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The chirality of icosahedral fullerenes: a comparison of the tripling (leapfrog), quadrupling (chamfering), and septupling (capra) transformations

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Fullerene polyhedra of icosahedral symmetry have the midpoints of their 12 pentagonal faces at the vertices of a macroicosahedron and can be characterized by the patterns of their hexagonal faces on the (triangular) macrofaces of this macroicosahedron. The numbers of the vertices in fullerene polyhedra of icosahedral symmetry satisfy the Goldberg equation $v = 20(h^2 + hk + k^2)$, where h and k are two integers and $0 < h \geqslant k \geqslant 0$ and define a two-dimensional Goldberg vector $\mathbf{G} = (h, k)$. The known tripling (leapfrog), quadrupling (chamfering), and septupling (capra) transformations correspond to the Goldberg vectors (1, 1), (2, 0), and (2, 1), respectively. The tripling and quadrupling transformations applied to the regular dodecahedron generate achiral fullerene polyhedra with the full I_h point group. However, the septupling transformation destroys the reflection operations of the underlying icosahedron to generate chiral fullerene polyhedra having only the I icosahedral rotational point group. Generalization of the quadrupling transformation leads to the fundamental homologous series of achiral fullerene polyhedra having $20n^2$ vertices and Goldberg vectors (n, 0). A related homologous series of likewise achiral fullerene polyhedra having $60n^2$ vertices and Goldberg vectors (n, n) is obtained by applying the tripling transformation to regular dodecahedral C_{20} to give truncated icosahedral C_{60} followed by the generalized operations (as in the case of quadrupling) for obtaining homologous series of fullerenes. Generalization of the septupling (capra) transformation leads to a homologous series of chiral C_{20m} fullerenes with the I point group and Goldberg vectors $\mathbf{G} = (h, 1)$ where $m = h^2 + h + 1$.

KEY WORDS: chirality, icosahedral symmetry, goldberg vectors, tripling transformation, leapfrog transformation, quadrupling transformation, chamfering, setupling transformation, capra transformation

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1. Introduction

Fullerenes are allotropes of carbon based on closed polyhedra containing only pentagonal and hexagonal faces. Each vertex of a fullerene polyhedron contains an sp^2 hybridized carbon atom so that all vertices have degree 3. Elementary topological considerations [1] indicate that all fullerene polyhedra have exactly 12 pentagonal faces but may have any number of hexagonal faces. In fullerenes of icosahedral symmetry (I or I_h) the midpoints of the 12 pentagonal faces form a large regular icosahedron, called the underlying macroicosahedron.

In 1937 Goldberg [2] showed that the numbers v of vertices in polyhedra of icosahedral symmetry can be related to two integers h and $k(0 < h \geqslant k \geqslant 0)$ by the following equation, conveniently called the *Goldberg equation*:

$$v = 20(h^2 + hk + k^2) = 20m. \tag{1}$$

The integers h and k in the Goldberg equation can be considered as components of a two-dimensional vector (h, k), hereafter called the *Goldberg vector,* **G**, and the variable m is the vertex multiplication factor.

The applicability of the Goldberg equation to fullerene polyhedra having icosahedral symmetry was first recognized in 1986 [3, 4] shortly after the discovery of C_{60}. Subsequently, a spiral construction was developed for the construction of such fullerenes of icosahedral symmetry based on the Goldberg equation and corresponding Goldberg vectors [5]. This paper explores the relationships of the Goldberg vector to various ways for the construction of fullerene polyhedra from smaller polyhedra that multiply the number of vertices, and hence the number of carbon atoms in the corresponding fullerene, by a small integer, typically 3, 4, and 7. Our approach indicates quite clearly which fullerenes are achiral with full icosahedral point group symmetry I_h and which fullerenes are chiral with only I point group symmetry.

2. Background

Consider the use of the C_{20} regular dodecahedron to generate fullerene structures by multiplication by factors, m, determined by the Goldberg vector $\mathbf{G} = (h, k)$ and equation (1). The initial regular dodecahedron corresponds to the "identity" Goldberg vector $\mathbf{G} = (1, 0)$. This identity Goldberg vector simply relates to the dual transformation of an underlying macroicosahedron into a dodecahedron. Other transformations of the regular dodecahedron giving larger Goldberg polyhedra can be characterized by the pattern of hexagons in a face of the underlying macroicosahedron. Since an icosahedron has 20 faces, each hexagon in a face of the underlying macroicosahedron corresponds to 20 hexagons in the corresponding fullerene polyhedron. Similarly, since an icosahedron has

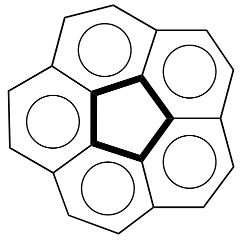

Figure 1. A corannulene unit showing the pentagon edges as bold lines and circles inside the hexagons.

30 edges, each hexagon on an edge corresponds to 30 hexagons in the corresponding fullerene polyhedron.

The fullerenes of interest corresponding to the most stable fullerenes satisfy the so-called *isolated pentagon rule* [6] (IPR) so that each pentagon must be surrounded by five hexagons to form a so-called *corannulene unit* (figure 1). In figure 1 and subsequent figures, the edges of the pentagon in a corannulene unit are bold for clarity and each corannulene hexagon is indicated by an internal circle. In the other figures hexagons without internal circles are not part of any corannulene units.

3. Achiral icosahedral fullerenes (I_h point group)

The two smallest non-identity Goldberg vectors $\mathbf{G_{Le}} = (1, 1) \Rightarrow m = 3$ and $\mathbf{G_Q} = (2, 0) \Rightarrow m = 4$ correspond to the tripling (leapfrog) [7–9] and quadrupling (chamfering) [10–12] transformations, respectively, which are the basis for fundamental processes generating all possible achiral icosahedral fullerenes. When applied to the dodecahedral C_{20} they generate C_{60} and C_{80}, respectively; C_{60} corresponds to the familiar truncated icosahedral fullerene whereas C_{80} is known in the form of some endohedral derivatives [13] such as $La_2@C_{80}$. Figure 2 shows the decoration of a face of the underlying macroicosahedron with hexagons for both the leapfrog and quadrupling transformations.

The leapfrog transformation used to generate C_{60} from C_{20} is characterized by a single hexagon in each face of the underlying macroicosahedron. Since the macroicosahedron has 20 faces, this transformation generates the 20 hexagonal faces found in the C_{60} structure. Furthermore each hexagonal face in C_{60} is part of three corannulene units. The leapfrog transformation adds the minimum number of hexagons to a regular dodecahedron so that no two pentagons have any edges in common. Therefore, C_{60} is the smallest fullerene that satisfies the isolated pentagon rule.

The quadrupling (chamfering) transformation used to generate C_{80} from C_{20} is characterized by a single hexagon on each edge of the underlying macroicosahedron. Since the macroicosahedron has 30 edges, this transformation

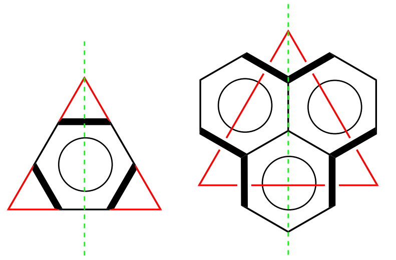

Figure 2. The patterns of hexagons on one of the 20 faces of the underlying macroicosahedron for the leapfrog and quadrupling transformations.

generates the 30 hexagonal faces found in the C_{80} structure. Each of these hexagonal faces of C_{80} is part of two corannulene units. In both the tripling and quadrupling transformations the altitudes of the (triangular) faces of the underlying macroicosahedron (dashed lines in figure 2) are symmetry planes so that these transformations, as well as combinations thereof, preserve the full I_h symmetry of the original dodecahedron leading to achiral polyhedra. In the leapfrog transformation the altitudes of the faces of the underlying macroicosahedron bisect the edges of the pentagonal faces. However, in the quadrupling transformation these altitudes pass through the pentagonal vertices.

The quadrupling transformation can be generalized to a series of analogous transformations with n hexagons on each edge of the underlying macroicosahedron. This generates the fundamental homologous series of C_{20n^2} fullerenes described by the Goldberg vectors $\mathbf{G} = (n, 0)$. One of the 20 macroicosahedral faces of each of the first three members of the fundamental homologous series is depicted in figure 3. Again the altitudes of the macroicosahedral faces (dashed lines in figure 3) generate a symmetry plane so that these structures have full icosahedral (I_h) symmetry. These altitudes pass through the pentagonal vertices as is the case for the simple quadrupling transformation.

A second homologous series of fullerenes of general formula C_{60n^2} with the Goldberg vectors (n, n) can be obtained by first applying the leapfrog transformation to the regular dodecahedron followed by the operations of the fundamental homologous series analogous to those in figure 3. This effectively corresponds to applying the operations of the fundamental homologous series to the truncated icosahedral C_{60} rather than to the dodecahedral C_{20} so that this homologous series of icosahedral fullerenes has the general formula C_{60n^2}. One of the 20 macroicosahedral faces of the first two members of this homologous series beyond C_{60}, namely C_{240} and C_{540} with Goldberg vectors (2, 2) and (3, 3), respectively, is depicted in figure 4. The altitudes of the macroicosahedral faces

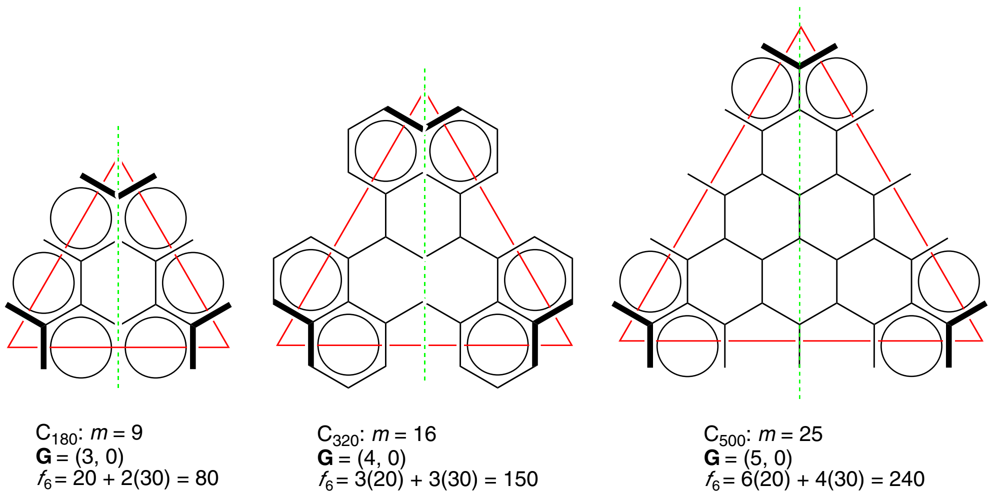

Figure 3. The patterns of hexagons on a face of the underlying macroicosahedron for the first three members of the fundamental homologous series C_{20n^2} of icosahedral fullerenes [$\mathbf{G} = (n, 0)$; $m = n^2$].

(dashed lines in figure 4) represent symmetry planes so that full icosahedral symmetry I_h is preserved leading to an achiral structure. These altitudes bisect edges of the pentagonal faces as in the simple leapfrog transformation. The molecular orbitals of the members of this C_{60n^2} homologous series have been of some interest [14, 15].

4. Chiral icosahedral fullerenes (I point group)

The smallest Goldberg vector not leading to an achiral fullerene is $\mathbf{G}_{Ca} = (2, 1)$ with a vertex multiplication factor of seven corresponding to the recently discovered [9, 16, 17] septupling or capra transformation. Figure 5 shows the pattern of hexagons on a face of the underlying macroicosahedron after a septupling transformation. The septupling transformation has the following distinctive features:

(1) It is the simplest transformation that preserves icosahedral rotational symmetry but destroys all reflection operations thereby leading to the chiral point group *I*. Note that the altitudes of the triangular faces are not symmetry planes.

(2) Each hexagon in the polyhedron resulting from the septupling transformation is part of exactly one corannulene unit. There are thus no "extra" hexagons that do not belong to some corannulene unit.

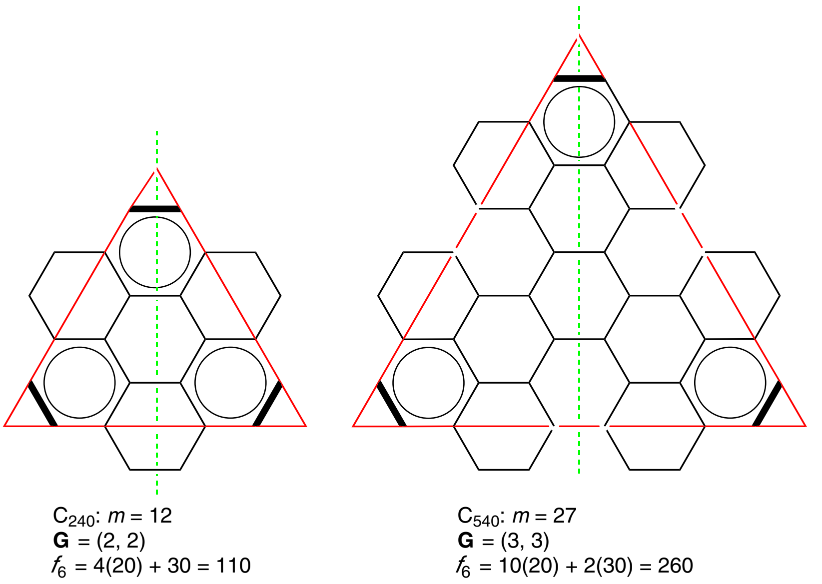

Figure 4. The patterns of hexagons on a face of the underlying macroicosahedron for the second and third members of the homologous series C_{60n^2} of icosahedral fullerenes [$\mathbf{G} = (n, n)$; $m = 3n^2$].

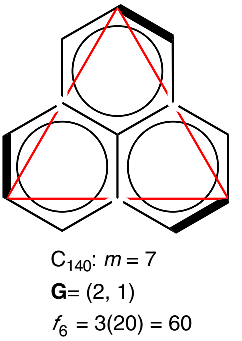

Figure 5. The patterns of hexagons on a face of the underlying macroicosahedron for the septupling (capra) transformation.

Since there are three hexagons in each face of the underlying macroicosahedron of the septupling transformation, the C_{140} icosahedral polyhedron generated from the C_{20} dodecahedron by the septupling process necessarily has 3(20) = 60 hexagonal faces.

The septupling transformation can be generalized to give a homologous series of chiral icosahedral fullerenes of general formula C_{20m}, where $m = h^2+$

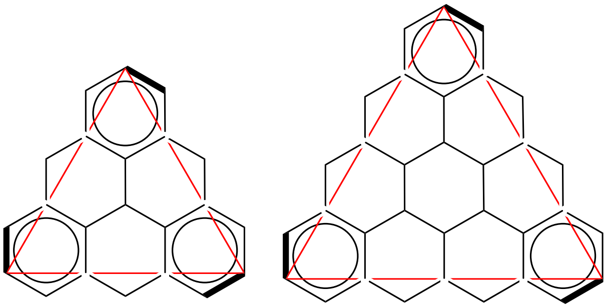

Figure 6. The patterns of hexagons on a face of the underlying macroicosahedron for the second and third members of the chiral homologous series C_{20m} of icosahedral fullerenes [$\mathbf{G} = (h, 1)$; $m = h^2 + h + 1$].

$h + 1$ (h integer) with a Goldberg vector $\mathbf{G} = (h, 1)$. The multiplication factors m found in this series are $m = 7, 13, 21, 31, 43, 57, 73, 91, 111, 133, \ldots$ The patterns of hexagons on the macroicosahedral faces of the second and third members of this chiral homologous series are given in figure 6.

5. Summary and outlook

The analysis in this paper describes the patterns of hexagons on the faces of the underlying macroicosahedron for the simplest series of fullerene polyhedra having icosahedral symmetry. This includes all of the possible achiral fullerenes having the full icosahedral point group I_h and Goldberg vectors of the types $\mathbf{G} = (n, 0)$ and (n, n) using the tripling (leapfrog) and quadrupling (chamfering) transformations. In addition a homologous series of chiral fullerenes having the icosahedral rotational group I and the Goldberg vectors $\mathbf{G} = (n, 1)$ is generated based on the septupling (capra) transformation. Similar methods to those outlined in this paper could undoubtedly be developed for generating larger chiral fullerenes having icosahedral rotational symmetry I and Goldberg vectors $\mathbf{G} = (h, k)(h \neq k; h \geqslant 2; k \geqslant 2)$.

Acknowledgments

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References

[1] R. B. King, *Applications of Graph Theory and Topology in Inorganic Cluster and Coordination Chemistry* Section 11.4 (CRC Press, Boca Raton, Florida, 1993).
[2] M. Goldberg, Tohoku Math. J. 443 (1937) 194.
[3] D. J. Klein, W. A. Seitz and T. G. Schmalz, Nature 323 (1986) 703.
[4] P. W. Fowler, Chem. Phys. Lett. 131 (1986) 444.
[5] P. W. Fowler and K. M. Rogers, J. Chem. Inf. Comput. Sci. 41 (2001) 108.
[6] X. Liu, T. G. Schmalz and D. J. Klein, Chem. Phys. Lett. 188 (1992) 550.
[7] P. W. Fowler and D. B. Redmond, Theor. Chim. Acta 83 (1992) 367.
[8] M. V. Diudea, P. E. John, A. Graovac, M. Primorac and T. Pisanski, Croat. Chem. Acta 76 (2003) 153.
[9] M. V. Diudea, Forma 19 (2004) 131.
[10] P. W. Fowler, J. E. Cremona and J. I. Steer, Theor. Chim. Acta 73 (1988) 1.
[11] A. Deza, M. Deza and V. P. Grishukin, Discrete Math. 192 (1988) 41.
[12] A. Ceulemans, R. B. King, S. A. Bovin, K. M. Rogers, A. Troisi and P. W. Fowler, J. Math. Chem. 26 (1999) 101.
[13] M. Moriyama, T. Sano, A. Yabe, K. Yamamoto, K. Kobayashi, S. Nagase, T. Wakahara and T. Akesaka, Chem. Lett. (2000) 524.
[14] A. C. Tang, F. Q. Huang, Q. S. Li and R. Z. Liu, Chem. Phys. Lett. 227 (1994) 579.
[15] R. B. King, Mol. Phys. 92 (1997) 293.
[16] M. V. Diudea, Stud. Univ. Babeş-Bolyai Chemia 48 (2003) 3.
[17] M. V. Diudea, J. Chem. Inf. Model. 45 (2005) 1002.