; 74_{5,20}$	$14^2; 74_{7,18}$	$30_{0,3}, 72_{12,12}$
36	$46_{0,7}, 62_{4,11}$	$16; 22^2_{0,1}, 48_{4,4}$	$12, 14; 36_{0,4}, 46_{1,7}$	$12, 14; 82_{19,11}$	$12, 16; 80_{20,8}$	$12; 30^2_{0,3}, 36_{0,4}$
	$14; 94_{12,28}$	$14^2; 30_{0,3}, 50_{0,9}$	$14^4; 26^2_{0,1}$	$46_{0,8}, 62_{4,12}$	$14^2; 30_{0,3}, 50_{0,9}$	$14^5; 38_{0,4}$
	$26^3_{0,1}, 30_{0,3}$	$14^4; 26^2_{0,1}$	$12^2, 14^6$			
38	$16; 98_{12,29}$	$16^3; 22^3_{0,1}$	$12; 102_{20,25}$	$16; 36_{0,4}, 62_{7,8}$	$114_{21,36}$	$114_{29,28}$
	$14, 16; 84_{11,18}$	$14; 26_{0,1}, 74_{5,17}$	$114_{27,30}$	$114_{19,38}$	$14; 38_{0,4}, 62_{2,13}$	$16; 48_{2,6}, 50_{1,8}$
	$14^2; 86_{9,22}$	$14^3; 26_{0,1}, 46_{0,8}$	$12^2, 14^2; 62_{1,14}$	$14^6; 30_{0,3}$	$14^4; 58_{1,12}$	

For any v, z-vectors are listed by fullerene, in spiral lexicographic order

Table 2.2 Zigzag structure of the IP fullerenes C_v with $v \leq 82$ and 4 (among 24) C_{84}: $84:19(D_{3d})$, $84:20(T_d)$, $84:23(D_{2d})$ and $84:24(D_{6h})$

v	z-vectors				
60	18^{10}				
70	$20^5; 110_{0,25}$				
72	$108_{0,24}, 108_{12,12}$				
74	$20^9; 42_{0,3}$				
76	$20; 56_{0,4}, 152_{8,40}$	$20^3; 42^4_{0,3}$			
78	$18^2; 198_{39,42}$	$38_{0,1}, 196_{22,58}$	$20^2; 64_{0,8}, 130_{4,31}$	$18^2; 198_{39,42}$	$42_{0,3}, 64^3_{0,8}$
80	$22^5; 130_{0,30}$	$22^2; 98^2_{0,16}$	$20, 22^2; 86_{2,13}, 90_{5,10}$	$20^3, 22^3; 114_{12,12}$	$42_{0,1}, 90_{5,10}, 108_{6,18}$
	$20^2; 90_{5,10}, 110_{15,10}$	20^{12}			
82	$20^2, 22^4; 118_{7,18}$	$20, 22^3; 160_{15,34}$	$22^2; 202_{23,58}$	$22^2; 202_{25,56}$	$42^2_{0,1}, 162_{17,32}$
	$20^2; 42^2_{0,1}, 122_{9,16}$	$42^3_{0,1}, 120_{12,12}$	$20^6; 42^3_{0,1}$	$20^4; 42^2_{0,1}, 82_{1,8}$	
84	$20^6, 22^6$	$42^6_{0,1}$	$42^6_{0,1}$	$20^6, 22^6$	

Table 2.3 z-uniform not z-knotted fullerenes F_v with $v \le 60$

Fullerene v:m	Group	Orbits	Zigzag	Int. vector
20:1	I_h	6	10	2^5
28:2	T_d	4, 3	12	2^6
40:40	T_d	4	$30_{0,3}$	8^3
44:73	T	3	$44_{0,4}$	18^2
44:83	D_2	2	$66_{5,10}$	36
48:84	C_2	2	$72_{7,9}$	40
48:188	D_3	3, 3, 3	16	2^8
52:237	C_3	3	$52_{2,4}$	20^2
52:437	T	3	$52_{0,8}$	18^2
56:293	C_2	2	$84_{7,13}$	44
56:349	C_2	2	$84_{5,13}$	48
56:393	C_3	3	$56_{3,5}$	20^2
60:1193	C_2	2	$90_{7,13}$	50
60:1197	D_2	2	$90_{13,8}$	48
60:1803	D_3	6, 3, 1	18	2^9
60:1812	I_h	10	18	2^9

Table 2.4 z-uniform not z-knotted IP fullerenes C_v with $v \le 100$

Fullerene v:m	Group	Orbits	Zigzag	Int. vector
60:1812	I_h	10	18	2^9
80:7	I_h	12	20	2^{10}
84:20	T_d	6	$42_{0,1}$	8^5
84:23	D_{2d}	4, 2	$42_{0,1}$	8^5
86:19	D_3	3	$86_{1,10}$	32^2
88:34	T	12	22	2^{11}
92:86	T	6	$46_{0,3}$	8^5
94:110	C_3	3	$94_{2,13}$	32^2
100:387	C_2	2	$150_{13,22}$	80
100:438	D_2	2	$150_{15,20}$	80
100:432	D_2	2	$150_{17,16}$	84
100:445	D_2	2	$150_{17,16}$	84

Table 2.3 lists z-uniform fullerenes F_v with $v \le 60$ vertices, and Table 2.4 lists the z-uniform IP fullerenes C_v with $v \le 100$ vertices. Note that in fullerenes $44 : 37(T), 52 : 437(T), 60 : 1812(I_h)$ each 6-gon is adjacent to exactly three 6-gons, while each 5-gon is adjacent to exactly 2, 1, 0 5-gons, respectively.

The smallest not z-balanced fullerene is a F_{52} (D_{2d}) with $\mathbf{z} = (16^4; 92_{12,12})$; not all of its zigzags of length 16 have the same intersection vector. The smallest *pure*

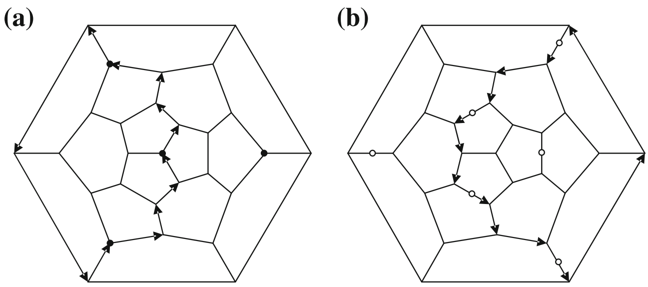


Fig. 2.1 The smallest fullerene, $F_{28}(T_d)$, that is z-uniform, $\mathbf{z} = 12^7$, but not z-transitive. The zigzag in (**a**) belongs to an orbit of size 4; the zigzag in (**b**) belongs to an orbit of size 3

not z-balanced fullerenes are $F_{108}(D_{2d})$ with $\mathbf{z} = (24^8, 26^4, 28)$ and $F_{144}(D_3)$ with $\mathbf{z} = (28^{12}, 32^3)$. Any z-uniform or tight pure fullerene F_v with $v \leq 200$ is z-balanced.

Icosahedral (i.e., of the symmetry I_h or I) fullerenes are called *Goldberg polyhedra*, since they are all available by the Goldberg–Coxeter construction (see [Gold37] and Chaps. 6 and 7) as GC_{kl} (Dodecahedron) with integers $0 \leq l \leq k$ specifying a net on the triangulation of the plane. Such fullerenes have $v = 20(k^2 + kl + l^2)$ vertices. The fullerene has I_h symmetry whenever $l = 0$ or $l = k$ and has I symmetry otherwise. The z-vectors of the icosahedral fullerenes C_v with $v < 2{,}000$ are listed in Table 2.5. All icosahedral fullerenes are IP and z-uniform, but they are z-transitive only for $gcd(k, l) = 1, 2$. It is sufficient to study only the case where k and l are coprime. In general, if the coprime parent (k, l) has $\mathbf{z} = s^t$, then the derived (ik, il) has $\mathbf{z} = is^{it}$ with $\lfloor \frac{i}{2} \rfloor$ orbits of size $2t$ and one orbit of size t, when i is odd. In fact [DuDe04], t is 6, 10 or 15; see Theorem 7.10. The icosahedral fullerenes may admit multiple solutions (k, l). There are fullerenes $C_{980}(I)$ with $(k, l) = (5, 3)$ (see Table 2.5) and $C_{980}(I_h)$ with $(k, l) = (7, 0)$ having $\mathbf{z} = 70^{42}$ and intersection vector 2^{35}.

2.2 Kekulé Graphs

A useful, though not infallible, indicator of stability of a π *framework* of molecule is that the corresponding plane graph should have a large number of perfect matchings, i.e., in chemical terms, *Kekulé structures*. Every fullerene has at least three [KlLi92] and typically very many more; $C_{60}(I_h)$ has 12,500 [KHCS85] and Borosphere (Fig. 1.13) has 286,224 of them. Call a *Kekulé graph* any 3-regular v-vertex plane graph admitting orientations of its zigzags, in which the number of edges of type I reaches the minimum $\frac{v}{2}$, according to the Proposition 1.2 (iii). A particularly simple perfect matching is formed by edges of type I of this graph.

Proposition 2.1 *Let G be a Kekulé graph with such orientation of its zigzags that the number e_I of edges of type I is $\frac{v}{2}$. If $p_i = 0$ for $i \geq 8$, then it holds*

Table 2.5 Icosahedral fullerenes C_v for $v \leq 2{,}000$. Only those cases defined by coprime pairs (k, l) are listed. N_z is the number of zigzags

v	k, l	N_z	Zigzag	Int. vector
20	1, 0	6	10	2^5
60	1, 1	10	18	2^9
140	2, 1	15	28	2^{14}
260	3, 1	10	$78_{0,3}$	8^9
380	3, 2	6	$190_{0,15}$	32^5
420	4, 1	6	$210_{5,10}$	36^5
620	5, 1	6	$310_{15,10}$	52^5
740	4, 3	6	$370_{0,25}$	64^5
780	5, 2	6	$390_{0,25}$	68^5
860	6, 1	10	$258_{0,9}$	$24^3, 28^6$
980	5, 3	10	$294_{0,9}$	$28^3, 32^6$
1140	7, 1	15	$228_{0,4}$	$14^8, 18^6$
1220	5, 4	15	$244_{0,4}$	$14^4, 18^{10}$
1340	7, 2	15	$268_{0,8}$	18^{14}
1460	8, 1	10	$438_{0,18}$	$42^3, 46^6$
1580	7, 3	10	$474_{0,18}$	$46^3, 50^6$
1820	6, 5	6	$910_{0,70}$	154^5
1820	9, 1	6	$910_{30,40}$	154^5
1860	7, 4	6	$930_{0,70}$	158^5
1920	8, 3	6	$970_{10,70}$	162^5

(i) *G has $f = \frac{v}{2} + 2$ faces, and two of them are* empty*, i.e., have no edges of type I, while others have exactly two such edges;*

(ii) *the two empty faces define uniquely the set of edges of type I over G; they are antipodal, in the sense that they span a diameter in the dual graph.*

Proof (i). Any 3-regular v-vertex plane graph has $2 + \frac{v}{2}$ faces by Euler's formula. By Proposition 1.2 (ii), and since $p_i = 0$ for $i \geq 8$, each face have either 0 or 2 edges of type I. By Proposition 1.2 (i), equality $e_I = \frac{v}{2}$ implies that the edges of type I form a perfect matching of G. So, the number of faces with two edges of type I is e_I.

(ii). Let $F_1, \ldots, F_p$. be the set of faces adjacent to one empty face F_0. Every pair F_i, F_{i+1} is incident to one edge, say e_i, that must be of type I since e_i is incident to one vertex of F_0. The face F_i is incident to edges e_i and e_{i-1} and so, all other edges of F_i are of type II. By induction, one is able to assign a type to every edge. □

2.3 z-knot Fullerenes

As a result of computations—all z-knotted simple polyhedra ($v \le 24$), all z-knotted fullerenes F_n ($v \le 74$) and all IP z-knotted fullerenes C_n ($v \le 120$)—we conjectured:

Conjecture 2.1 [DDF04] *For any z-knotted 3-regular plane graph, e_1 is odd.*

The condition of 3-regularity is necessary, as, for example, the dual of the odd-gonal $Prism_m$ has $e_1 = 2m$; see Table 1.1.

There are only two z-knotted F_v with $v \le 40$ vertices; they are shown in Fig. 2.2. Tables 2.6, 2.7 and 2.8 give the statistics of z-knotted ones among 3-regular polyhedra, general fullerenes, and IP fullerenes. Their proportion among fullerenes should be small, because [ScZJ04] implies: for any m, the proportion, among 3-regular v-vertex plane graphs of those having at most m zigzags goes to 0 with $v \to \infty$. In fact, z-knot fullerenes account for only 19 out of a total of 2,706 IP fullerenes with $v \le 100$, and of these 19 only 7 are Kekulé z-knotted ones (Table 2.8).

The unique zigzag of a z-knot fullerene must transform into itself (up to reversal of all arrows) under all symmetry operations belonging its group, G. Thus each sets of e_1 edges of type I and of e_2 edges of type II must comprise an integer number of orbits of G. Recall that, in a polyhedron, the site symmetry of an edge is C_{2v} or one of its subgroups C_2, C_s, or C_1. The orbits that may occur in the edge-sets are therefore limited to sizes $\frac{|G|}{4}$, $\frac{|G|}{2}$, or $|G|$.

The Conjecture 2.1 implies that the set of edges of type I must be spanned by an odd number of orbits of odd size. So, centrosymmetric groups are not possible for z-knot fullerenes with odd e_1. Application of the orbit-parity argument to the list of all 28 fullerene point groups reduces it to 11 candidates for z-knot fullerene groups: D_{5h}, D_5, D_{3h}, D_3, C_{3h}, C_{3v}, C_3, C_{2v}, C_2, C_s, C_1.

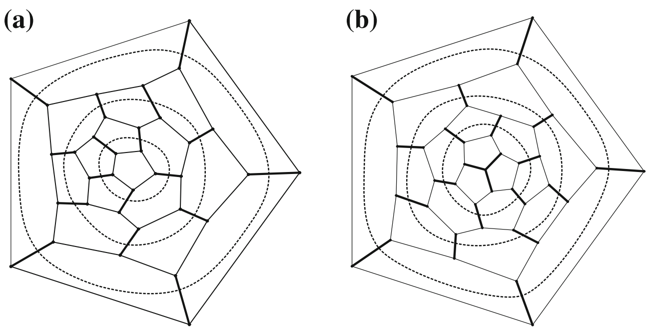


Fig. 2.2 **a** The smallest z-knot fullerene, 34:1 (C_2), with $\mathbf{z} = 102_{17,34}$. The $\frac{v}{2} = 17$ edges of self-intersection of type I are marked by *thick lines*. They span a perfect matching (Kekulé structure). *Dotted curves* indicate lines of latitude of the Föppl structure [Fö77] of the vertices. **b** The smallest *near-Kekulé* (i.e., $e_1 = \frac{v}{2} + 1$) z-knot fullerene 40:22 (C_1) with $\mathbf{z} = 120_{21,39}$

Table 2.6 Statistics of occurrence of knots in small 3-regular polyhedra

v	N_P	N_{knot}	$N_{\min}$	Symmetries
4	1	0	0	–
6	1	1	1	$D_{3h}(1)$
8	2	0	0	–
10	5	3	1	$C_{2v}(1)$,$C_{3v}(1)$,$D_{5h}(1)$
12	14	4	0	$C_1(2)$,$C_s(2)$
14	50	22	4	$C_1(8)$,$C_2(3)$,$C_{2v}(4)$,$C_s(6)$,$D_{7h}(1)$
16	233	70	0	$C_1(53)$,$C_s(15)$,$C_{3v}(2)$
18	1249	482	13	$C_1(398)$,$C_s(45)$,$C_2(27)$,$C_{2v}(10)$,$D_{3h}(1)$,$D_{9h}(1)$
20	7595	2955	0	$C_1(2816)$,$C_s(138)$,$C_3(1)$
22	49566	17901	168	$C_1(17306)$,$C_s(366)$,$C_2(196)$,$C_3(5)$,$C_{2v}(33)$,$D_{11h}(1)$
24	339722	114642	0	$C_1(113604)$,$C_s(1026)$,$C_{3v}(8)$,$C_3(4)$

At each number v of vertices, N_P is the number of non-isomorphic polyhedra, N_{knot} and $N_{\min}$ are the number of z-knotted and Kekulé z-knotted ones among them. The final column gives their breakdown by symmetry

Table 2.7 Statistics on z-knot fullerenes with $v \leq 74$ vertices

v	N_{full}	N_{knot}	$N_{\min}$	$N(C_1)$	$N(C_2)$	$N(C_3)$	$N(D_3)$
34	6	1	1	0	1	0	0
36	15	0	0	0	0	0	0
38	17	4	1	1	2	0	1
40	40	1	1	1	0	0	0
42	49	6	2	2	3	0	1
44	89	9	6	9	0	0	0
46	116	15	2	6	9	0	0
48	199	23	13	23	0	0	0
50	271	30	6	21	8	0	1
52	437	42	13	42	0	0	0
54	580	93	16	69	23	0	1
56	924	87	26	87	0	0	0
58	1205	186	11	155	30	1	0
60	1812	206	63	206	0	0	0
62	2385	341	20	297	41	2	1
64	3465	437	148	436	0	1	0
66	4478	567	64	507	59	0	1
68	6332	894	203	892	0	2	0
70	8149	1048	139	967	80	1	0
72	11190	1613	255	1612	0	1	0
74	14246	1970	200	1865	104	0	1

At each v, N_{full} is the number of such fullerenes; N_{knot}, $N_{\min}$, and $N(G)$ are the number of z-knotted, Kekulé z-knotted, and those with symmetry G among them. The group D_5 appears 1-st for z-knot fullerene F_{90}

Table 2.8 IP z-knot fullerenes C_v with $v \le 98$ vertices

v	Signature		Kekulé?
86	43, 86	C_2:2	Yes
90	47, 88	C_1:7	No
	53, 82	C_2:19	No
	71, 64	C_2:6	No
94	47, 94	C_1:60; C_2:26, C_2:126	Yes
	65, 76	C_2:121	No
	69, 72	C_2:7	No
96	49, 95	C_1:65	Near
	53, 91	C_1:7, C_1:37, C_1:63	No
98	49, 98	C_2:191, C_2:194, C_2:196	Yes
	63, 84	C_1:49	No
	75, 72	C_1:29	No
	77, 70	C_1:5; C_2:221	No

For each v and signature e_1, e_2, they are listed by symmetry and position in the spiral lexicographic order

All five pure rotation groups in above list (and only they) have been found as groups of some z-knot fullerene. So, in [DDF04] we conjectured that all z-knot fullerenes are chiral and that the set D_5, D_3, C_3, C_2, C_1 is the complete list of their point groups. The smallest D_5 z-knot fullerene is the unique $F_{90}(D_5)$ and smallest cases other 4 groups are given in Table 2.7. Trivial symmetry appears to dominate.

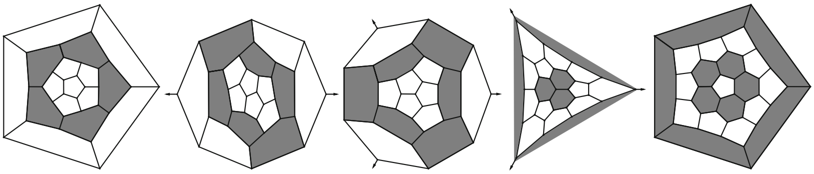
2.4 Railroads in Fullerenes

We conjectured in [DDF04] on the basis of calculations on fullerenes with $v \le 74$ (general) and $v \le 120$ (IP fullerenes) that there is at least one tight fullerene for each $v \ge 20$, $v \ne 22$. First and 7-th fullerenes on Fig. 2.3 are not tight.

The smallest fullerene with a belt is the 1-st on Fig. 2.3. See on Fig. 2.4 the smallest icosahedral fullerene with a belt. Figure 2.5a shows the smallest fullerene with a double self-intersection of a railroad, and Fig. 2.6a the smallest such IP fullerene (Figs. 2.7 and 2.8). A fullerene with a triple self-intersection of a railroad (conjectured to be such smallest) is shown in Fig. 2.9a.

Railroads without triple self-intersection can be seen as projections of alternating knots, and every fullerene with simple or doubly intersecting railroads has therefore an associated list of knots (Tables 2.9 and 2.10).

The *Conway graph* $(k \times m)^*$ (see, for example, [Kaw96]) is, for $k = 2$, $APrism_m$; for $k > 2$, it comes from $((k-1) \times m)^*$ by inscribing an m-gon in the 1-st of its two m-gons. The group of $(k \times m)^\star$ is D_{mh} for k even, and D_{md} for k odd, apart from



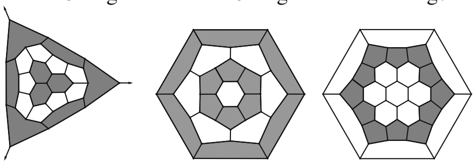
30, D_{5h} all 6-gons in 5-belt

32, D_2 all 6-gons in 6-ring

32, D_{3d} all 6-gons in 6-ring

32, D_{3h} all 6-gons in 2 rings

40, D_{5d} all 6-gons in 2 rings



38, C_{3v} all 6-, 5- in 4 rings

36, D_{6h} all 5-gons in 2 rings

48, D_{6d} all 5-gons in alt. ring

Fig. 2.3 Some fullerenes with 6- or 5-gons, organized in rings. First four and 6-th, 7-th are given as 1-st, 2-nd, 3-rd, 5-th and 16-th, 5-th for $v = 30, 32, 32, 32$ and $38, 36$, respectively, in Table 2.1

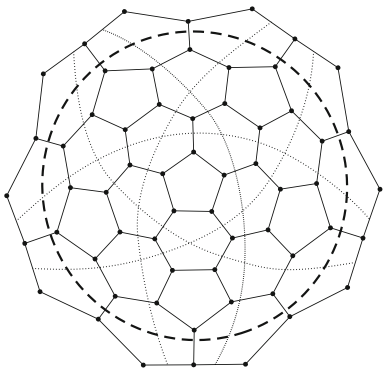


Fig. 2.4 $C_{80}(I_h)$, the smallest icosahedral fullerene with a belt, has $\mathbf{z} = 20^{12}$ and 6 belts

$(2 \times 3)^{\star}$ (i.e., Octahedron) and $(3 \times 4)^{\star}$ (i.e., Cuboctahedron) where it is O_h. In terms of links, $(2 \times 2)^{*} = 4_1$, $(2 \times 3)^{\star} = 6_2^3$, $(2 \times 4)^{*} = 8_{18}$.

In the open nanotubes and the *graphite sheet* $\{6; 3\}$, both zigzags and railroads can become doubly infinite rays (which can be seen as circuits including the point at infinity). The graphite sheet has three parallel classes of infinite railroads, each of them simple; accordingly, it has three parallel classes of infinite simple zigzags (Fig. 2.7) that form a single orbit. *Nanotubes* are formally constructed by rolling up the graphite sheet, with each tube identified by a two-parameter lattice vector, and their zigzag structure derives from that of graphite itself. The three types of nanotube, *zigzag*, *armchair* and *chiral* [DDE96] have parameter signatures $(n, 0)$, (n, n), (n, m) $(n \neq m)$. Zigzag structures of these three types are:

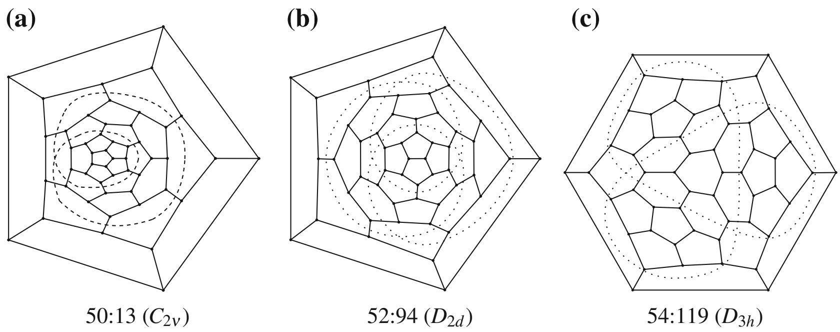


Fig. 2.5 Smallest fullerenes with self-intersecting railroads (indicated by *dashed lines*): **a** The smallest fullerene with a railroad that is a non-minimal projection of the trivial knot 0_1; **b** the smallest fullerene with a railroad that is a projection of a nontrivial knot (in this case the figure-of-eight knot 4_1); it is also the smallest not z-balanced fullerene; **c** the smallest fullerene with a railroad that is a projection of Trefoil knot 3_1

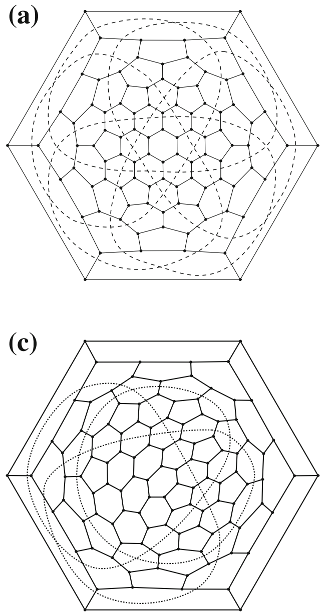


Fig. 2.6 IP fullerenes with self-intersecting railroads (indicated by *dashed lines*): **a** The smallest such fullerene, 96:187 (D_{6d}) $= GC_{2,0}(F_{24})$, has a railroad that is a projection of the knot $(4 \times 6)^*$. **b** 104:823 (D_{3h}) is the smallest fullerene with a railroad that is a projection of the knot 9_{40}. **c**, **d** 112:3341 has railroads corresponding to projections of two knots: the 4_1 (**c**) and the knot 8_{18} (**d**)

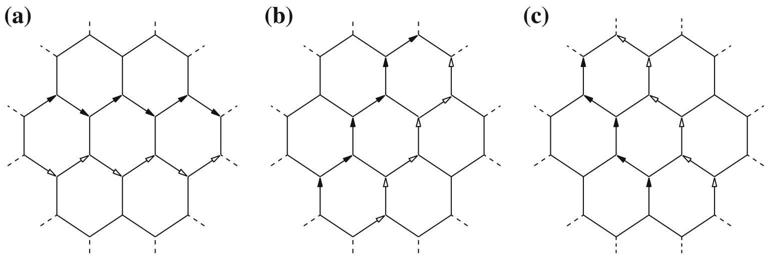


Fig. 2.7 The three parallel classes of zigzags in the graphite sheet {6; 3}

(a) for $(n, 0)$: two orbits of simple zigzags, one composed of concentric circuits of length $2n$ around the body of the tube, the other of two parallel classes of doubly infinite rays, related by reflection.
(b) for (n, n): two orbits of simple zigzags, both consisting of doubly infinite rays, one 'vertical' and one 'oblique'.
(c) for (n, m), $n \neq m$: 3 orbits of doubly infinite rays, each consisting of a parallel class of helically wound zigzags wrapping around the long axis of the tube.

In all 3 cases, the stack within each parallel class of zigzags corresponds to a stack of doubly infinite railroads.

2.5 Fullerenes 5_v with Simple Zigzags

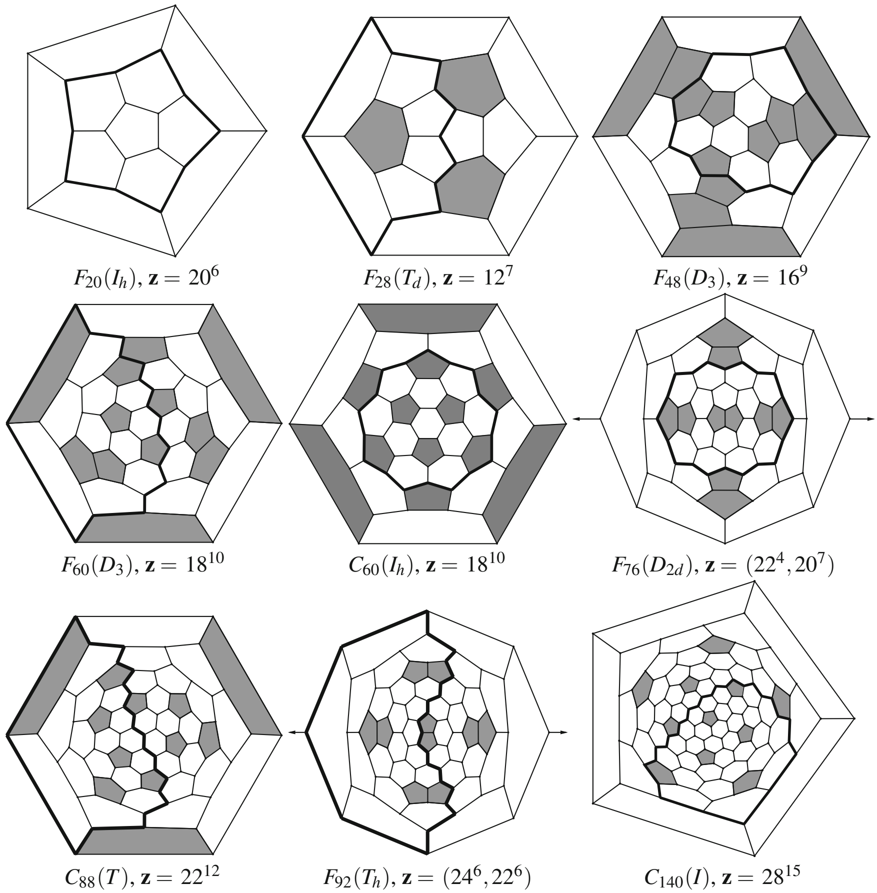
Figure 2.8 gives all tight pure 5_v, $v \leq 200$; we conjecture that this list is complete. (Among them only $5_{60}(I_h)$, $5_{88}(T)$, $5_{140}(I)$ are IP and only $5_{76}(D_{2d})$ has 6 isolated pairs of adjacent pentagons.) The largest one, $5_{140}(I)$, has $\mathbf{z} = 28^{15}$; by Theorem 2.5, any tight pure 5_v has at most 15 zigzags. We expect that any tight 5_v has at most 15 zigzags. Also, we conjecture that a tight 5_v exists for any even $v \geq 20$, $v \neq 22$.

The central circuits of seven z-uniform pure fullerenes from Fig. 2.8 produce seven new *Grünbaum arrangements* of Jordan curves, defined in Sect. 1.3.

Theorem 2.1 *For any even number $h \geq 2$, there exists a fullerene 5_v, with $v = 18h - 8$, having two simple zigzags intersecting in exactly h edges. For $h = 2$, it is $5_{28}(T_d)$; for $h \geq 4$, it has symmetry D_{2h}, D_{2d} if $\frac{h}{2}$ is even, odd respectively.*

Proof For any even $h \geq 2$, there exists a unique h-vertex 4-regular plane graph H, whose faces are four 2-goons (in two pairs of adjacent ones) and $\frac{h}{2} - 2$ 4-gons only, and having two simple central circuits (see [DeSt03]). 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 identify the two central circuits of H with 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 5_v, which we will construct, and so, the local Euler formula (Theorem 3.1) can be



v	Group	z-vector	Orbit 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	$22^6, 24^6$	6,6	2^{11} and $2^{10}, 4$
140	I	28^{15}	15	2^{14}

Fig. 2.8 All pure tight fullerenes 5_v with $v \leq 200$; no others are expected for larger v

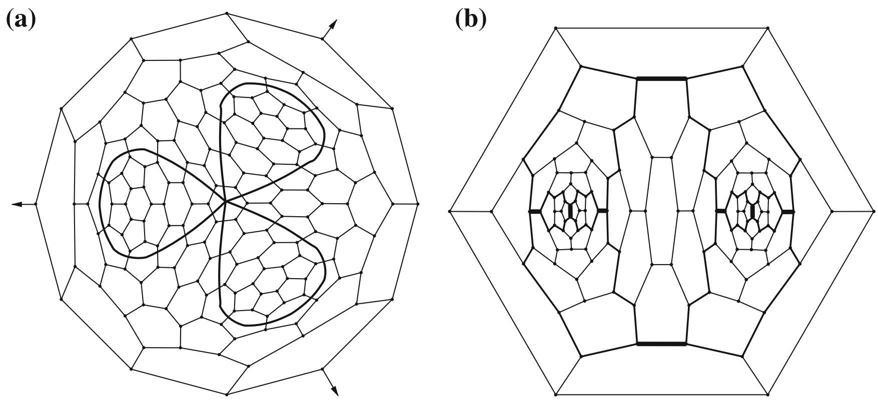


Fig. 2.9 Two particular fullerenes. **a** $5_{172}(C_{3v})$ with triple self-intersecting railroad (Trifolium). **b** Two simple zigzags Z, Z' in $5_{136}(D_{2h})$ with $|Z \cap Z'| = 8$ (8 underlined edges)

Table 2.9 Fullerenes F_n ($n \leq 60$) with self-intersecting railroads are listed below by position in the spiral lexicographic order, with the sizes of the orbits of zigzags and their r- (i.e., railroad) knots

Fullerene	Group	Orbits	z-vector	r-knots
50:13	C_{2v}	2,1,1	20; $\mathbf{24}^2_{0,1}$, $82_{14,5}$	0_1
52:94	D_{2d}	2,2	$38^2_{0,3}$, $\mathbf{40}^2_{0,4}$	4_1
54:13	C_2	2,2,1,1	20^3; $\mathbf{24}^2_{0,1}$, $54_{2,5}$	0_1
54:119	D_{3h}	3,2,1	16^3; $\mathbf{36}^2_{3,0}$, $42_{0,3}$	3_1
60:27	C_s	1,1,1,1	14; $\mathbf{26}^2_{0,1}$, $114_{18,14}$	0_1
60:34	C_s	1,1,1	$\mathbf{26}^2_{0,1}$, $128_{19,23}$z	0_1
60:207	C_s	1,1,1	$\mathbf{28}^2_{0,1}$, $124_{17,21}$	0_1
60:208	C_{2v}	2,1,1	$\mathbf{28}^2_{0,1}$, $60_{0,8}$, $64_{8,2}$	0_1
60:1379	C_{2v}	2,2	$\mathbf{28}^2_{0,1}$, $62^2_{2,6}$	0_1

A bold entry in a z-vector shows the origin of a significant knotted railroad. Knots are named in the Rolfsen notation [Rol76, Kaw96] and illustrated in Fig. 1.4

applied. Fix a face F of H; one 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 below the graph for the 1-st values of h.

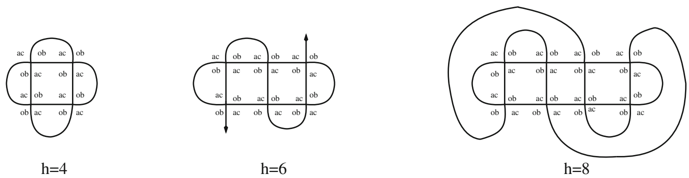
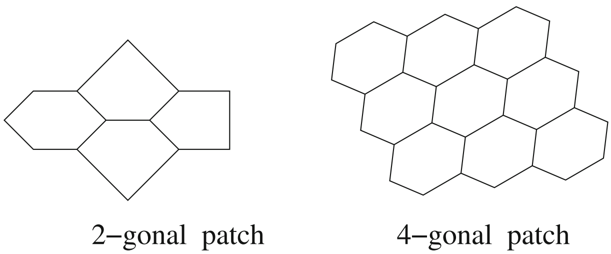


Table 2.10 IP fullerenes C_v ($v \leq 114$) having self-intersecting railroads

Fullerene	Group	Orbits	z-vector	r-knots
96:187	D_{6d}	2,2	$24^2;\mathbf{120}^2_{12,12}$	(0_1); $(4 \times 6)^*$
104:823	D_{3h}	3,3,2	$24^6;\mathbf{84}^2_{0,9}$	$(0_1)^3$; $9_{40} \equiv (3 \times 3)^*$
106:624	C_{3v}	3,1,1	$50^3_{0,1},\mathbf{84}^2_{0,9}$	$9_{40} \equiv (3 \times 3)^*$
108:897	D_{3h}	6,2	$26^6;\mathbf{84}^2_{0,9}$	$9_{40} \equiv (3 \times 3)^*$
112:3341	D_2	2,2,2	$24^2;\mathbf{64}^2_{0,4},80^2_{0,8}$	4_1, $8_{18} \equiv (2 \times 4)^*$
114:9	C_{2v}	2,2,1	$\mathbf{40}^2_{0,1},86^2_{2,6},90_{3,6}$	0_1
114:1738	C_1	1,1,1,1,1	$50_{0,1},\mathbf{64}^2_{0,4},82_{0,8},82_{1,7}$	4_1
114:2338	C_{2v}	1,1,1,1	$42_{0,1},\mathbf{80}^2_{0,8},140_{14,12}$	$8_{18} \equiv (2 \times 4)^*$
114:3419	C_2	1,1,1	$\mathbf{64}^2_{0,4},214_{13,46}$	4_1

Where the Rolfsen notation is not available, the Conway graph notation [Kaw96] is used

So, 2-gonal patches will contain three pentagons, while 4-gonal patches will contain only 6-gons. We replace 2- and 4-gonal faces of H by patches depicted below.



The obtained graph has $p_6 = 9(h-2)+4$, and so, $v = 18h - 8$ vertices. The symmetry group is the same as the one of H, except for the 1-st values $h = 2, 4$. See Fig. 2.9b for the corresponding graph with $h = 8$. □

2.6 Tight Fullerenes

Theorem 2.2 *The number of zigzags of a tight fullerene is at most* 15.

Proof For a zigzag z, we have two sides and the condition that it is tight implies that on each side there is at least one pentagon.

For $1 \leq i \leq 4$, denote by n_i the number of sides incident to exactly i pentagons. Denote by n_5 the number of sides incident to at least 5 pentagons. We denote by n_{sec}, n_{sec2}, and n_{sec3} the number of sides in the configurations depicted on Fig. 2.10 with n_{sec2} and n_{sec3} excluding n_{sec}.

If we have a lonely side, i.e., a side that contains only a single 5-gon, then we have the configuration of Fig. 2.11. The dashed side will eventually close itself, but

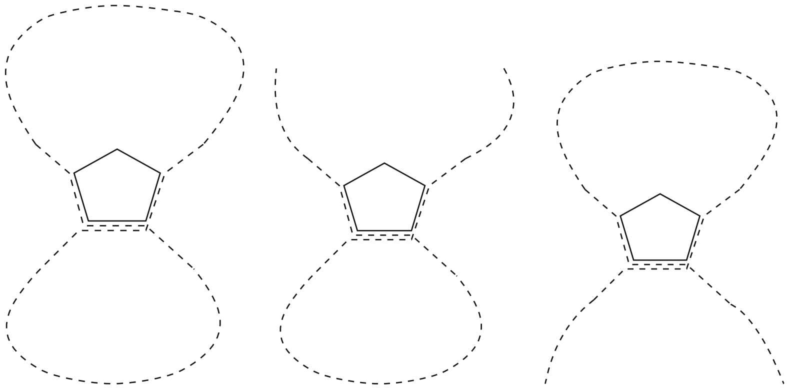


Fig. 2.10 Possible local configurations corresponding to a lonely side

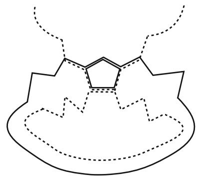


Fig. 2.11 Possible local configurations corresponding to a fourth configuration

it may or may not have another pentagon. Therefore, we are either in configuration n_{sec} or n_{sec2} and this gives the following equation:

$$n_1 = n_{sec} + n_{sec2}.$$

We denote by n_{4sec}, n_{4sec2} the number of sides that contain the configurations of Fig. 2.12. Let us take a configuration n_{sec} or n_{sec3} and add the opposing side passing by the 5-gon, according to Fig. 2.13. When doing this we get a sequence of 6-gon coming from the 5-gon. This sequence has to end on a 5-gon. Therefore, we get a configuration n_{4sec} or n_{4sec2}. This gives the equality:

$$n_{sec} + n_{sec3} = \frac{1}{2} n_{4sec} + n_{4sec2}.$$

The following other inequalities are easy to prove:

$$\begin{cases} n_1 \le 12 \\ n_{4sec} + n_{4sec2} + n_{sec2} + n_{sec3} \le n_3 + n_4 + n_5 \\ n_1 + 2n_2 + 3n_3 + 4n_4 + 5n_5 \le 60 \\ n_{sec} \le n_2 \\ n_{4sec2} \le n_5 \\ n_{4sec} \le n_4 \end{cases}$$

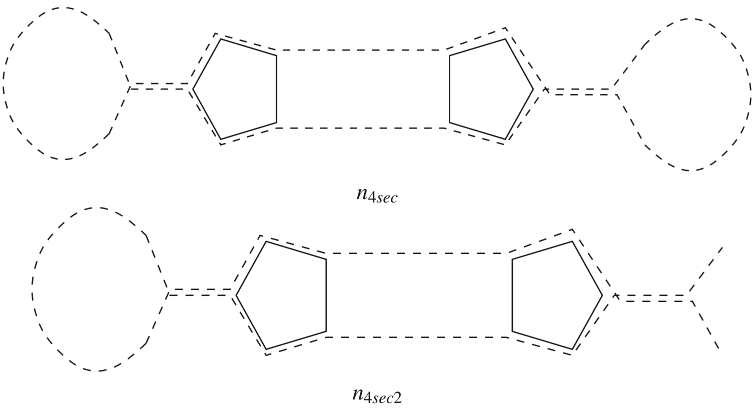


Fig. 2.12 A lonely side in overlined drawing and the corresponding side

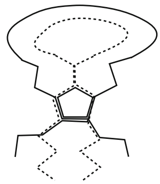


Fig. 2.13 A second configuration and the corresponding side

The objective function giving the number of zigzags is $\frac{1}{2}(n_1 + n_2 + n_3 + n_4 + n_5)$ and the maximum found value of the linear programming problem is 15 as obtained from [Fu]. □

2.7 Disk-Fullerenes

This section is based partly on [DDS13a, DDS13b].

Given a ({5, 6, c},3)-sphere with $c \neq 5, 6$ and $p_c = 1$, call it a *c-disk-fullerene* (or $c - DF$) if the c-gon has no self-intersections (i.e., it can be seen as the boundary of a disk) and call it a *c-multidisk-fullerene* (or $c - MDF$), otherwise. Denote such spheres $c - DF_v(G)$ or $c - MDF_v(G)$ if they have v vertices and the group G of symmetry. So, the fullerenes can be seen as $c - DF$'s with $c = 5, 6$. The unique c-gon is a negatively curved face if and only if $c \geq 7$.

In general, a $c - DF$ and a c-disk, obtained from it by deleting the c-gon, are different geometrical objects; but they have the same skeleton. Since we consider only their combinatorial properties, we will, by abuse of language, treat them as the same object. We will use the term *disk* but present a picture for sphere. Also, a "group" means here the group of a sphere, not only of its skeleton. Call a $c - DF$ with $c \neq 5, 6$ *tight* if it has no *belts*, i.e., simple railroads.

Call a *c-disk-nearfullerene* (or $c - DNF$) a c-disk, in which vertices have degree 3, interior faces are 5- or 6-gons, boundary faces have gonality within $\{2, 3, 4, 5, 6\}$, and at least one boundary face is neither 5, nor 6-gon. Any $c - MDF$ has (only) 1-connected graph—a tree of following possible components, connected by *bridges* (edges between components, i.e., edges of self-intersection of the c-gon):

1. vertex having (i.e., from which emanate) 3 bridges;
2. empty disk having 5 or 6 bridges;
3. disk-fullerene, having bridges on some (at least one) of its boundary 5-gons;
4. disk-nearfullerene, having $5 - t$ or $6 - t$ bridges on boundary t-gons, $2 \leq t \leq 5$.

One can slightly generalize $c - DNF$, in order to incorporate cases 2. and 3. in it. Also, a theory of c-multidisk-fullerenes with infinite c will be of interest.

Call a $c - MDF$ *extensible* if among faces, adjacent to the boundary c-gon, there is a 5-gon; call it *nonextensible*, otherwise, i.e., if all boundary faces are 6-gons.

Let D be a component $c' - DF$ or $c' - DNF$ of a $c - MDF$. One can check that $c' > 6 - t$ if there is a t-gon among the boundary faces of D; so, $c' \geq 2$. Hence, a $c - MDF$ exists if and only if $c \geq 8$, since $c \geq (2 + 1) + 2 + (2 + 1) = 8$. See a minimal $8 - MDF_v$ on Fig. 2.14. Four pictures there are "dumbbells" of two $2 - DF_{38}$, of $2 - DF_{38}$ and $3 - DF_{34}$, of two F_{20} and of two $6 - DNF_{22}$. This $6 - DNF_{22}$ comes from F_{24} by deleting edge connecting a 5-gon with the 6-gon nonadjacent to it.

It is easy to check that $(\{a, b, c\}, k)$-sphere with $p_c = 1$ and $p_b = 0$ has $c = a$, i.e., it is the k-regular map $\{a, k\}$ on the sphere. We conjecture that a $(\{a, b, c\}, k)$-sphere with $p_c = p_b = 1 < a, c$ has $c = b$, i.e., it is a $(\{a, b\}, k)$-sphere with $p_b = 2$.

Theorem 2.3 *The possible symmetry groups of a c-disk-fullerene with* $c \neq 5, 6$ *or a c-multidisk-fullerene are* C_k, $C_{k\nu}$ *with* $k \in \{1, 2, 3, 5, 6\}$ *and k dividing c.*

Proof Any symmetry of such sphere should stabilize unique c-gon. So, the possible groups are only C_k and $C_{k\nu}$ with k $(1 \leq k \leq c)$ dividing c. Moreover, $k \in \{1, 2, 3, 5, 6\}$, since the axis has to pass by a vertex, edge, or face. Remind that $C_s = C_{1\nu}$. □

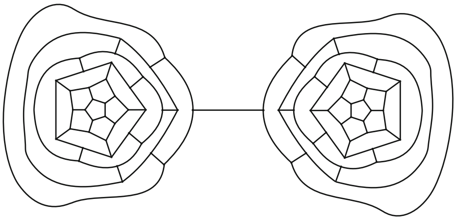
Let $m(c, G)$ denote the smallest value of p_6 in a $c - DF(G)$ if $c = 1, 2$ and, in a 3-connected $c - DF(G)$, if $c \geq 3$; Table 2.11 gives $m(c, G)$ for small c and, in parenthesis, such values for $c - MDF(G)$, when they exist, i.e., for $c \geq 8$.

Proposition 2.2 [DDS13b]

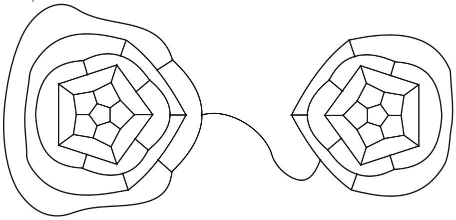
(i) The skeleton of any $c - DF$ *is* 2*-connected if and only if* $c > 1$.
(ii) The skeleton of any $c - DF$ *is* 3*-connected if and only if* $3 \leq c \leq 7$.

Clearly, for $c = 1, 2$, the skeleton S of a $c - DF$ is only c-connected. For $c \geq 3$, it can be only 2- but not 3-connected, when the intersection of the c-gonal boundary with a face is not connected. Then the group of $c - DF$ can be a proper subgroup of $Aut(S)$. Also, the plane realization can be not unique; see, for example, Fig. 2.15.

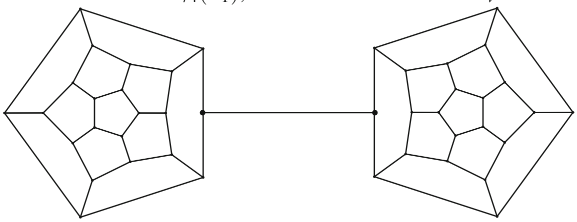
Such 2-connected skeleton admits a convex realization in $\mathbb{R}^2$, but in $\mathbb{R}^3$ it can be realized only as a convex polyhedral surface with nonplanar boundary.



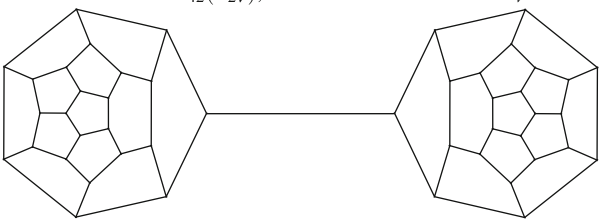
a $8-MDF_{78}(C_{2v})$; it is the minimal $8-MDF_v$ and a $c-MDF_v$ with smallest c



a $9-MDF_{74}(C_1)$; it is the minimal $9-MDF_v$



a $14-MDF_{42}(C_{2v})$; it is the minimal $14-MDF_v$



a $16-MDF_{46}(C_{2v})$; it is the minimal $16-MDF_v$

Fig. 2.14 Some *minimal*, i.e., with minimal v, c-multidisk-fullerenes $c-MDF_v$

Clearly, any $c-DF$ or $c-MDF$ has $p_5 = c+6$, $v = 2(p_6+c+5)$ vertices and there is an infinity of $c-DF$'s for any $c \geq 1$ and of $c-MDF$'s for any $c \geq 8$.

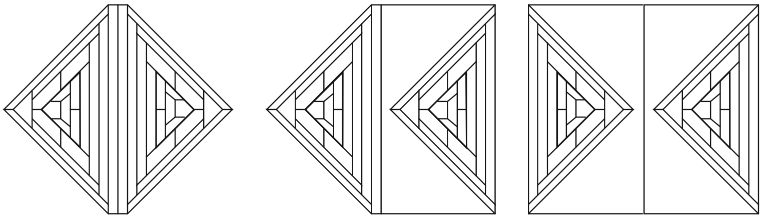
A $(\{5,6\};3)$-*polycycle* (cf. [DeDu08]) is the following relaxation of a $c-DF$: some—say, v_2'—of the vertices of the c-gon have degree 2. Clearly, $p_5 = c+6-2v_2'$.

Let $m(c)$, $m_3(c)$, and $m_2(c)$ denote the smallest value of p_6 in a any $c-DF$, in a $c-DF$ whose skeleton is 3-connected and, respectively, 2- but not 3-connected.

Theorem 2.4 *(i) There are eight $c-DF$ with $p_6 \leq 3$ (all are 3-connected): unique ones $5-DF_{20}$, $6-DF_{24}$, $6-DF_{26}$, $4-DF_{22}$, $3-DF_{22}$, $7-DF_{30}$, and two $6-DF_{28}$; their p_6 is* 0, 1, 2, 2, 3, 3, 3, 3*, respectively.*

Table 2.11 Minimal values of p_6 in a $c - DF(G)$ with small c not dividing 5 and 6; in parenthesis, minimum values of p_6 for $c - MDF(G)$, when they exist (i.e., if $c \geq 8$), are given

G	C_1	C_s	C_2	C_{2v}	C_3	C_{3v}
$m(1, G)$	18	14	–	–	–	–
$m(2, G)$	10	9	8	6	–	–
$m(3, G)$	7	5	–	–	9	3
$m(4, G)$	5	3	4	2	–	–
$m(7, G)$	5	3	–	–	–	–
$m(8, G)$	6(?)	5(?)	6(?)	4(26)	–	–
$m(9, G)$	7(23)	6(?)	–	–	12(?)	6(?)
$m(11, G)$	8(10)	8(9)	–	–	–	–
$m(13, G)$	5(5)	5 (4)	–	–	–	–
$m(14, G)$	5(4)	4(3)	5(6)	4(2)	–	–
$m(16, G)$	5(3)	4(3)	4(4)	6(2)	–	–
$m(17, G)$	5(4)	5(3)	–	–	–	–
$m(19, G)$	6(6)	6(5)	–	–	–	–



$8 - DF_{74}(C_{2v})$ $9 - DF_{74}(C_{2v})$ $10 - DF_{74}(C_{2v})$

Fig. 2.15 Three disk-fullerenes with isomorphic skeletons; also each of them is tight and contains two simple disjoint zigzags of length 10 nonintersecting the boundary

(ii) If $c \leq 11$, then all $c - DF$ realizing $m(c)$, $m_2(c)$, and $m_3(c)$ are 23, 6, *and* 19 *$c - DF$'s given for $c \leq 11$ in the Table* 2.12, *where the number of $c - DF$'s is given in parentheses if it is not* 1*; see also Figs.* 2.16 *and* 2.17.
(iii) If $c \geq 12$, then:
(iii1) $m_2(c) = 4$ and $m(c) = m_2(c)$ for $c \equiv 4, 5, 6 \ (mod\ 10)$;
(iii2) $m_2(c) = 5$ for $c \equiv 2, 3, 7, 8 \ (mod\ 10)$;
(iii3) $m_2(c) = 6$ and $m(c) = m_3(c)$ for $c \equiv 0, 1, 9 \ (mod\ 10)$;
(iii3) $4 \leq m_3(c) \leq 6$; we conjecture that $m_3(c) = 6$ and is realized only by the c-pentatube *(it is checked it for $12 \leq c \leq 21$).*

For $c \geq 12$, the *c-pentatube* is the 3-connected $c - DF_{2(c+11)}$—of symmetry C_2, C_s for even and odd c, respectively—depicted in the end of Fig. 2.16 for $c = 12, 13$. For any c, it consists of the same left and right subgraphs separated by $c - 12$ pentagons. A c-pentatube with c not divisible by 5 has z-vector 10^4; $6c + 26_{3c-3,0}$.

Table 2.12 Minimal values of p_6 in a c-disk-fullerene

c	1	2	3	4	5	6	7	8	9	10	11
$m(c)$	14	6	3	2	0	1	3	4	6 (2)	7 (3)	8 (10)
$m_2(c)$	–	6	–	–	–	–	–	23	17 (2)	10	8 (2)
$m_3(c)$	–	–	3	2	0	1	3	4	6 (2)	7 (3)	8 (8)
c	12	13	14	15	16	17	18	19	20	21	$c \geq 22$
$m(c)$	5	5	4	4	4	5	5	6	6	6	$\min(m_2, m_3)$
$m_2(c)$	5	5	4	4	4	5	5	6	6	6	Theorem 2.4
$m_3(c)$	6	6	6	6	6	6	6	6	6	6	$4 \leq m_3(c) \leq 6$

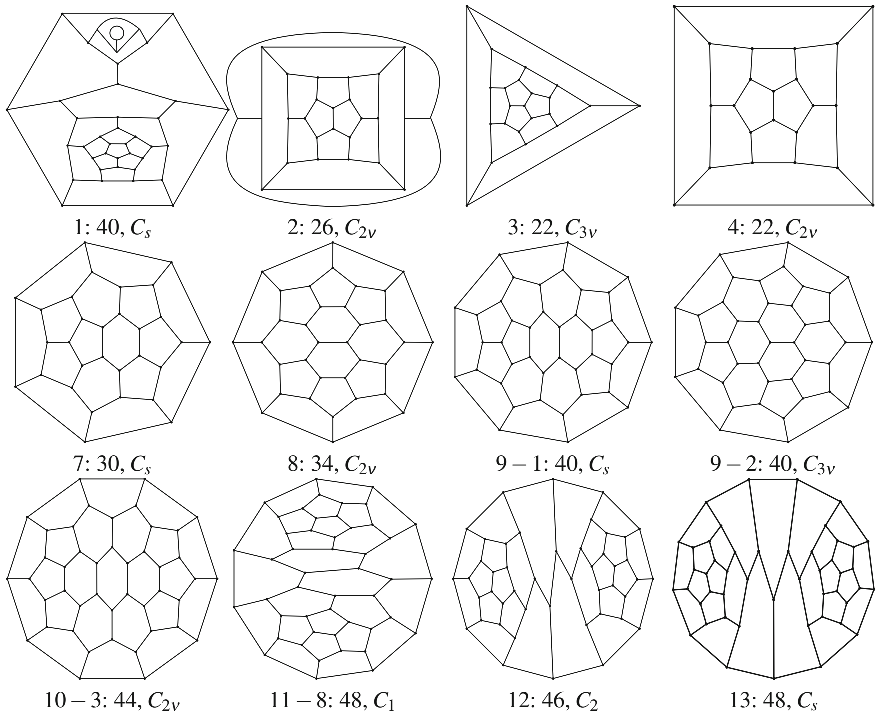


Fig. 2.16 Minimal $c - DF$ with $c = 1, 2$ and minimal 3-connected $c - DF$ with $3 \leq c \leq 13$, $c \neq 5, 6$; for $c = 10$ and 11 only one of 3 and, respectively, one of 8 is given

Conjecture 2.2 *A $c - DF_v$ exists—except the cases $(c, v) = (1, 42)$, $(3, 24)$, $(5, 22)$—if and only if v is even and $v \geq 2(m(c) + c + 5)$.*

Call *c-thimble* any 2-nd condition is necessary: see Fig. 2.21. It exists if and only if $c \geq 5$ and its skeleton is always 3-connected. One can consider also *c-multi-thimble*,

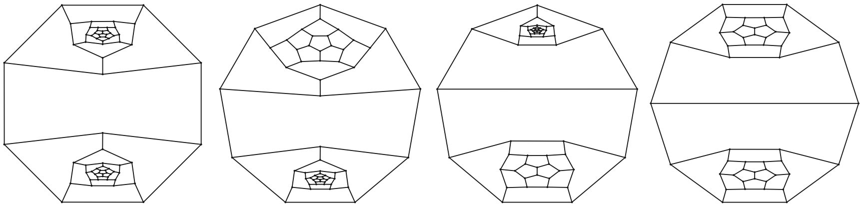


Fig. 2.17 Minimal only 2-connected $c - DF$ with $3 \le c \le 10$

i.e., $c - MDF$ such that the c-gon is adjacent only to 5-gons and only once to each of them; one example is $16 - MDF_{46}(C_{2v})$ from Fig. 2.14.

For $c \ge 5$, let $m_t(c)$ denote the smallest value of p_6 in a c-thimble.

Proposition 2.3 [DDS13a] *and* [DDS13b] *It holds* $c - 6 \le m_t(c) \le \left\lfloor \frac{3(c-5)}{2} \right\rfloor$.

We expect that $m_t(c) = \left\lfloor \frac{3(c-5)}{2} \right\rfloor$. It holds for $5 \le c \le 10$: all minimal $c - DF$ with $5 \le c \le 9$, as well as the 3-rd minimal $10 - DF_{44}$ (see Fig. 2.16), are c-thimbles.

A *fullerene c-patch* is a partial subgraph of fullerene bounded by a c-gon; so, it has $p_5 \le 12$. Such ({5, 6}; 3)-polycycle is a $c - DF$ if and only if $c \in \{5, 6\}$. Let us cut a fullerene with a belt along the middle line of such railroad. Then each 6-gon splits into two 5-gons, and the fullerene splits into two thimbles. These thimbles are not necessarily identical, and not fullerene patches.

Remark 2.1 In any $c - DF$ it holds the following:

- (i) If two zigzags intersect, then each connected component of their intersection consists of a single edge. In each of them the intersection is transverse, that is, the segments of the zigzags near their common edge are on different sides.
- (ii) Each of c pairs of adjacent edges on the boundary generates a zigzag. These are the only zigzags which intersect the boundary; their number is at most c, while exactly 7 zigzags of length 20 in a $7 - DF_{72}$ on Fig. 2.18a intersect the boundary.
- (iii) If an edge does not belong to the boundary, but both ends of the edge belong to it, then any zigzag containing this edge is self-intersecting. If a simple zigzag intersects the boundary, then any two boundary edges in it alternate with at least two non-boundary edges.
- (iv) A shortest simple zigzag is the one bounding the half of Dodecahedron; it consists of 10 edges. So, if all zigzags are simple, then there are at most $\frac{e}{5} = \frac{3v}{10}$ of them, since each edge belongs to at most two zigzags.
- (v) Adjacent edges of a face in a $c - DF$ cannot belong to its boundary, since the graph is 3-regular. So, a 6-gon has at most three (and a 5-gon has at most two) edges on the boundary. Each 6-gon in a $c - DF$ belongs to at most three railroads.

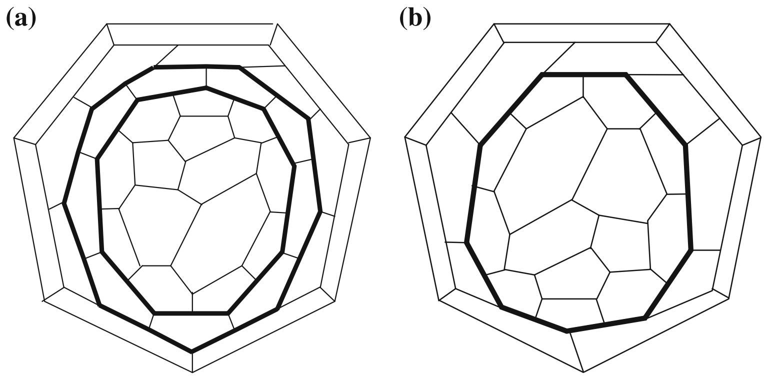


Fig. 2.18 Reduction of a $7 - DF_{72}$ (unique pure $c - DF$ with $p_6 \leq 25$ and $c \leq 15$, $c \neq 5, 6$) to a tight $7 - DF_{54}$; all its zigzags, except two of the length 18 intersect pairwise in two edges. **a** A reducible pure $7 - DF_{72}(C_1)\mathbf{z} = 20^9, 18^2$. **b** One of its reductions, $7 - DF_{54}(C_1)\mathbf{z} = 18$; $144_{24,39}$

(vi) The number of faces adjacent to a simple zigzag on any side is equal to half its length. There is one exception: when counting the number of faces adjacent to a zigzag on the exterior side, the boundary edges of the zigzag are not considered.

Proposition 2.4 *The intersection of a face in a c-disk-fullerene with a simple zigzag is connected.*

Proof A face in a disk-fullerene cannot have just one common edge with a zigzag. A nonempty intersection of a 5-gon with a simple zigzag contains exactly two adjacent edges. Let us prove by contradiction that two opposite pairs of adjacent edges of a 6-gon cannot belong to a simple zigzag. We first prove this for a fullerene. If two opposite pairs of adjacent edges of a 6-gon belong to a simple zigzag, then the face adjacent to the 6-gon along an edge, which does not belong to the zigzag, has a disconnected intersection with the zigzag. So, this face is another 6-gon. There is a third 6-gon which is adjacent to the second and has a disconnected intersection with the zigzag, and so on. All possible ways of termination of this process (in any direction) give an m-gon with $m \neq 5, 6$, i.e., are not possible for a fullerene.

In the case of a disk-fullerene the proof is similar, but the following modification is needed. Consider the 1-st 6-gon which intersects the zigzag in two opposite pairs of adjacent edges. If this 6-gon is on the interior side of the zigzag, then the proof is the same. If the 1-st 6-gon is on the exterior side, then we choose a 2-nd 6-gon on the same side as the part of the zigzag which is interior with respect to the cycle consisting of the other part of the zigzag and an edge of the 1-st 6-gon not belonging to the zigzag. This 2-nd 6-gon is adjacent to a 3-rd 6-gon which also has a disconnected intersection with the zigzag, and so on. As in the case of a fullerene, this process (in only one direction) cannot terminate at a 6-gon. □

Lemma 2.1 *All the boundary 5-gons of a thimble form a cylinder, one of whose edges is the boundary of the thimble and the other is a simple zigzag.*

Proof Consider the cyclic sequence of 5-gons adjacent to the boundary of a thimble. The 5-gons in it are all different. Indeed, each 5-gon has a single edge on the boundary. Neighboring 5-gons in the sequence have a common edge with an endpoint on the boundary of the thimble. We will prove that non-neighboring 5-gons do not intersect. Assume that they do intersect, and consider the following two cases:

Case 1. Two non-neighboring 5-gons have a common vertex A which is opposite to the boundary edge of each 5-gon. The two 5-gons have a common edge AB, since the graph is 3-regular. The star of the vertex B contains a third face, which has a common edge BC with one 5-gon and a common edge BD with the other 5-gon. The vertices C and D belong to the boundary of the thimble. Since there are only 5-gons adjacent to the boundary, the third face in the star of B is a 5-gon, which has a disconnected intersection with the boundary. This is a contradiction.

Case 2. Two neighboring 5-gons have a common edge AB, where the vertex A is opposite to the boundary edge of one 5-gon, and the vertex B is opposite to the boundary edge of the other 5-gon. The star of B contains a 3-rd face, which has a common edge with the 1-st 5-gon of the sequence. One of the ends of this edge belongs to the boundary of the thimble. Hence, the 3-rd face in the star of B is a 5-gon. The 3-rd and the 2-nd 5-gons have a common edge, say BC. The star of C consists of the 2-nd 5-gon, the 3-rd 5-gon, and some 4-th 5-gon. The 4-th and 3-rd 5-gons have a common edge CD, and so on. The sequence $ABCD \ldots$ can be continued indefinitely. (Indeed, two sequences of 5-gons, one indexed by even numbers and the other by odd numbers, cannot close up into a cylinder with two boundary components, but they also cannot close up into a Möbius band with only one boundary component.) Again, we end up with a contradiction. □

In a thimble, pairs of edges of boundary 5-gons with a common vertex, which is opposite to a boundary edge of a 5-gon, form a simple zigzag, because all faces adjacent to the boundary of a thimble are different 5-gons. If all the boundary faces of an $c - DF$ are 5-gons, but the $c - DF$ is not a thimble (see one in Fig. 2.21a), then these pairs of edges form a self-intersecting zigzag. But if all the boundary faces of an $c - DF$ are 5-gons forming a cylinder whose second boundary component is a simple zigzag, then this $c - DF$ is a thimble.

Proposition 2.5 *A disk D cut out from a c-disk-fullerene by a simple zigzag Z contains exactly six pentagons.*

Proof The degrees of the vertices of Z in D alternate between 3 and 2. We attach a 5-gon to each pair of boundary edges of D with a common vertex of degree 3; the number of the attached 5-gons equals half the length of the zigzag. By identifying edges of the 5-gons with vertices of degree 2 in D we obtain a thimble. Besides the boundary 5-gons, this thimble contains exactly six 5-gons belonging to D. □

Lemma 2.2 *If a disk-fullerene has a simple zigzag, such that all the adjacent faces on one of its sides are* 6*-gons, then these* 6*-gons form a belt.*

Proof A 6-gon adjacent to a zigzag contains a pair of zigzag edges with a common vertex (see Proposition 2.4). The number of such 6-gons is half the number of edges in the zigzag; see Remark 2.1 (vi). Take two neighboring 6-gons in the cyclic sequence. They have a common edge. One end of this edge belongs to the zigzag. Denote the other end by A and assume that A belongs to a 3-rd 6-gon which is adjacent to the zigzag along the two edges with common vertex opposite to A. This 3-rd 6-gon is adjacent to the first two 6-gons. Let AB be the common edge of the 3-rd and 2-nd 6-gons. The vertex B belongs to some 4-th face, because the graph is 3-regular. Since one of the ends of the common edge of the 4-th and 3-rd faces belongs to the zigzag, the 4-th face is a 6-gon adjacent to the zigzag. Let BC be the common edge of the 4-th and 2-nd 6-gons. The vertex C belongs to some 5-th face, which is a 6-gon adjacent to the zigzag (by the same reason as for the 4-th face). Let CD be the common edge of the 5-th and 4-th 6-gons. Then the vertex D belongs to a 6-th 6-gon, which is adjacent to the zigzag, and so on.

If we now swap the 2-nd and the 3-rd hexagons, then we obtain two sequences of 6-gons, one indexed by even numbers and the other by odd numbers, that are adjacent along the middle polygonal line $ABCD\dots$, which is infinite. Indeed, it cannot close up, for suppose that it does close up. It has either an even or an odd number of edges. However, both cases are impossible. In the first case two sequences of 6-gons cannot close up into a cylinder, which has two boundary components. In the second case the two sequences cannot close up into a (forbidden, see above) Möbius band, even though it has one boundary component. We got a contradiction.

So, adjacent 6-gons on one side of the zigzag cannot intersect unless they are neighboring in the cyclic sequence. It follows that these 6-gons form a belt. □

Lemma 2.1 can be viewed as a particular case of Lemma 2.2: one can cut the belt along its middle line and get a thimble.

Proposition 2.6 *If a fullerene has two disjoint simple zigzags, then*

(i) the fullerene has at least one belt
(ii) and both zigzags have the same length.

Proof (i) Two simple zigzags Z_1 and Z_2 cut the fullerene into two disks and an *annulus* (a region bounded by two concentric zigzags). Each disk contains six 5-gons, so the annulus contains only 6-gons. By Lemma 2.2, there exists a belt.

(ii) Since there are only 6-gons between Z_1 and Z_2, we can apply Lemma 2.2. If the first boundary component of the belt is Z_1 and the second boundary component is not Z_2, then there is another belt. If the second boundary component of the second belt is not Z_2, then there is a third belt, and so on. After a finite number of steps we get a belt whose second boundary component is Z_2. Then all the boundary components of all these belts have the same length. □

By Proposition 2.5, a simple zigzag intersects the boundary of a thimble in $s \leq 3$ connected components (pairs of edges); the disk cut by this zigzag has $2s$ boundary 5-gons. See Fig. 2.1 for $s = 0, 1$ and Fig. 2.19b for $s = 0, 2, 3$. On Fig. 2.19a, three longest zigzags, i.e., those of length 72 and 66, have $s = 0$, while each of remaining 15 zigzags has $s = 2$.

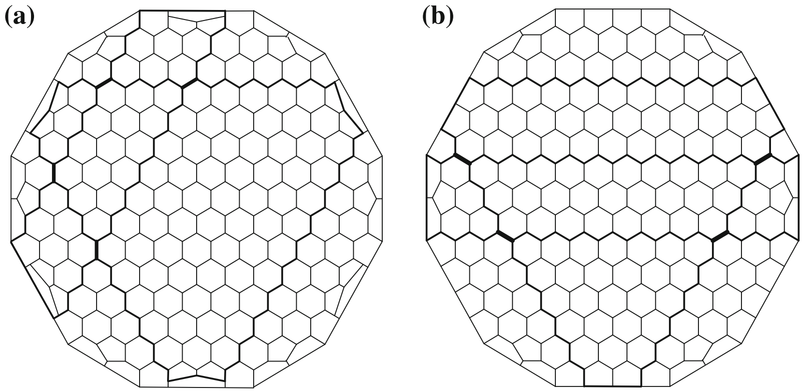


Fig. 2.19 Two special disk-fullerenes. **a** a tight pure $30-DF_{36}(C_{6\nu})$ with $\mathbf{z} = 72, 66^2, 58^6, 56^3, 48^6$. **b** a tight 36-thimble ($C_{6\nu}$) with two simple zigzags having 2 or 3 boundary components

Proposition 2.7 *If two simple zigzags in a c-thimble do not intersect the boundary and do not intersect each other, then:*

(i) the thimble has at least one belt
(ii) and the two zigzags have the same length.

Proof (i) By Proposition 2.5, each simple zigzag cuts a disk containing six 5-gons off the thimble. They are all not adjacent to the boundary, because the zigzag does not intersect the boundary. If the disks cut off from the thimble by the two zigzags do not intersect, then the thimble contains 12 rather than 6 non-boundary 5-gons, which is impossible since $p_5 = c + 6$. So, one disk is contained in the other, and all six 5-gons are contained in the smaller disk. Since there are only 6-gons between the zigzags, the existence of a belt follows from Lemma 2.2.

(ii) If the second boundary component of the belt does not coincide with the second zigzag, then there are only 6-gons adjacent to the belt from the other side. These 6-gons form another belt, and so on. After a finite number of steps, we end up at a belt whose boundary component is the second given zigzag. Both boundary components of each belt have the same length. □

Any disk-fullerene can be turned into a tight disk-fullerene by a finite number of the following *reductions steps*. If a $c-DF$ has a belt, call *z-reduction* of this $c-DF$ the operation of deleting the interior of such railroad with subsequent identification of its boundary zigzags. This step is not uniquely defined.

If the belt does not intersect the boundary of the $c-DF$, then after deleting the interior of such a belt with inner boundary Z_1 and outer boundary Z_2 we obtain a disk with boundary Z_1 and an annulus with inner boundary Z_2. They can be united into a new $c-DF$ in z different ways, where z is the number of edges of the simple zigzag Z obtained after identifying the zigzags Z_1 and Z_2.

If Z_2 intersects the boundary of the $c - DF$, then we attach an c-gon to this boundary, obtaining a sphere. By removing from it the interior of the belt, we obtain two disks with boundaries Z_1 and Z_2. We identify them in one of z ways and remove the attached c-gon. As a result, we obtain a new $c-DF$. The number of simple zigzags can increase under z-reduction (the number of simple central circuits *decreases* under cc-reduction; see Sect. 4.1. But p_6 always decreases. So, any disk-fullerene can be reduced to a tight one in a finite number of steps.

See z-reduction of a pure $7-DF$ on Fig. 2.18. See also first and seventh fullerenes on Fig. 2.3: a 5-thimble $F_{30}(D_{5h})$ (with $\mathbf{z} = 10^2, 70_{15,10}$ and a belt of five 6-gons) reduces to 5-thimble $F_{20}(I_h)$ with $\mathbf{z} = 10^6$ and pure 6-thimble $F_{36}(D_{6h})$ (with $\mathbf{z} = 12^2, 14^6$ and 6-belt) reduces to 6-thimble $F_{24}(D_{6d})$ with $\mathbf{z} = 12; 60_{12,12}$.

A disk-fullerene with a simple zigzag Z can be extended by cutting it into two parts along Z and inserting a belt joining them. The *extending* operation is the reverse of the reduction operation and is also not uniquely defined. A disk-fullerene without simple zigzags cannot be extended or reduced. Any tight thimble can be extended along its unique simple zigzag not intersecting the boundary.

Lemma 2.3 *A c-thimble is tight if and only if at least one of its non-boundary* 5*-gons is adjacent to a boundary* 5*-gon.*

Proof A c-thimble has c boundary 5-gons. Since we have a non-boundary 5-gon adjacent to a boundary 5-gon, there is a set of at least $c + 1$ pentagons whose union is connected. If the thimble had a belt, all these pentagons would be on the same side of the belt. Then on the other side of the belt there would be at most five pentagons, which contradicts Proposition 2.5. If none of the non-boundary 5-gons is adjacent to a boundary 5-gon, then the thimble has a belt by Lemma 2.2. □

The next Proposition follows from Proposition 2.6.

Proposition 2.8 *(i) Any two simple zigzags of a tight fullerene intersect.*
(ii) A non-tight disk-fullerene has at least two simple zigzags of the same length.

Lemma 2.4 *If a fullerene or thimble is not tight, then all its belts with pairwise nonintersecting interiors form a cylinder. Both boundary components of this cylinder are adjacent to* 5*-gons.*

Proof In a fullerene, there are two disks on the different sides of the belt, each containing six 5-gons (see Proposition 2.5). Any other belt, which has no common interior point with the 1-st belt, is inside one of these disks. If two belts have no common boundary points, then there is a cylinder (an annulus) between them consisting only of 6-gons. By Lemma 2.2, this cylinder contains a sequence of belts in which two neighbors are adjacent along a zigzag. The belts in this sequence fill another cylinder. If there are only 6-gons adjacent to this cylinder from outside, then they form a belt by Lemma 2.2. We join this belt to the cylinder. After a finite number of steps, we obtain a cylinder with only 5-gons adjacent to its boundary from outside.

In the case of a c-thimble, all c boundary 5-gons are on the same side of any belt in the thimble, because they form an connected annulus homeomorphic to the lateral surface of a round cylinder. We prove by contradiction that the remaining six 5-gons are all on the other side of the belt. Assume that there are fewer than six 5-gons there. Consider the middle edge cycle splitting the belt into two cylinders. It cuts out a disk from the thimble and this disk is a new thimble. The number of 5-gons in this new thimble must be equal to the number of boundary 5-gons plus six. However, by assumption there are fewer than six old 5-gons inside the new thimble. This is a contradiction. Therefore, there are exactly six 5-gons on the other side of the belt. All of them are non-boundary faces of the thimble.

The same six 5-gons are on the disk side of another belt, because only these 5-gons are not adjacent to the boundary. Indeed, if the two disks did not intersect, then the thimble would contain 12 non-boundary 5-gons, which is excluded by $p_5 = c+6$. So, one disk is inside the other, and all six 5-gons are in the smaller disk. The complement of the smaller disk in the larger one is a cylinder.

There are only 6-gons between the belts in the cylinder. The cylinder has a sequence of belts in which any two neighbors are adjacent along a zigzag. These belts fill the cylinder. (The cylinder can consist of only two original belts if they are adjacent.) There are 6 non-boundary 5-gons on one side of the cylinder, and c boundary 5-gons on the other side. If there are only 6-gons adjacent to the boundary of the cylinder from the outside, then they form a belt by Lemma 2.2. We attach this belt to the cylinder. After a finite number of steps, we obtain a cylinder with only 5-gons adjacent to its boundary components from the outside. There is at least one non-boundary 5-gon adjacent to a boundary component, and all c boundary 5-gons are adjacent to the other boundary component. So, all belts constructed above form a cylinder with only 5-gons adjacent to its boundary from the outside. □

We note that all the belts in a thimble are pairwise nonintersecting and belong to a single cylinder. Each 6-gon in a thimble belongs to at most one belt. If there is a belt containing a given 6-gon, then when trying in one of the two other possible ways to construct a belt containing this 6-gon and corresponding to each of the two other pairs of edges opposite to it, we come to one of the c boundary 5-gons of the thimble. Any other $c - DF$ can contain several cylinders.

Lemma 2.1 and Remark 2.1 (ii) imply that the number of simple zigzags in a tight c-thimble is within $[1, c + 1]$:

Proposition 2.9 *(i) Any c-thimble has at least one simple zigzag nonintersecting its boundary.*

(ii) A tight c-thimble has exactly one such zigzag, and so, the number of its simple zigzags is at most $c + 1$.

Above boundary is best possible: a tight pure 5-thimble $F_{20}(I_h)$ and tight pure 6-thimble $F_{28}(T_d)$ have $\mathbf{z} = 10^6$ and $\mathbf{z} = 12^7$, respectively. A pure 6-thimble $F_{36}(D_{6h})$, given as 7-th on Fig. 2.3, have $\mathbf{z} = 12^2, 14^6$ but it is not tight.

But a tight disk-fullerene, which is not a tumble, can have several simple disjoint zigzags nonintersecting the boundary; see example on Fig. 2.15.

Lemma 2.5 *In a tight fullerene or tight c-thimble, each simple zigzag has at least one adjacent* 5*-gon on each side.*

Proof If a simple zigzag in a thimble intersects the boundary, then it has at least two adjacent 5-gons on each side. Therefore, we may assume that the zigzag does not intersect the boundary.

We prove the statement by contradiction. If there are no adjacent 5-gons on some side of a simple zigzag, then all faces adjacent to it are 6-gons. By Lemma 2.2 they would form a belt, implying that the fullerene or thimble is non-tight. □

Each of five pairs of adjacent edges in a 5-gon belongs to a zigzag, possibly self-intersecting. The number of zigzags adjacent to 5-gons in a fullerene is at most $5p_5 = 60$. By Lemma 2.5, there are at least two 5-gons adjacent to each simple zigzag of a tight fullerene. So, such a fullerene has at most 30 simple zigzags. But this bound is not the best possible.

Each of c pairs of adjacent edges on the boundary of a thimble generates a zigzag, possibly self-intersecting. This zigzag intersects the boundary and so has at least two adjacent 5-gons on each side. A tight thimble has no belts; hence, it has only one simple zigzag nonintersecting the boundary.

Lemma 2.6 *Assume that a fullerene has a simple zigzag with only one adjacent* 5*-gon on one of its sides. Then this fullerene also has a self-intersecting zigzag.*

Proof Assume that there is only one adjacent 5-gon on one of the sides of a simple zigzag Z. All the other adjacent faces are 6-gons, which form an open chain. By Proposition 2.4, each 6-gon in this chain has only two edges in Z (equivalently, all the 6-gons in the chain are different).

Let us prove that non-neighboring 6-gons in the chain do not intersect (in boundary points). Two neighboring 6-gons in the chain have a common edge. Only one end of this edge belongs to Z (see above). If the other end of the edge (denote it by A) belongs to a third 6-gon, which is adjacent to Z along two edges with a common vertex opposite to A. Then these three 6-gons split Z into two parts.

We can assume without loss of generality that the 2-nd 6-gon is adjacent to that part of the zigzag which is adjacent only to the 6-gons from the open chain. The 3-rd 6-gon is adjacent to each of the 1-st two. Let the edge AB be the intersection of the 3-rd and 2-nd 6-gons. Since all vertices are of degree 3, the vertex B belongs to a 4-th face. But one end of the common edge of the 3-rd and 4-th faces belongs to Z. Hence, the 4-th face is a 6-gon adjacent to Z. Let the edge BC be the intersection of the 4-th and 2-nd 6-gons. Then the vertex C belongs to a 5-th face which is a 6-gon adjacent to Z (as in the case of the 4-th face). Let the edge CD be the intersection of the 5-th and 4-th 6-gons. Then, as above, the vertex D belongs to a sixth 6-gon which is adjacent to the zigzag, and so on. If we swap the 2-nd and 3-rd 6-gons, then we obtain two chains of 6-gons, one indexed by even numbers and the other by odd numbers. These two chains are adjacent along the polygonal line $ABCD\ldots$, which must be infinite. This is a contradiction.

Therefore, any two 6-gons in the open chain do not have common boundary points unless they are neighboring in the chain.

In the 6-gons of the open chain, pairs of adjacent edges that are opposite to pairs of adjacent edges belonging to Z form a polygonal line Λ which is a proper part of a zigzag containing an edge passed through twice that is in the original 5-gon and is opposite to the 5-gon's vertex at which the two of its edges belonging to Z are adjacent. (The open polygonal line Λ together with this edge forms a closed polygonal contour which is not a zigzag but is part of the zigzag.) □

The following alternative is a trivial corollary of Lemma 2.6.

Corollary 2.1 *If a fullerene has only simple zigzags, then among the faces adjacent to any zigzag from one side there are either at least two* 5*-gons, or only* 6*-gons.*

So, Lemma 2.6 justifies Proposition 8 (iii) from [DDF04]. Note that Theorem 2.2 prove, by another way, a more general result than (ii) in Theorem 2.5.

Theorem 2.5 *If all zigzags in a fullerene are simple and pairwise intersecting, then:*

(i) there are at least two 5*-gons adjacent to any zigzag on each side;*
(ii) the number of all zigzags is at most 15 *(this bound is the best possible).*

Proof (i) Clearly, there are no belts. By Corollary 2.1, there are two 5-gons adjacent to any zigzag on each side.
(ii) Each 5-gon is adjacent to at most five zigzags. So, the number of zigzags is at most $5p_5 = 60$. By (i), there are at least four 5-gons adjacent to any simple zigzag. Therefore, the fullerene has at most $\frac{5p_5}{4} = 15$ zigzags. □

All the pairwise nonintersecting belts in a fullerene form a cylinder which has only 5-gons adjacent to its boundary components from the outside. It gives:

Corollary 2.2 *In a fullerene, the number of cylinders formed by pairwise nonintersecting belts is at most* 15*. (Recall that in a thimble, the number of cylinders formed by all its belts is at most* 1*.)*

Theorem 2.6 *If a $c-DF$ is tight and all the zigzags not intersecting its boundary are simple, then:*

(i) there are at least two 5*-gons adjacent to each side of any such zigzag;*
(ii) the number of such zigzags is at most $\frac{5(c+6)}{4}$.

The proof is similar to the proof of Theorem 2.5. As regards a non-tight $c-DF$, if only two 5-gons are adjacent to such a zigzag and all the zigzags are simple, then both 5-gons are on the same side of the zigzag.

Remark 2.2 (i) If all the zigzags in an $c-DF$ are simple, then their number is at most $c+\frac{5p_5}{4} = c+\frac{5(c+6)}{4}$. This follows from Theorem 2.6 (ii) and Remark 2.1 (ii).

(ii) For any $c = 4k+12$, $v = 20k+54$, where $k \in \mathbb{N}$, there is a tight $c-DF_v$ with $2k+1$ simple and 4 self-intersecting zigzags. For $k = 5$, it is shown in Fig. 2.20.

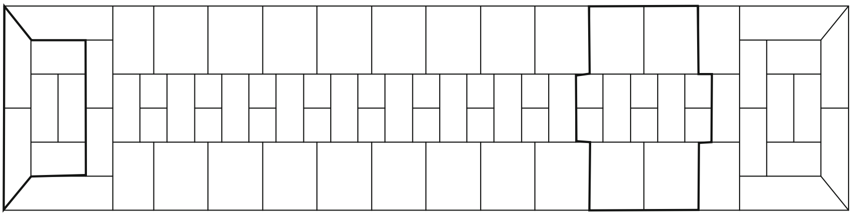


Fig. 2.20 The case $k = 5$ of a tight $c - DF_v(C_{2v})$ with $c = 4k + 12$, $v = 20k + 54$ and many simple zigzags (both types of them are shown): $\mathbf{z} = 10^2, 16^{2k-1}; 36^2_{0,3}, (14k + 30)_{k+1,0}, (14k + 56)_{k+4,4}$

The number of simple zigzags grows with k. So, this number in a tight disk-fullerene can be arbitrarily large. It would be interesting to know for which c there exist tight $c - DF$'s with an arbitrarily large number of simple zigzags.

Examples of other, besides disk-fullerenes, interesting $(\{5, 6, c\}, 3)$-maps follow.

- Haeckel, 1887: $(\{5, 6, c\}, 3)$-spheres with $c = 7, 8$ representing skeletons of radiolarian zooplankton *Aulonia hexagona*.
- *G-fulleroids*, i.e., $(\{5, c\}, 3)$-spheres with $c > 6$ and symmetry G.
- *Azulenoids*, i.e., $(\{5, 6, 7\}, 3)$-$\mathbb{T}^2$; such tori have $p_5 = p_7$.
- *Schwartzits*, i.e., $(\{5, 6, c\}, 3)$-maps on minimal surfaces of constant negative curvature (of genus $g \geq 2$) with $c = 7, 8$.

Also, *plane fullerenes* (or *nanocones*) are $(\{5, 6\}, 3)$-$\mathbb{E}^2$. Such planes have $0 \leq p_5 \leq 6$. Their number is 1 if $p_5 = 0, 1$ and infinity if $2 \leq p_5 \leq 6$; they are just *nanotubes* (see Sect. 2.4) if $p_5 = 6$. The number of their equivalence (isomorphism up to a finite induced subgraph) classes is [KlBa06] 2, 2, 2, 1 for $p_5 = 2, 3, 4, 5$.

[DDD10, DD12] considered *space fullerenes*, i.e., tilings of $\mathbb{E}^3$ by fullerenes, while [DeSt99] treated *fullerene manifolds*, i.e., $(d-1)$-dimensional d-valent compact connected manifolds whose 2-faces are 5- and 6-gons; they exist for $2 \leq d \leq 5$ (Fig. 2.21).

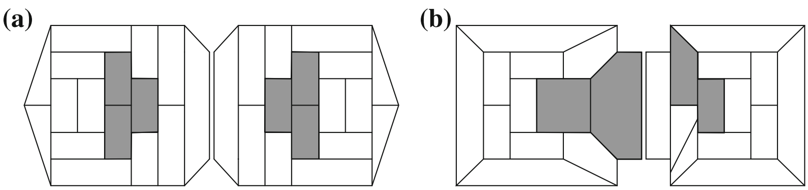


Fig. 2.21 Two only 2-connected $c - DF$ split in two parts with the same p_6 and the number of simple zigzags of length 10 in each; all those zigzags are adjacent to the boundary in two edges. **a** $20 - DF_{62}(C_{2v})$: not a 20-thimble, but all its 18 boundary faces are 5-gons; $\mathbf{z} = 10^2; 30^2{}_{0,3}, 40_{2,0}, 66_{4,5}$. **b** $15 - DF_{48}(C_1)$ split in two parts with $p_6 = 2$ and 2 simple zigzags of length 10 each; $\mathbf{z} = 10^4; 40_{0,4}, 64_{4,8}$

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