The smallest fullerene without a spiral

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Abstract

In this note we give the result of a computer search for the smallest fullerene that does not allow a face spiral code as used by Manolopoulos and Fowler and adopted in IUPAC recommendations for fullerene nomenclature. The search enumerated all the small fullerenes on up to 400 vertices and the conclusion is that the smallest fullerene without a face spiral has 380 vertices.

Keywords: fullerene, spiral, IUPAC

The first algorithm to construct lists of fullerenes was the *spiral algorithm* of Manolopoulos and Fowler [1][2]. It constructs fullerenes by enumerating encodings of *face spirals*. A clockwise (resp. counterclockwise) face spiral of a fullerene with k faces is a sequence of distinct faces $(f_1, f_2, \ldots, f_k)$ with the property that f_1 and f_2 share an edge and that for $3 \leq i \leq k$ face f_i has a connected intersection with $\{f_1 \cup f_2 \cup \ldots \cup f_{i-1}\}$ and shares an edge e with f_{i-1} that is the last of those edges of f_{i-1} in clockwise (resp. counterclockwise) orientation around f_{i-1} that belong to no face in $\{f_1, f_2, \ldots, f_{i-2}\}$. For fullerenes such face spirals can be encoded as sequences of 5s and 6s giving the face sizes, or more compactly as a sequence of length 12 giving the position of the 12 pentagons in the spiral.

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Already in [3] Manolopoulos and Fowler gave an example of a fullerene with 380 vertices that does not allow any face spirals and therefore would be missed by the algorithm. The question was whether this is the smallest counterexample. In [4] it is shown that in the more general class of all cubic polyhedra, the smallest counterexample has only 18 vertices, so one might have expected a smaller counterexample also in the class of fullerenes. For efficiency reasons, when applying the spiral algorithm for the generation of fullerenes, Manolopoulos and Fowler restricted the generation to spirals starting with a pentagon (see [2]). It is known that the smallest fullerene that is missed in this way is one isomer of C_{100}. Table 1 and Table 2 give the numbers of fullerenes up to 400 vertices that do not allow spirals starting at a pentagon. The structures can be downloaded from `http://hog.grinvin.org/Fullerenes`.

After a much more efficient and also complete algorithm for fullerene enumeration was developed [5], there were no longer algorithmic reasons to ask for the smallest fullerenes without spirals, but as an IUPAC proposal recommended the use of face spirals as a basis for fullerene nomenclature [6], it is still important to know the smallest fullerenes to which such a nomenclature could not be applied.

In [7] a new and faster algorithm using a recursive structure for the class of fullerenes [8] was developed that could generate and test all fullerenes up to 400 vertices. The result is that the fullerene with 380 vertices depicted in Figure 1 is the smallest fullerene without a spiral. This fullerene was already given in [3] but at that time minimality could not be proven. For computational results independent checks are very important to minimize the chance of errors, and so we independently confirmed this minimality result with the program from [5]. In the range from 382 to 400 vertices, fullerenes were generated and tested by the first program alone. In this range, the fullerene with 384 vertices depicted in Figure 2, is the only fullerene without a spiral. Again, this example was obtained earlier by construction (in [9]).

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vertices	fullerenes	vertices	fullerenes	vertices	fullerenes
100	1	150	0	200	36
102	0	152	3	202	25
104	1	154	0	204	59
106	0	156	3	206	35
108	0	158	0	208	66
110	1	160	1	210	37
112	0	162	1	212	89
114	0	164	10	214	57
116	0	166	3	216	85
118	0	168	10	218	62
120	0	170	4	220	87
122	0	172	8	222	64
124	1	174	2	224	172
126	0	176	14	226	99
128	0	178	6	228	198
130	0	180	8	230	141
132	1	182	9	232	194
134	1	184	16	234	141
136	1	186	10	236	316
138	0	188	18	238	205
140	1	190	6	240	400
142	0	192	33	242	259
144	2	194	13	244	468
146	0	196	34	246	397
148	2	198	18	248	634

Table 1: Counts of fullerenes without a spiral starting at a pentagon. These counts have been independently confirmed with the program fullgen [5].

vertices	fullerenes	vertices	fullerenes	vertices	fullerenes
250	411	300	5 548	350	30 885
252	615	302	4 388	352	41 747
254	467	304	6 193	354	35 180
256	851	306	4 938	356	47 021
258	562	308	7 673	358	39 661
260	881	310	6 242	360	51 978
262	623	312	9 165	362	44 499
264	1 083	314	7 261	364	57 767
266	863	316	10 302	366	50 370
268	1 270	318	8 464	368	66 261
270	1 037	320	11 854	370	58 003
272	1 558	322	9 745	372	77 534
274	1 133	324	14 356	374	68 670
276	1 968	326	12 344	376	89 284
278	1 525	328	17 926	378	77 802
280	2 529	330	15 397	380	100 355
282	2 002	332	21 182	382	86 960
284	3 011	334	17 986	384	112 914
286	2 473	336	23 625	386	101 046
288	3 413	338	19 571	388	131 212
290	2 783	340	26 885	390	117 963
292	4 215	342	22 801	392	152 483
294	3 401	344	31 476	394	134 408
296	4 996	346	26 842	396	171 302
298	3 797	348	35 834	398	150 285
				400	189 662

Table 2: Counts of fullerenes without a spiral starting at a pentagon (continued). The counts for up to 380 vertices were independently confirmed with the program fullgen [5].

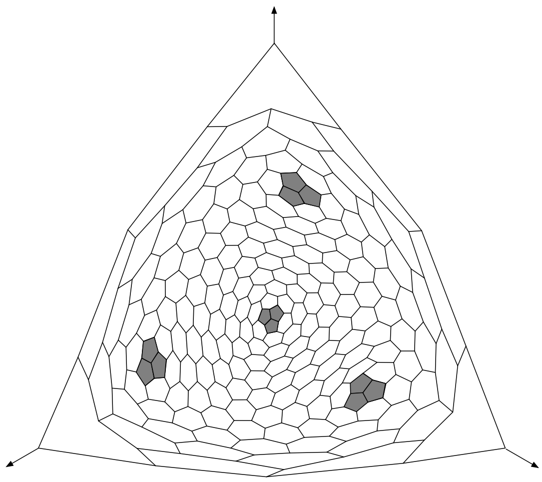

Figure 1: The smallest fullerene without a spiral. It has 380 vertices and was first described in [3]. In order to show the rotational symmetry with vertices as centres of rotation, one vertex has to be chosen at infinity. The fullerene has chiral tetrahedral symmetry.

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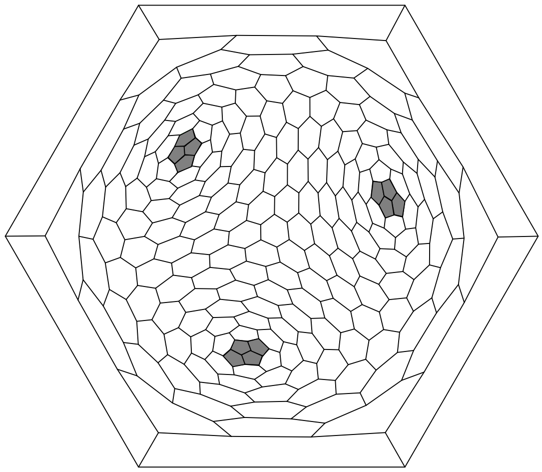

Figure 2: The second smallest fullerene without a spiral. It has 384 vertices and was first described in [9]. The fullerene has D_3 symmetry.

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