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Symmetry of a toroidal fullerene

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Suppose G is a molecular graph with atoms labeled by numbers 1, 2, … n. The adjacency matrix A = [a_{ij}] of G is a 0-1 matrix with a_{ij} = 1 if and only if there is a bond connecting atoms i and j. A Euclidean graph associated to a molecule M is defined by a weighted graph with the adjacency matrix D = [d_{ij}], where for $i \neq j$ d_{ij} is the Euclidean distance between the nuclei i and j. In this matrix d_{ii} can be taken as zero if all the nuclei are equivalent. In this work a new method is presented by which it is possible to calculate the symmetry of fullerenes.

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1. Introduction

Symmetry generally conveys two primary meanings. The first is an imprecise sense of harmonious or aesthetically pleasing proportionality and balance such that it reflects beauty or perfection. The second meaning is a precise and well-defined concept of balance or "patterned self-similarity" that can be demonstrated or proved according to the rules of a formal system: by geometry, through physics or otherwise.

Since the discovery of the first fullerene molecule in 1985, the fullerenes have been objects of interest to scientists all over the world [1]. The name fullerene was given to cubic carbon molecules in which the atoms are arranged on a sphere in pentagons and hexagons. Many properties of fullerene molecules can be studied using mathematical tools and results [2].

Let F be a fullerene molecule with exactly p pentagons, h hexagons, n carbon atoms and m bonds. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is n, the number of edges is m = 3/2n and the number of faces is f = 2m = 3n This implies that such molecules made up entirely of n carbon atoms and having 2m hexagonal faces.

In algebra, a group action is a way of describing symmetries of objects using groups. The essential elements of the object are described by a set and the symmetries of the object are described by the symmetry group of this set, which consists of bijective transformations of the set. In this case, the group is also called a permutation group. A group action is a flexible generalization of the notion of a symmetry group in which every element of the group "acts" like a bijective transformation (or" symmetry") of some set, without being identified with that transformation. This allows for a more comprehensive description of the symmetries of an object, such as a polyhedron by allowing the same group to act on several different sets, such as the set of vertices ,the set of edges and the set of faces of the polyhedron. If *G* is a group and *X* is a set then a group action may be defined as a group homomorphism from *G* to the symmetric group of *X* .The action assigns a permutation of *X* to each element of the group in such a way that i) the permutation of *X* assigned to the identity element of *G* is the identity transformation of *X*; ii) the permutation of *X* assigned to a product *gh* of two elements of the group is the composite of the permutations assigned to *g* and *h*.

A permutation matrix is a square matrix whose entries are all 0's and 1's, with exactly one 1 in each row and exactly one 1 in each column. Examples of these matrices are as follows:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Multiplying any matrix A by a permutation matrix P on the left has the effect of rearranging the rows of A. The identity I is a permutation matrix, every elementary matrix is a permutation matrix and product of elementary matrices is again a permutation matrix. In fact, every permutation matrix is a product of elementary matrices, because you can arrange the rows in any order by a sequence of two-row exchanges. Finally, the inverse of a permutation matrix is the same as its transpose: $P^{-1} = P^{T}$.

Randic [3,4] showed that a graph can be depicted in different ways such that its point group symmetry or three dimensional perception may differ, but the underlying connectivity symmetry is still the same as characterized by the automorphism group of the graph. However, the molecular symmetry depends on the coordinates of the various nuclei which relate directly to its three dimensional geometry. Although the symmetry as perceived in graph theory by the automorphism group of the graph and the molecular group are quite different, it showed by Balasubramanian [5-10] that the two symmetries are connected.

2. Main results

Suppose G is a molecular graph with atoms labeled by numbers 1, 2, … n. The adjacency matrix $A = [a_{ij}]$ of G is a 0-1 matrix with $a_{ij} = 1$ if and only if there is a bond connecting atoms i and j. A Euclidean graph associated to a molecule M is defined by a weighted graph with the adjacency matrix $D = [d_{ij}]$, where for $i \neq j$ d_{ij} is the Euclidean distance between the nuclei i and j. In this matrix d_{ii} can be taken as zero if all the nuclei are equivalent.

Our computations of the symmetry properties of molecules were carried out with the use of GAP [11]. GAP contains several functions for working with finite groups. In this paper, we use freely these functions and the reader is encouraged to consult the manual of GAP, as well as papers by Ashrafi and his co-workers [12-16]. We also encourage the readers to consult papers [17-30] for background material as well as basic computational techniques.

Consider the equation $(P_\sigma)^t A P_\sigma = A$, where A is the adjacency matrix of the weighted graph G. Suppose $Aut(G) = \{\sigma_1, \sigma_2, \ldots, \sigma_m\}$. The matrix $S_G = [s_{ij}]$, where $s_{ij} = \sigma_i(j)$ is called a solution matrix for G. Clearly, for computing the automorphism group of G, it is enough to calculate a solution matrix for G.

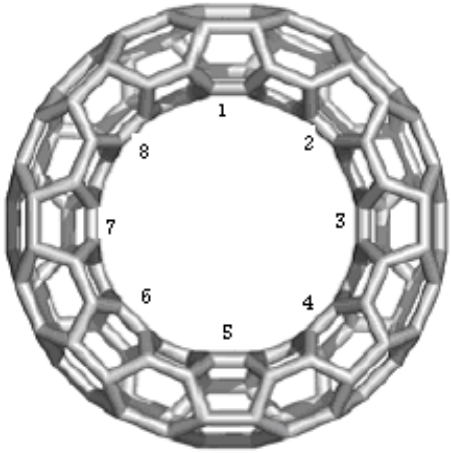

Fig. 1. A Polyhex Toroidal Fullerene.

Suppose G is a group and N is a subgroup of G. N is called a normal subgroup, if it is invariant under conjugation; that is, for each element n in N and each g in G, the element gng^{-1} is still in N. Normal subgroups are important because they can be used to construct quotient groups from a given group. A semidirect product describes a particular way in which a group can be put together from two subgroups, one of which is normal. Let G be a group, N a normal subgroup of G and H a subgroup of G. We say that G is a semidirect product of N and H, or that G splits over N, if every element of G can be written in one and only one way as a product of an element of N and an element of H.

Suppose L is the 2-dimensional lattice of a Toroidal fullerene containing p vertical zig-zag and q row, Fig. 2. It is clear that p is even. Put

a = (1, 2, …, p/2),
b = (2 , p/2)(3 , p/2 – 1)(4 , p/2 – 2)…(p/4 , p/4 + 2),
(2 , p/2)(3 , p/2 – 1)(4 , p/2 –2)…((p/2 + 1)/2,(p/2 + 3)/2),

when p/2 is even or odd, respectively. Then the group H generated by a and b is a subgroup of the symmetry group of a polyhex carbon nanotorus V. But a vertical plane determines a symmetry element c of V such that $c \notin H$. Consider V = <H,c> then V is the symmetry of the carbon polyhex nanotorus. Since |H| = 1/2|V|, H is a normal subgroup of V. This implies that V is a semidirect product of H by a cyclic group of order 2. Thus the group V of the symmetry of a polyhex nanotorus is a semidirect product of $D_{p/2}$ by Z_2, where Z_2 is the cyclic group of order 2.

References

[1] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R. E. Smalley, Nature, **318**, 162 (1985).
[2] P. W. Fowler, D. E. Manolopoulos, An Atlas of Fullerenes, Oxford Univ. Press, Oxford, 1995.
[3] M. Randic, Chem. Phys. Letters **42**, 283 (1976).
[4] M. Randic, J. Chem. Phys. **60**, 3920 (1974).
[5] K. Balasubramanian, Chem. Phys. Letters **232**, 415 (1995).
[6] K. Balasubramanian, J. Chem. Phys. **72**, 665 (1980).
[7] K. Balasubramanian, Intern. J. Quantum Chem. **21**, 411 (1982).
[8] K. Balasubramanian, Chem. Rev. **85**, 599 (1985).
[9] K. Balasubramanian, Studies Phys. Theor. Chem. **23**, 149 (1983).
[10] K. Balasubramanian, J. Chem. Phys. **75**, 4572 (1981).
[11] M. Schönert, H. U. Besche, Th. Breuer, F. Celler, B. Eick, V. Felsch, A. Hulpke, J. Mnich, W. Nickel, G. Pfeiffer, U. Polis, H. Theißen, A. Niemeyer, GAP, Groups, Algorithms and Programming, Lehrstuhl De für Mathematik, RWTH, Aachen, 1995.
[12] A. R. Ashrafi, M. Hamadanian, Croat. Chem. Acta **76**, 299 (2003).
[13] M. Hamadanian, A. R. Ashrafi, Croat. Chem. Acta **76**, 305 (2003).
[14] A. R. Ashrafi, Chem. Phys. Letters, **406**, 75 (2005).
[15] A. R. Ashrafi, M. R. Ahmadi, Cent. Eur. J. Chem., **3**, 647 (2005).
[16] A. R. Ashrafi, MATCH Commun. Math. Comput. Chem., **53**, 161 (2005).
[17] A. R. Ashrafi, M. Ghorbani, MATCH Commun. Math. Comput. Chem., **59**, 595 (2008).
[18] A. R. Ashrafi, M. Ghorbani, M. Jalali, J. Theor. Comput. Chem., **7**, (2212008).
[19] H. Yousefi-Azari, B. Manoochehrian, A. R. Ashrafi, Appl. Math. Lett., **21**, 624 (2008).
[20] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, Discrete Appl. Math. **156**, 1780 (2008).
[21] A. R. Ashrafi, M. Ghorbani, Fullerenes, Nanotubes

and Carbon Nanostructures, **18**, 198 (2010).
[22] A. R. Ashrafi, M. Ghorbani, Jalali, Fullerenes, Nanotubes and Carbon Nanostructures, **18**, 107 (2010).
[23] A. R. Ashrafi, M. Ghorbani, J. Serb. Chem. Soc., **75**, 368 (2010).
[24] A. R. Ashrafi, F. Rezaei, A. Loghman, Revue Roumaine de chimie, **54**, 823 (2009).
[25] A. R. Ashrafi, H. Shabani, Optoelectron. Adv. Mater.- Rapid Commun., **3**(4), 356 (2009).
[26] A. R. Ashrafi, M. Ghorbani, Optoelectron. Adv. Mater.- Rapid Commun., **3**(6), 596 (2009).
[27] A. R. Ashrafi, M. Ghorbani, M. Jalali, Optoelectron. Adv. Mater.- Rapid Commun., **3**(8), 823 (2009).
[28] A. R. Ashrafi, M. Ghorbani, M. Hemmasi, Dig. J. Nanomat. Bios., **4,** 483 (2009).
[29] M. J. Nadjafi-Arani, G. H. Fath-Tabar, A. R. Ashrafi, Appl. Math. Lett., **22**, 1838 (2009).
[30] A. R. Ashrafi, A. Karbasioun, Dig. J. Nanomat. Bios., **4**, 663 (2009).

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