

Spiral Coding of Leapfrog Polyhedra

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Statistical connections are made between the constructibility of a cubic polyhedron by leapfrog transformation (omnicapping + dualization of a planar graph) and its representability by face-spiral coding. It is proved that all truncations of cubic polyhedra with more than four vertices are nonspiral. More qualitatively, several million examples show leapfrogs from cubic polyhedral parents to be less likely to have spirals than their parents. Exhaustive search shows that the smallest fullerene polyhedron without a spiral, whatever it may turn out to be, has more than 176 and not more than 380 vertices and is not a leapfrog.

INTRODUCTION

Chemical interest in polyhedral frameworks is growing, fueled by the discoveries of the fullerenes,^{1,2} nanotubes,³ and their heteronuclear analogues.^{4,5} The present note connects two constructions that are useful in the systematic treatment of polyhedral carbon cages. These are the *face-spiral algorithm*⁶ and *leapfrog transformation*.⁷ Each construction is described briefly before turning to a survey of some millions of small cases that provides data on the relative abundance of leapfrog and nonspiral polyhedra among the cubic polyhedra. The results imply, perhaps unexpectedly, that leapfrogging typically reduces the chances of a cubic polyhedron having a spiral code. They also motivate a proof that the truncate of a cubic polyhedron of more than four vertices (equivalently, the leapfrog of its deltahedral dual) is always unspirallable.

THE SPIRAL ALGORITHM

The spiral algorithm gives a coding and construction of each cubic (i.e., trivalent) polyhedron that can be unwrapped as a single tightly wound spiral strip of edge-sharing faces. It was proposed specifically for enumeration of fullerenes (carbon cages based on trivalent spherical polyhedra made up entirely of pentagonal and hexagonal faces) but has been applied more widely. The initial conjecture⁶ that *every* fullerene would have at least one such face spiral was disproved by construction of a counterexample with 380 vertices;⁸ it is not known whether this counterexample is minimal, but it has been verified using the algorithm described by Brinkmann and Dress⁹ that all fullerene isomers with <178 vertices have at least one spiral.

The construction itself has proved useful in generation of sets of isomers for testing chemical, physical, and mathematical hypotheses about the fullerene class, and is incorporated in IUPAC proposals for nomenclature.¹⁰ For the general class of cubic polyhedra, completeness breaks down very much earlier (at 18 vertices) and the statistics suggest a decreasing ratio of spirallable to unspirallable cubic

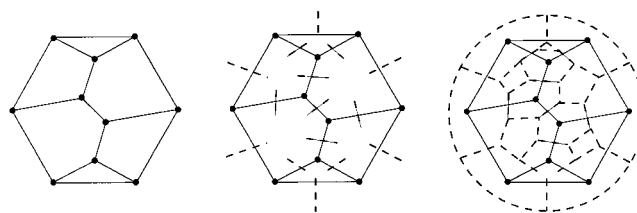


Figure 1. The leapfrog transformation of a polyhedron by edge replacement on the Schlegel diagram. The new graph has edges (dotted) traversing those of the parent (full lines), which are then joined to produce the new (staggered) faces inside those of the parent.

polyhedra as the number of vertices increases.¹¹ Within the many billions of fullerenes on 380 to 1000 vertices there are now known several hundred sporadic counterexamples to the spiral conjecture, and all are chiral.^{8,12–14} Almost all of them have highly destabilizing crowding of pentagons; very few isolated pentagon counterexamples have been found so far.

There is interest in devising systematic constructions for fullerenes without spirals, with the twin aims of tightening the bounds on the range of applicability of the conjecture and identifying common symmetry or other characteristics.

THE LEAPFROG TRANSFORMATION

Any planar graph may be converted to a specific derivative polyhedron with three times as many edges by the process of *leapfrogging*.⁷ This transformation may be described in several equivalent ways. Three of these are: capping on all faces followed by dualization;⁷ dualization followed by truncation on all vertices;¹⁵ and replacement of every edge of the parent by a transverse edge connecting interior points on the two adjacent faces, endpoints of distinct new edges being connected when they lie on the same parent face and arise from neighboring parent edges (Figure 1).¹⁶

The faces of the resulting *leapfrog* polyhedron comprise one for every original face and equal to it in size, plus one for every original vertex, of size equal to twice the vertex degree. Thus when the parent is cubic, the leapfrog consists of copies of all the original faces, separated from one another by hexagons; in particular, leapfrog fullerenes have isolated

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pentagons. The leapfrog polyhedron is cubic and has at least one Clar coloring (i.e. a disjoint subset of its faces covering every vertex once and only once¹⁷). Leapfrogs are those cubic polyhedra with precisely one or three Clar colorings. Those with three have all faces of even size and are derived from parent graphs without odd faces; those with one Clar coloring have at least one odd-sized face, but no adjacent odd faces.¹⁷ The even faces of a Clar coloring are not necessarily all hexagonal.

The chemical interest of the leapfrog construction lies in the fact that leapfrogs of a wide class of trivalent polyhedra that includes the fullerenes have properly closed-shell eigenvalue spectra.^{7,18} Thus, they have half positive and half negative eigenvalues and, when they are considered as neutral Hückel systems of carbon atoms, they have exactly enough bonding orbitals to accommodate their π electrons. Leapfrog fullerenes are therefore ideal structures from the purely π -electronic point of view, though usually poorer in terms of steric strain and therefore total energy than some non-leapfrogs within the isolated-pentagon class.

Of the known fullerene counterexamples to the spiral conjecture, just one published case (with $n = 924$ vertices⁸) is a leapfrog (see later for new examples). On the other hand, the smallest general cubic polyhedron without a spiral (at $n = 18$) is itself the leapfrog of the unique five vertex deltahedron or—equivalently—the truncation of the trigonal bipyramid, and several others among the first few general nonspiral polyhedra are also leapfrogs.¹¹ Two questions naturally arising from these observations are: how common among the cubic polyhedra are leapfrogs and, are they less or more likely to have spirals than nonleapfrogs of the same size? These two questions are now explored by explicit enumeration, construction, and testing for spirals of leapfrog and nonleapfrog cubic polyhedra.

STATISTICS

Powerful methods for the rapid construction and enumeration of cubic polyhedra are available, as are programs for checking whether a given cubic polyhedron has a spiral code.¹¹ A program for leapfrogging a given starting graph was written for the current exploration, as was a program to count the number of parents (0, 1, 3) of a given cubic polyhedron considered as a putative leapfrog. The latter task is equivalent to counting the Clar colorings, not necessarily nonisomorphic, of the test polyhedron. A combination of these programs was used to answer a series of questions on the statistical relations between spiral and leapfrog constructions.

It was noted in the previous survey of spiral and nonspiral cubic polyhedra¹¹ that (i) the proportion of polyhedra without spirals increases rapidly with vertex count, and (ii) the class of unspirallable polyhedra is dominated by those with a wide range of face sizes. Triangle-free cubic polyhedra, for example, are about twice as likely to have spirals as general cubic polyhedra in the range of n studied.

Tables 1–3 show how these trends are affected by taking leapfrogs. For the general cubic polyhedra (Table 1), leapfrogging increases the number of nonspirals by a large factor, though the effect becomes less pronounced as the number of vertices increases. Again this property is

Table 1. How Does Leapfrogging Affect the Probability of Finding a Spiral for General Cubic Polyhedra?^a

n	N_T	N_S	N_L
4	1	0	0
6	1	0	0
8	2	0	0
10	5	0	0
12	14	0	1
14	50	0	3
16	233	0	13
18	1 249	1	149
20	7 595	11	1 514
22	49 566	184	14 858
24	339 722	2 800	138 521
26	2 406 841	41 763	1 237 136
28	17 490 241	612 755	10 709 072

^a Comparison for general cubic polyhedra on n vertices of the total number of polyhedra (N_T), the number of them without spirals (N_S) and the number of nonspiral polyhedra produced by leapfrogging the originals (N_L).

Table 2. How Does Leapfrogging Affect the Probability of Finding a Spiral for Triangle-Free Cubic Polyhedra?^a

n	N_T	N_S	N_L
4	0	0	0
6	0	0	0
8	1	0	0
10	1	0	0
12	2	0	0
14	5	0	0
16	12	0	0
18	34	0	0
20	130	0	0
22	525	1	1
24	2 472	8	7
26	12 400	79	71
28	65 619	751	669
30	357 504	6 924	6 032
32	1 992 985	61 784	52 947
34	11 284 042	526 159	451 049

^a Comparison as in Table 1 but for triangle-free cubic polyhedra only.

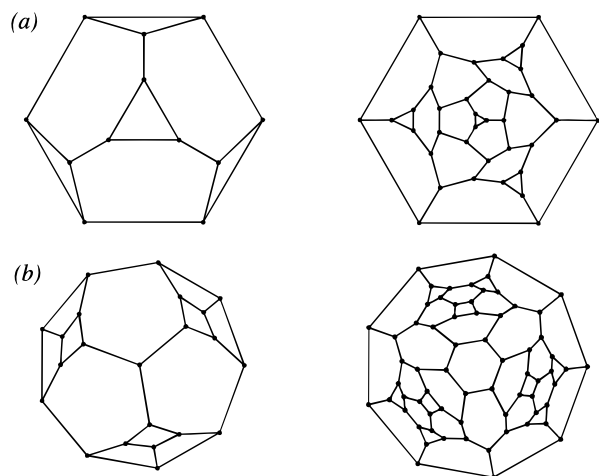
predominantly of those parent polyhedra that have a large range of face sizes. When the parent is triangle-free (Table 2), the proportion of nonspiral cases is actually reduced on leapfrogging, and when the parent has no face larger than a hexagon (Table 3), the increase in the small number of nonspiral cases is slight. Particular results from the tables are the smallest general ($n = 12$) and the smallest triangle-free ($n = 22$) cubic polyhedron whose leapfrogs are cubic polyhedra without spirals. The parents and leapfrogs are illustrated in Figure 2. The 12 vertex example is also the smallest with no face larger than a hexagon to leapfrog to a nonspiral polyhedron.

Restricting the polyhedra of Table 3 further, to those that have no face smaller than a pentagon or larger than a hexagon, gives the fullerenes. Combination of the leapfrog and spiral testing programs with a fast fullerene generator⁹ allows further comment on the nature of the minimal counterexample to the fullerene spiral conjecture. All fullerenes C_n with $58 \leq n \leq 128$ vertices were constructed, leapfrogged to give fullerenes in the range $174 \leq n \leq 384$, and tested for spirals. All were found to have at least one spiral. The significance of this test is that these leapfrogs span the gap between the highest vertex count where all

Table 3. How Does Leapfrogging Affect the Probability of Finding a Spiral for Cubic Polyhedra with Faces Smaller than a Hexagon?^a

n	N_T	N_S	N_L	n	N_T	N_S	N_L
4	1	0	0	58	41 007	0	0
6	1	0	0	60	52 293	0	1
8	2	0	0	62	65 724	0	0
10	5	0	0	64	82 953	1	2
12	10	0	1	66	103 022	0	0
14	15	0	0	68	128 343	0	1
16	30	0	0	70	158 191	0	1
18	44	0	0	72	194 954	0	1
20	77	0	0	74	237 866	0	1
22	115	0	0	76	290 728	0	2
24	184	0	0	78	351 678	0	0
26	267	0	0	80	425 998	1	2
28	420	0	1	82	511 817	0	3
30	595	0	0	84	614 595	1	2
32	883	0	0	86	733 120	0	3
34	1 242	0	0	88	874 872	1	3
36	1 783	1	0	90	1 036 004	1	0
38	2 445	0	1	92	1 227 511	0	2
40	3 443	0	2	94	1 446 160	1	1
42	4 622	0	0	96	1 702 224	2	3
44	6 319	0	0	98	1 993 449	2	4
46	8 406	0	0	100	2 334 060	2	4
48	11 247	0	1	102	2 717 962	0	1
50	14 676	0	0	104	3 165 259	0	3
52	19 345	0	1	106	3 669 287	1	1
54	24 884	0	0	108	4 249 410	0	3
56	32 219	0	0				

^a Comparison as in Table 1 but only for those cubic polyhedra that have no face larger than a hexagon.

**Figure 2.** Minimal parent and leapfrog pairs where the parent but not the leapfrog has a spiral: (a) for a general cubic parent (12 \rightarrow 36), (b) for a triangle-free cubic parent (22 \rightarrow 66).

fullerenes are known to have spirals (176) and the lowest where at least one fullerene is known to be unspirallable (380); the result shows that the minimal fullerene counterexample to the spiral conjecture is not a leapfrog.

Some further information on the existence of spirals for leapfrog fullerenes was obtained by transforming all IPT (isolated pentagon-triple) nonspiral polyhedra on $n \leq 1000$ vertices.¹² The leapfrog of the T -symmetric C_{380} counterexample has a spiral⁸ and, of the full set of 312 isomers, 137 gained a spiral after one leapfrog transformation, though all had nonspiral double leapfrogs. A similar pattern was observed for the five isolated-pentagon tetrahedral counterexamples:⁸ three gained a spiral on leapfrogging once, but all five double leapfrogs were without spirals.

Table 4. Effects of Repeated Leapfrogging on Non-Spiral Cubic Polyhedra^a

n	N_1	N_2	N_3
18	1	1	1
20	11	11	11
22	184	183	181
24	2 800	2 772	2 744
26	41 763	41 021	40 519
28	612 755	597 467	590 123

^a The leapfrog transformation is here applied *only* if the polyhedron is without a spiral. Of the general cubic polyhedra on n vertices, N_1 have no spiral, of which N_2 still have no spiral after leapfrogging, of which N_3 still have no spiral after leapfrogging a second time.

The fullerenes, with 12 pentagonal faces and all others hexagonal, form a subclass of Goldberg's trivalent *medial* polyhedra,¹⁹ which in general have only p -gonal ($p = 3, 4, 5$) and hexagonal faces. Leapfrogging any medial polyhedron trivially gives another with the same value of p ; when p is odd, the *parent* of any leapfrog member of the medial series is unique and also a medial polyhedron. Isomer counts in the medial series with $p < 5$ are nonmonotonic and grow more slowly than for fullerenes, so that a complete survey up to, for example, $n = 400$, is feasible.

Systematic results from these related series can be used to shed light on the fullerene class itself. The triangle/hexagon series ($p = 3$, four triangles, $n = 4 + 4k$, $k \neq 1$) contains small nonspiral examples; for example, on 36 (L), 64, 84 (L), 100, 112, 120 (L), 124, 136, 140, 144 (L), 148, 156 (L), ... vertices, where L denotes a leapfrog polyhedron. Leapfrogging increases the likelihood of nonspirality, with for example at least one nonspiral isomer on $3n$ vertices for all $n > 60$ in the range investigated.

In the square/hexagon series ($p = 4$, six squares, $n = 8 + 2k$, $k \neq 1$) the smallest examples without a spiral are much larger: at 306 (one of 1057 isomers), 356 (one of 2838), and 384 (one of 2500). The smallest nonspiral leapfrogs in this series are at 384, 486, 564, ... vertices. It is tempting to see in the higher onset of nonspirality as p increases from 3 to 4 some support for a still higher value for the vertex count of the smallest fullerene without a spiral, suggesting that the fullerene counterexample at 380 vertices may be close to minimal.

It is apparent from Table 1 that leapfrog transformation of a general cubic polyhedron gives a product that is less likely to have a spiral; iteration of the procedure by leapfrogging *only* the nonspiral polyhedra at each generation (Table 4) shows that a small fraction of nonspiral polyhedra regain spirals by repeated leapfrogging. This result is compatible with the earlier observations on face signature, given the fact that leapfrogging does not change the range of the face sizes for any cubic polyhedron that already has a hexagonal or larger face.

Although all leapfrogs are cubic polyhedra,¹⁷ it is not necessary for the parent to be either cubic or polyhedral. Tables 5 and 6 show the distribution among cubic polyhedra of leapfrogs derived from parents of any kind. As the number of leapfrog polyhedra with n vertices grows as the number of graphs on $n/3$ edges (the two counts differing because a leapfrog may have up to three nonisomorphic parents), at large n the proportion of leapfrogs among the general cubic polyhedra will fall steeply with n . There are

Table 5. Distribution of Leapfrogs Amongst General Cubic Polyhedra and General Cubic Polyhedra without Spirals^a

<i>n</i>	<i>N_T</i>	<i>N_{T0}</i>	<i>N_{T1}</i>	<i>N_{T3}</i>	<i>N_S</i>	<i>N_{S0}</i>	<i>N_{S1}</i>	<i>N_{S3}</i>
4	1	1	0	0	0	0	0	0
6	1	0	1	0	0	0	0	0
8	2	1	0	1	0	0	0	0
10	5	3	2	0	0	0	0	0
12	14	11	2	1	0	0	0	0
14	50	42	7	1	0	0	0	0
16	233	215	16	2	0	0	0	0
18	1 249	1 193	54	2	1	0	1	0
20	7 595	7 426	161	8	11	11	0	0
22	49 566	48 947	611	8	184	179	5	0
24	339 722	337 358	2 332	32	2 800	2 786	14	0
26	2 406 841	2 397 157	9 627	57	41 763	41 605	154	4
28	17 490 241	17 449 138	40 918	185	612 755	611 893	857	5
30	129 664 753	129 484 024	180 263	466	8 495 726	8 488 211	7 475	40

^a Of *N_T* polyhedra on *n* vertices, *N_{T0}* have no parent (i.e., are not leapfrogs), *N_{T1}* have one parent, and *N_{T3}* have three (not necessarily nonisomorphic) parents. The left-hand side of the table shows a similar breakdown for the subset of *N_S* nonspiral polyhedra, *N_{Si}* being the number with *i* parents.

Table 6. Distribution of Leapfrogs Amongst Triangle-Free Cubic Polyhedra and Triangle-Free Cubic Polyhedra without Spirals^a

<i>n</i>	<i>N_T</i>	<i>N_{T0}</i>	<i>N_{T1}</i>	<i>N_{T3}</i>	<i>N_S</i>	<i>N_{S0}</i>	<i>N_{S1}</i>	<i>N_{S3}</i>
4	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0
8	1	0	0	1	0	0	0	0
10	1	0	1	0	0	0	0	0
12	2	1	0	1	0	0	0	0
14	5	2	2	1	0	0	0	0
16	12	8	2	2	0	0	0	0
18	34	22	10	2	0	0	0	0
20	130	103	19	8	0	0	0	0
22	525	445	72	8	1	1	0	0
24	2 472	2 233	207	32	8	6	2	0
26	12 400	11 572	771	57	79	64	11	4
28	65 619	62 703	2 731	185	751	655	91	5
30	357 504	346 506	10 532	466	6 924	6 395	489	40

^a Notation as for Table 5.

indications that at large *n* the leapfrog fraction falls faster for nonspiral than spiral polyhedra. Thus, for the general trivalents of Table 5 with *n* = 22, 24, ...30, the leapfrog fractions are *f_S* = (*N_{S1}* + *N_{S3}*)/*N_S* = 0.0272, 0.0050, 0.0038, 0.0014, and 0.0009, and *f_T* = (*N_{T1}* + *N_{T3}*)/*N_T* = 0.0125, 0.0070, 0.0040, 0.0024, 0.0014, giving a reduction factor of *f_S*(22)/*f_S*(30) = 31 compared with *f_T*(22)/*f_T*(30) = 9. The trend is less pronounced for the triangle-free polyhedra of Table 6, where *f_S*(24)/*f_S*(30) = 3.3, only just above *f_T*(24)/*f_T*(30) = 3.1.

The overwhelming majority of the cubic polyhedra without spirals are not themselves leapfrogs, yet the statistical data obtained so far point to one class of leapfrogs that should be very rich in nonspiral polyhedra. This class is based on a particular type of parent graph that automatically leads to a leapfrog product with a wider spread of faces (i.e., the planar triangulation or deltahedron).

The leapfrog of an *n*-face deltahedron is identical to the polyhedron derived by truncation of its *n*-vertex cubic dual. The deltahedron on four faces is self-dual, and its 12-vertex leapfrog, the truncated tetrahedron, has a spiral. The next smallest case, the five-faced trigonal bipyramid, leapfrogs to the 18-vertex truncated trigonal prism, and this is notoriously without a spiral, being the smallest nonspiral cubic polyhedron.¹¹ Explicit search on triangulations with 6–17 vertices failed to reveal any other example of a

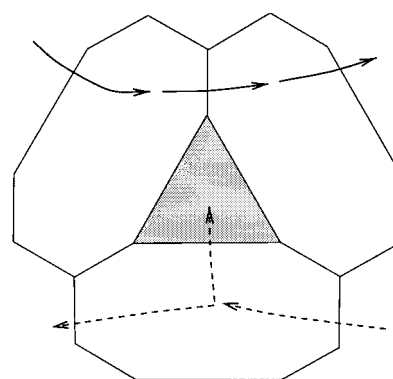


Figure 3. A triangular trap. Here the attempted spiral has passed through two neighbors of the central triangle (full arrows), visited other faces and has returned through the third neighbor. The dotted lines indicate Scylla and Charybdis: either visit the triangle and end there, or miss it altogether and thereby fail.

deltahedron whose leapfrog has a spiral. In the following section it is proved that nonspirality is a property of *all* leapfrogs whose parents are deltahedra of more than four faces. An equivalent statement of the result is that the tetrahedron is the only cubic polyhedron whose truncate has a spiral.

AN INFINITE CLASS OF LEAPFROGS WITHOUT SPIRALS

We begin by defining the notion of a trap. Leapfrogs of deltahedra have no adjacent triangular faces — every face is either a triangle surrounded by even faces or is an even face surrounded by alternately triangles and other even faces. A *trap* is produced when a tentative spiral unwinding of the polyhedron gives rise to a triangle that is not itself yet included in the spiral but has at least two neighbors that are already in the spiral (Figure 3) and if there are only two then neither neighbor is the latest face included in the spiral. In the case of three neighbors in the spiral, either the triangle will be next and the spiral ends, or it is already isolated, so the spiral will never reach it. In case of two neighbors in the spiral, when the spiral reaches the third neighbor of the trapping triangle, it must then either enter the triangle on the next step, and terminate, or leave this triangle forever unvisited. Thus the existence of two distinct trapping

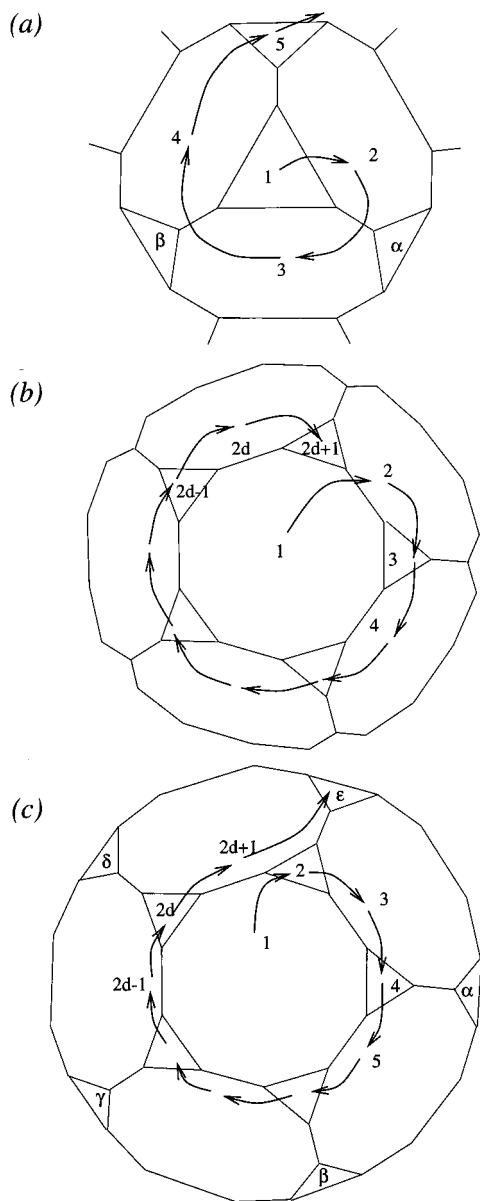


Figure 4. The three ways to start a spiral on a truncated cubic polyhedron: (i) from a triangle, (ii) from a pair of even faces, or, (iii) from an even face followed by a triangle.

triangles at any stage of the construction is sufficient to guarantee failure of the given putative spiral.

Now consider the ways that an attempt to construct a spiral on a truncated cubic polyhedron might start (Figure 4). It could begin on (i) a triangle, (ii) an even face followed by another even face, or (iii) an even face followed by a triangle.

In case (i) the spiral starts in triangle 1, visits its even neighbors 2, 3, 4, then triangle 5. The triangles α , β , and 5 are different as a consequence of the fact that the graph is 3-connected. Therefore the spiral has two traps α and β and cannot complete. Thus, no spiral of a truncated cubic polyhedron can start with a triangle.

In case (ii) the spiral starts on the even face 1 (of size $2d$), visits the even-triangular-even-triangular...neighbors 2, 3,... $2d$, and, having reached the triangle $2d+1$, has no exit to a new face. Thus, no spiral of a truncated cubic polyhedron can start with a pair of even faces. Note that again, because of 3-connectedness, the triangles 3, 5,... $2d+1$ and the even faces 2, 4,... $2d$ are distinct.

In case (iii) the spiral starts on the even face 1, visits its neighbors in the sequence triangular-even-triangular-..., 2, 3, $2d+1$. As in (ii), all triangles 2, 4,... $2d$ and the even faces 3, 5,... $2d+1$ must be distinct, and because the graph is a leapfrog, each free edge leaving these triangles must end in a vertex of a triangle that—again implied by 3-connectedness—has not been counted so far. Call the number of distinct triangles at the ends of free edges, which may be 1, 2, 3, or more, t . Case (iii) now splits into three subcases. If $t = 1$, all free edges terminate on the same triangle, $2d$ must be 6, the polyhedron is the truncated tetrahedron, and there is a spiral. If $t \geq 3$, the free edges terminate on three or more new triangles, at least two of which are traps, and hence there is no spiral. Last, if $t = 2$, say there are triangles α , β , the Jordan Curve Theorem²⁰ implies that all triangles adjacent to α (or equivalently β) must follow each other on the boundary of face 1. So if we have three triangles adjacent to α (or β), we have a 2-cut (i.e., a pair of edges whose removal will disconnect the graph). So we have $d \in \{3, 4\}$ and each of α , β is adjacent to at most two triangles on the boundary of face 1. Checking these two cases separately, again a 2-cut is detected or the structure closes to give the truncated trigonal prism (a case that can be checked separately by hand and is known to have no spiral); so, in fact, no polyhedron exists in case $t = 2$. Thus, a successful spiral of a truncated cubic polyhedron starting with an even face followed by a triangle is possible, but only for the truncated tetrahedron. In summarizing, the truncated tetrahedron has 24 copies of the unique distinct spiral 6 3 6 3 6 3 6 3, but no other truncated cubic polyhedron has a spiral.

Further extension of this result is likely to be possible. We note that double or triple leapfrogging of deltahedra on 5–15 vertices failed to find any spiral polyhedra. Four consecutive leapfrog transformations of deltahedra on 5–14 vertices and six on 5–12 vertices gave no polyhedra with spirals. Leapfrogs of the tetrahedron itself give a more complicated pattern: double leapfrogging leads to a polyhedron without a spiral, triple leapfrogging to one with a spiral, and in fact for all cases $1 \leq n \leq 8$, the n^{th} leapfrog of the tetrahedron has a spiral if and only if n is odd. Testing the case $n = 8$ is already a substantial task because the polyhedron has 26 244 vertices and therefore 157 464 potential spiral starts, all of which fail. These results prompt the question whether *any* multiple leapfrogs of deltahedra on >4 vertices can be unwound in a spiral.

CONCLUSIONS

It has been shown that the leapfrog transformation can multiply examples of nonspiral cubic polyhedra. The connection between leapfrog and spiral constructions claimed in the *Introduction* to this paper is exhibited by the general tendency of leapfrogged cubic polyhedra to be nonspiral and by a specific theorem forbidding spirals for the infinite class of truncated cubics. Truncated cubics, as a subclass of cubic polyhedra, are potential models for carbon cages. For example, all cubic polyhedra composed of 20 neutral carbon atoms have been found to correspond to local minima in a semiempirical potential surface.²¹ Their π -electronic characteristics have been studied previously: the Hückel orbital energies of a truncate follow directly from those of the parent

cubic and whenever this parent is a nonalternant, the π -configuration is formally closed with a multiply degenerate nonbonding HOMO and equisymmetric with that of the leapfrog of the parent cubic.²² Their energetic characteristics will doubtless be dominated by the strained three-membered rings, implying poor stability relative to frameworks drawn from the triangle-free class, and in particular with respect to fullerene polyhedra. The present result shows that if such molecules were to be synthesized, they would fall outside the recent IUPAC formulation of spiral-based rules for nomenclature of fullerenes and fullerene-like cages.¹⁰ Other codes capable of representing them exist.^{11,23} Finally, the computational part of the present work has placed a further limitation on the much sought-after smallest counterexample to the fullerene spiral conjecture: it is not a leapfrog polyhedron.

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