Version of Zones and Zigzag Structure in Icosahedral Fullerenes and Icosadeltahedra

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A circuit of faces in a polyhedron is called a *zone* if each face is attached to its two neighbors by opposite edges. (For odd-sized faces, each edge has a left and a right opposite partner.) Zones are called *alternating* if, when odd faces (if any) are encountered, left and right opposite edges are chosen alternately. Zigzag (Petrie) circuits in cubic (= trivalent) polyhedra correspond to alternating zones in their deltahedral duals. With these definitions, a full analysis of the zone and zigzag structure is made for icosahedral centrosymmetric fullerenes and their duals. The zone structure provides hypercube embeddings of these classes of polyhedra which preserve all graph distances (subject to a scale factor of 2) up to a limit that depends on the vertex count. These embeddings may have applications in nomenclature, atom/vertex numbering schemes, and in calculation of distance invariants for this subclass of highly symmetric fullerenes and their deltahedral duals.

1. INTRODUCTION

This paper deals with the concept of *zones* in polyhedra, specifically in the graphs of fullerenes of centrosymmetric icosahedral symmetry (I_h) and their deltahedral duals. Zones give a multiple covering of a polyhedron by closed cycles of faces, as will be described in detail below.

They are worth studying in chemical and biological contexts for several reasons. First, for the particular subset of chemically relevant polyhedra constituted by the I_h fullerenes, it turns out that a binary encoding of the vertices of a fullerene, which can be derived from its zones, and which relates these 3D polyhedral cages to cubes in much higher dimension, has a useful property. This encoding preserves distances, subject to a scaling by a factor of 2, up to a maximum distance that is large and is always at least a third of the graph diameter. These results give examples of extensions of the theory of isometrical embeddings (up to a scale factor) which has been described elsewhere for general metrics[1] and for planar graphs.[2,3] This coding may have practical applications in the calculation of distance-based graph invariants, which are themselves known to correlate with chemical and physical properties of fullerene cages.[5] Codings of vertices that additionally preserve many of the graph distances could also offer a useful scheme for nomenclature.[6,7]

Second, it is clear from the variety of theories used to study the structure, energetics, dynamics, and reactivity of chemical polyhedra that it may be profitable at different times to concentrate on edge-, vertex-, or face-based descriptions. For example, bonding theories for polyhedral systems from the saturated spheroalkanes, through the unsaturated fullerenes, to the electron deficient deltahedral boranes, are cast respectively in terms of σ bonds along edges, π orbitals on vertices, and multicenter bonds on faces. Zones add a new decomposition of fullerene cages, a partition into overlapping closed rings of pentagons and hexagons, suggesting a fragment analysis of the electronic structure of the cage in terms of conjugated π systems.

Third, as well as providing structures for hypothetical large boranes,[8] the duals of icosahedral fullerenes (icosadeltahedra) describe the capsid structures of many of the known viruses.[9−11]

The results of this investigation can be stated essentially pictorially, and the end result is a clear structural classification of I_h fullerenes and their duals. The paper is organized as follows. After some preliminary definitions (§2), we review some properties of the zones of icosahedral fullerenes and their duals (the icosadeltahedra), showing how they produce embeddings of these graphs in high-dimensional *(half)cubes*, leading to useful encodings of the fullerenes (§3). It is found that there are embeddings which preserve (up to a scale factor of 2) all distances below some critical value for each centrosymmetric icosahedral fullerene and its dual. A complete description of zigzag structure for the I_h fullerenes and their duals is then given.

2. DEFINITIONS

We consider planar, three-connected graphs without loops or multiple edges, i.e. the graphs that correspond to the skeletons of spherical polyhedra.

A *circuit* in such a graph is constructed as a cyclic sequence of vertices, each connected to its successor in the sequence by an edge: the connecting edges therefore form a closed path. A circuit is *simple* if it has no self-intersection. A circuit (whether simple or not) is *Petrie*,[12] *geodesic*,[13] *left-right*,[14] or *zigzag* if it includes alternately the extreme left and extreme right edges emanating from successively visited vertices. In a Petrie circuit, each consecutive pair of edges,

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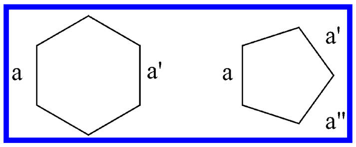

Figure 1. Opposite edges in even and odd polygons. In a hexagon, and all other even polygons, there is a unique edge a' opposite to the edge a; in a pentagon, and all other odd polygons, there are two edges a' and a'' opposite to a.

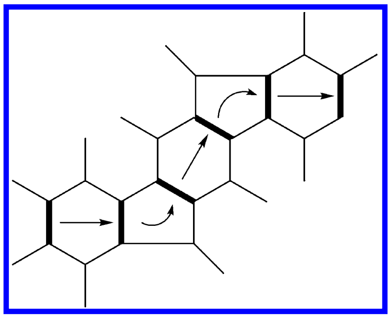

Figure 2. A segment of an alternating zone in a planar graph. The bold lines denote the edges making up the underlying cut.

but no consecutive triple of edges, belongs to the same face of the polyhedron.

In an even face (a face with an even number of edges), every edge has a unique opposite partner, but in an odd face every edge has two opposite (i.e. most distant) partners, one left and one right (Figure 1). An *(opposite) cut* is a cyclically ordered sequence of edges, e_1, e_2, ... e_n, $e_{n+1} = e_1$, such that any two consecutive members are opposite edges of the same face. As with circuits, cuts may be simple, alternating, neither, or both. An opposite cut is *alternating* if, when an odd face is entered in the sequence of edges, the next member of the sequence in cyclic order is chosen as the left or right opposite edge of that face, the choice alternating with the parity of i, the counter for the odd faces; between odd faces there may be a number of even faces, but for each of these there is no choice as the exit is through the unique opposite of the entry edge (Figure 2).

The sequence of consecutive faces traversed by a cut is called a *zone*. A cut can be seen as a kind of skeleton of a zone. Mostly we will be interested in zones that correspond to alternating cuts, and these will be termed *alternating zones*. Those alternating zones that consist entirely of triangles correspond to Petrie circuits of vertices in the dual. General alternating zones correspond to *quasi-central* circuits in the dual: having entered a vertex along one edge, such a circuit takes as exit the edge that is straight ahead (if uniquely defined), and otherwise takes one of the two edges closest to the straight-ahead direction (alternately choosing the left and right member of the pair); if all vertices in the circuit are of even degree, there is a unique straight-ahead choice at each of them, and the circuit is *central*. When the graph is trivalent, the Petrie circuit, in which extreme left and right exit edges are chosen alternately, coincides with a quasi-central circuit. Zones are either *straight*, containing only even-sized faces, or *crooked*, containing some odd-sized faces. These concepts are illustrated by examples in Figures 3 and 4, where it is seen that a polyhedron may have one or many Petrie circuits, simple or not. Clearly, if the Petrie circuit is unique, it cannot be simple, as each edge is then at a self-intersection. Equally, it is easily shown that the set of

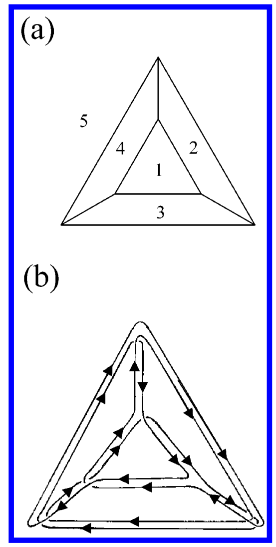

Figure 3. Zones and Petrie circuits in the trigonal prism. (a) The trigonal prism has one simple (straight) zone, which consists of the cycle of square faces 2−3−4, and one self-intersecting alternating zone consisting of the cycle 1−2−5−4−1−3−5−2−1−4−5−3 in which each triangle is visited three times and each square face twice. (b) The single Petrie circuit on the edges of the trigonal prism has a self-intersection on every edge. In the dual trigonal bipyramid, this corresponds to one alternating zone with triple self-intersection in each of the six triangles.

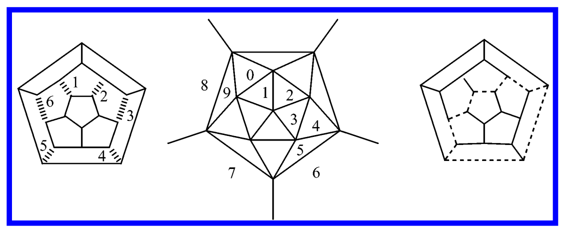

Figure 4. (a) One of the 10 alternating zones made up of six faces in the dodecahedron (each edge of the zone is marked by a double bond). (b) One of the six alternating zones made up of 10 faces (marked 1, 2, 3, ... 9, 0) in the icosahedron. (c) A Petrie circuit (denoted by dotted lines) in the dodecahedron that corresponds to a zone in the dual icosahedron.

Petrie circuits of a polyhedron is an exact double cover of the set of edges i.e., every edge appears twice in the set, either twice in the same or once in two different Petrie circuits (see e.g. ref 15). Alternating cuts also cover the edges of a polyhedron but in a less regular manner. To achieve an exact double cover, we should count twice those alternating cuts that are skeletons of straight zones (see Figure 4). The same convention is used in counting the zones themselves. Each original straight zone is represented by two copies, taken formally to be distinct, in the extended set of zones of the polyhedron.

3. VERTEX CODES

We can interpret this double covering of edges by the extended set of zones in various ways, one of which is as a way of labeling the edges of a polyhedron, P. The zones are numbered 1, 2, ..., n_Z in some order; the order itself is not important, provided that every crooked zone and each copy of every straight zone receive distinct numbers. Every edge is then labeled with the numbers of the two zones to which it belongs. This label is clearly not unique to a particular edge; for example, all edges in a given straight zone are in its copy, and all therefore receive the same pair of integers as a label. However, in favorable circumstances, these pairs can be used in their turn to give a unique label to each vertex. Consider an arbitrarily chosen starting vertex i and a shortest path, not necessarily unique, from it to some other vertex j, passing through vertices

$$i, i + 1, i + 2, ... j - 2, j - 1, j$$

and traversing edges

$$e_1, e_2, e_3, ...$$

which have been assigned zone-pair labels

$$\{e_{1a}, e_{1b}\},\{e_{2a}, e_{2b}\}, ...$$

Now, each vertex on the path from i to j can be labeled by a *set* constructed from those attached to the previous edges in the path. The process starts by assigning the empty set ϕ to vertex i, as there are no previous edges. The next vertex $i + 1$ is assigned the symmetric difference $\phi\Delta\{e_{1a}, e_{1b}\}$, the next (vertex $i + 2$) is assigned $\phi\Delta\ \{e_{1a}, e_{1b}\}\ \Delta\ \{e_{2a}, e_{2b}\}$, the next $\phi\Delta\{e_{1a}, e_{1b}\}\ \Delta\ \{e_{2a}, e_{2b}\}\ \Delta\ \{e_{3a}, e_{3b}\}$, and so on until j is reached. [The symmetric difference of two sets A and B is the difference of their union and their intersection, *i.e.* $A \triangle B = A \cup B - A \cap B$; ϕ denotes the empty set.] Working out from i, with different choices of j, labels i.e., *sets* can eventually be attached to all vertices. In favorable circumstances, the procedure will be consistent and will lead to distinct, unique sets for every vertex of the polyhedron. Once an addressing of this type is found, equivalent labelings can be generated by replacing each vertex label by its symmetric difference with any fixed set. Figure 5 illustrates the process for the icosahedron and the dodecahedron.

Suppose now that such a vertex labeling in terms of sets has been found for some polyhedron P. From the set a binary address can be extracted. Each set on a vertex contains any one of the n_Z zones exactly once or not at all, so each vertex can be assigned a binary address of fixed length n_Z containing a 1 for every zone present. By the symmetric-difference construction, each address will contain an even number of 1's. The addresses will also have other mathematical properties, and in order to appreciate these it is necessary to recall the definitions of the cubes and half-cubes in n dimensions.

The graph of the n-dimensional (hyper)cube H_n may be interpreted in several ways (see e.g. ref 1). In terms of sets, given an original set S of n elements, the vertices of H_n correspond to the 2^n possible subsets of S. The shortest-path distance between any two vertices is then the cardinality of the symmetric difference between their sets, and, in particular, two vertices are adjacent if and only if their sets differ by the presence of exactly one element. Each subset of S is characterized by a binary sequence of length n, and so, in terms of binary sequences, the vertices are the 2^n sequences of length n, and the shortest-path distance is the *Hamming distance* between sequences. In the present case, the Hamming distance between two binary sequences is also the square of the usual Euclidean distance of the corresponding vertices.

The *half cube*, $^1/_2H_n$, is constructed from H_n by taking only the subsets of even size *or* binary sequences containing an even number of 1's. Vertices in $^1/_2H_n$ are adjacent if their

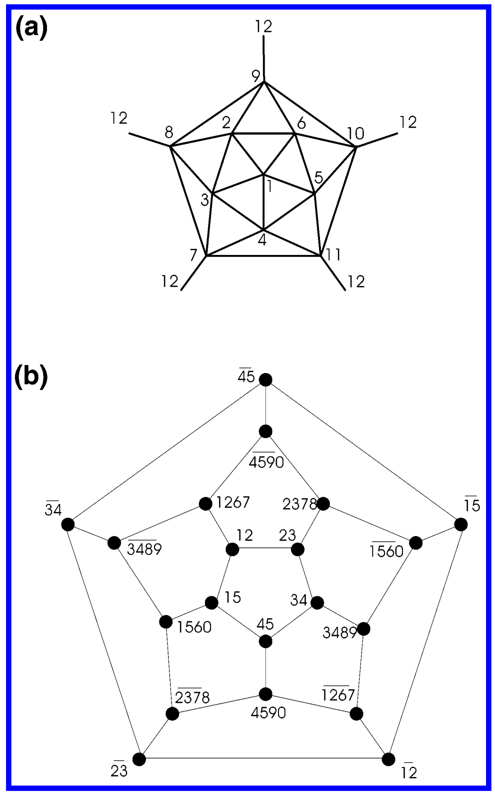

Figure 5. Labeling of vertices by sets for (a) the icosahedron and (b) the dodecahedron. The constructions given in the text provide embeddings in the six- and ten-dimensional half-cubes, respectively. In (a) the vertices 1−12 have set labelings ϕ, {12}, {23}, {34}, {45}, {51}, {$\overline{51}$}, {$\overline{45}$}, {$\overline{34}$}, {$\overline{23}$}, {$\overline{12}$}, $\overline{\phi}$ = {123456}, where the symbol $\overline{B}$ denotes the complement of the set B. In (b) the sets are shown directly on the diagram and use the range 0−9.

sets differ in *two* elements *or* the Hamming distance between their sequences is 2. The shortest-path distance between two vertices in $^1/_2H_n$ is half the corresponding distance between them in H_n.

The binary addresses derived for the vertices of the polyhedron P have various properties. The address of the starting vertex i is 000 ... 000, with as many zero entries as P has zones. This can be seen as the origin of coordinates in a Euclidean space R^{n_Z}, where each member of the extended set of zones plays the role of a spatial dimension. As every address contains an even number of 1's, the vertices of P have been inscribed vertex-to-vertex in the half-cube $^1/_2H_{n_Z}$. By construction, as i was taken as the origin, all Hamming distances of vertices with respect to i are also twice the graph distance in P. In the best case, this equality of shortest-path distances in the half cube and P holds for *any* pair of vertices, not only those that contain i. This case applies when the original graph is an isometric subgraph of $^1/_2H_{n_Z}$, expressed symbolically as $P \rightarrow {}^1/_2H_{n_Z}$. An equivalent statement is that P embeds with scale two in the half-cube H_{n_Z}.

Among fullerenes and their duals this full embedding is known in four icosahedral cases: $C_{20} \rightarrow {}^1/_2\ H_{10}$, $C_{20}^* \rightarrow {}^1/_2\ H_6$, $C_{60}^* \rightarrow {}^1/_2H_{10}$, $C_{80} \rightarrow {}^1/_2H_{22}$ (where C_n^* is the fullerene on n vertices and C_n^* is its dual). The present work shows that this list is complete in I_h symmetry; five examples are known in lower symmetries, $C_{26}(D_{3h}) \rightarrow {}^1/_2H_{12}$, $C_{28}^*\ (T_d) \rightarrow {}^1/_2H_7$, $C_{36}^*\ (D_{6h}) \rightarrow {}^1/_2H_8$, $C_{40}(T_d) \rightarrow {}^1/_2H_{15}$, $C_{44}(T) \rightarrow {}^1/_2H_{16}$, and no more occur for $n \leq 60$.[11]

The more general case is that the equality of distances will be preserved for pairs only up to some limit $t < D$ where D is the diameter (i.e. the maximum of the pairwise distances) of the graph.[2] The present paper uses the concept of zones to describe the maximum t for this weaker form of embedding for the achiral icosahedral fullerenes and their duals.

4. ZONES IN FULLERENES

A fullerene is a cubic polyhedron with exactly 12 pentagonal faces and all other faces hexagonal. An n-vertex fullerene has $n/2-10$ hexagonal faces.[16] The straight zones in a fullerene therefore consist entirely of hexagons, and the *crooked* zones contain some pentagons. Straight zones are therefore entirely straight-ahead, entering and leaving each face through uniquely defined opposite edges, but the crooked zones may in principle be alternating or not, and both types will be encountered in the zone description of icosahedral fullerenes.

Each pentagon of a fullerene occurs five times in the set of all zones and each hexagon occurs three times, so the number of crooked zones is at most 60 for a fullerene, whereas the number of straight zones can increase with n.

In a general fullerene, description and classification of zones becomes complicated. However in one case, the fullerenes of the highest attainable symmetry, I_h, it is possible to make a compact description.

Molecular graphs for I_h fullerenes are all available by the Goldberg−Coxeter construction,[17,10] in which two integer parameters specify a net on the triangulation of the plane. The vertex counts of I and I_h fullerenes are

$$n = 20(i^2 + ij + j^2)$$

with $i > 0$, $j \leq i$, $j \geq 0$. The fullerene has I_h symmetry whenever $j = i$ or $j = 0$ and has I symmetry, otherwise. Thus, I_h fullerenes have either $20k^2$ or $60k^2$ vertices.

When $n = 20k^2$, the diameter D is $6k - 1$, and for the dual the diameter is $3k$. When $n = 60k^2$, the diameter is $10k - 1$, and for the dual the diameter is $5k$.

The classification of the zone structures is described by four cases.

(i) C_n with $n = 20k^2$: Fullerenes. The fullerene embeds in the half-cube $^1/_2H_{n_Z}$ up to distance t. The dimension n_Z is the number of zones, counting all straight zones twice, as noted earlier. For $k = 1$, t is 5, and for $k \geq 2$, t is $2k + 7$. Thus, for $k = 1$ and 2 only, t is equal to the diameter of the graph, i.e., *full* embedding is possible only for the dodecahedron (C_{20}) and the chamfered dodecahedron (C_{80}) among the I_h fullerenes with $20k^2$ vertices. For all k, $n_Z = 2D = 12k - 2$.

The zone structure has 10 crooked zones, all of length $6k$, each alternating, and consisting of six pentagons spaced by strings of $(k - 1)$ hexagons. Considered as a circle cutting a sphere, each crooked zone partitions the remaining pentagons into three in the interior and three in the exterior regions.

The straight zones are $6(k-1)$ in number, each of length $5k$ hexagons. Two zones are called *parallel* if they do not intersect. It can be seen that the straight zones in the $20k^2$ icosahedral fullerenes fall into six classes of $(k-1)$ mutually parallel elements. It is easy to see that each straight zone partitions the 12 pentagons into interior and exterior sets of six. Figure 6 shows typical zones for the C_{80} I_h fullerene.

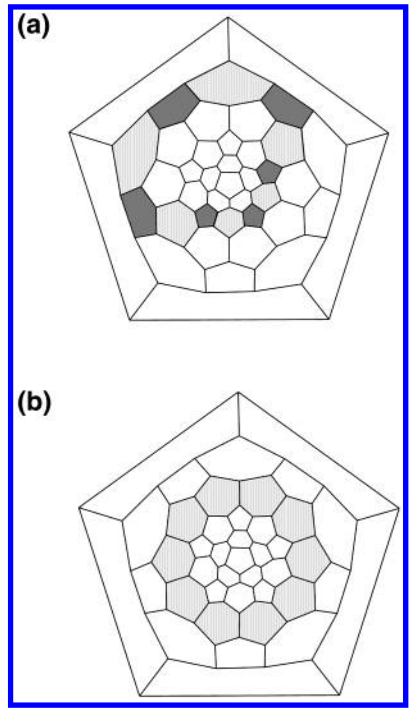

Figure 6. Zones in the icosahedral C_{80} fullerene ($n = 20k^2$, $k = 2$): (a) the symmetry-unique crooked alternating zone and (b) the symmetry-unique straight zone.

(ii) C_n^* with $n = 20k^2$: Fullerene Duals. The embedding has $t = 3$ for $k = 1$ (the icosahedron) and $t = 2k$ for $k > 1$. The only case where the embedding is full is for $k = 1$. The dimension n_Z of the half cube is $6k = 2D$. Now the zone structure consists of $6k$ zones, all alternating, and of length $10k$ each, which fall into six parallel classes. As alternating zones in the dual correspond to Petrie circuits in the fullerene, the $20k^2$ fullerenes therefore have $6k$ Petrie circuits, all simple, of length $10k$ and falling into six classes, each consisting of k disjoint elements.

The dodecahedron has six Petrie circuits of length 10, every pair having two antipodal edges in common and any larger member of the $20k^2$ class is an inflation in which each single Petrie circuit of the original dodecahedron is replaced by a stack of parallel Petrie circuits in the final fullerene.

(iii) C_n with $n = 60k^2$: Fullerenes. The embedding has $t = 6k + 1$, and as $t < D = 10k - 1$, full embedding is never possible. The dimension n_Z is $20k = 2(D + 1)$. There are 20 crooked zones, each of length $9k$ and *non*alternating, each containing three pentagons, spaced by $(3k-1)$ hexagons. These zones partition the remaining pentagons into a sets of 3 and 6. There are $10(k-1)$ straight zones also of length $9k$ each. The full set of the $10(k+1)$ zones is partitioned into 10 parallel classes, each consisting of a stack of $(k-1)$ straight zones sandwiched between a pair of crooked zones.

Figure 7 illustrates the unique crooked zone for C_{60}.

For C_{60} itself, the embedding in $^1/_2H_{20}$ with $t = 7$ has an interesting geometrical interpretation[2] in which each of the 20 *hexagons* of C_{60} labels a dimension, and every vertex is labeled by the set of seven hexagons that can reached from it by paths of length at most two. Each vertex is therefore

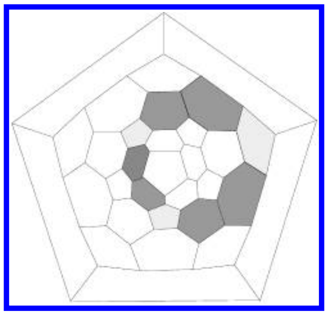

Figure 7. Zones and Petrie circuits in the icosahedral C_{60} fullerene ($n = 60k^2$, $k = 1$): (a) the symmetry-unique crooked (nonalternating) zone and (b) the symmetry-unique Petrie circuit (which corresponds to the symmetry-unique crooked zone in the dual).

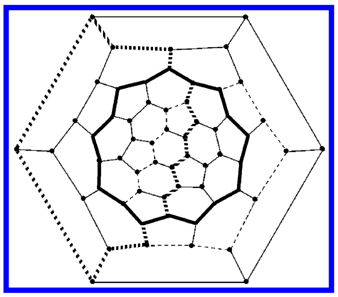

Figure 8. The D_3 C_{60} fullerene isomer that has Petrie circuits with the same number (10), length (18), and pattern of pairwise intersection (in two edges) as the icosahedral isomer. Each of the three orbits of circuits is illustrated by a set of distinguished edges: the unique equatorial circuit (thick solid line), a representative of the orbit of size 3 (hatched line), and of the orbit of size 6 (thin dotted line).

labeled by its nearby chemical environment. The present labeling can be recovered by taking symmetric differences of all vertex labels with that of any one vertex.

(iv) C_n^* with $n = 60k^2$: Fullerene Duals. The embedding has $t = 3k + 2$, and since $D = 5k$, full embedding exists only for $k = 1$ (the omnicapped dodecahedron, the dual of the C_{60} truncated icosahedron). The dimension n_Z is $10k = 2D$. There are $10k$ zones, each of length $18k$ and all alternating. They are again divided into 10 parallel classes.

The correspondence of alternating zones in the dual and Petrie circuits in the fullerene implies that the zigzag structure of icosahedral C_{60} consists of 10 Petrie circuits of length 18, each pair having two common edges. Curiously, there is exactly one other fullerene on 60 vertices (isomer 60:1803, in the notation of ref 16, with D_3 symmetry) that has the same zigzag structure, though neither it nor its dual is fully embeddable (Figure 8). This isomer has three pentagon−pentagon fusions. While in icosahedral C_{60} the I_h group acts transitively on the Petrie circuits, the 10 circuits of 60:1803 are partitioned by the action of the D_3 group into three orbits consisting of the unique equatorial circuit, a set of three circuits of C_2 site symmetry, and a set of six circuits of only C_1 symmetry. The existence of the pair of nonisomorphic 60-vertex fullerenes with the same zigzag structure[18] settles a question raised by a remark of Grünbaum. (‘No example is known to disprove the conjecture that the numbers p_i, together with the specification of the different types of closed Petri-curves and their numbers, determine the combinatorial type of 3-polytopes.’, see ref 19, p 296.)

5. CONCLUDING REMARKS

The present discussion has shown that the zone structure of all I_h fullerenes is described by just two cases. When $j = 0$ and $i = k$, the fullerene has $20k^2$ vertices and $6k$ Petrie circuits of length $10k$; when $i = j = k$, the fullerene has $60k^2$ vertices and $10k$ Petrie circuits of length $18k$. Extension to the chiral I fullerenes will be presented in a forthcoming paper.[20] The zone and zigzag structure for the trivalent T_d-symmetric polyhedra composed of 3- and 6-gons, and the O_h-symmetric polyhedra composed of 4- and 6-gons, can also be described by direct analogy with the I_h fullerenes. Polyhedra of these types are given by the Goldberg−Coxeter construction with the same i, j pairs as the I_h fullerenes and have $n = 4(i^2 + ij + j^2)$, $n = 8(i^2 + ij + j^2)$ vertices, respectively. Their zigzag properties will be discussed elsewhere.

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