

Computing symmetry group of fullerene C_{80}

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Fullerene era was started with the discovery of stable cluster of C_{60} fullerene by Harry Kroto in 1895. An Euclidean graph associated with a molecule is defined by a weighted graph with adjacency matrix $M = [d_{ij}]$, 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. Otherwise, one may introduce different weights for distinct nuclei. The aim of this paper is to compute the automorphism group of the Euclidean graph of a big fullerene C_{180} . We prove this fullerene graph is isomorphic with I_h point group.

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1. Introduction

An object is called symmetrical if some movement or operation leaves the object in a position indistinguishable from its original position. The symmetry of molecules and solids is a very powerful tool for developing and understanding of bonding and physical properties used to predict the nature of molecular orbitals. Chemists and physicists classify molecules in terms of their symmetry. It is of some value to recognize that all molecules that have the same basic "shape" share a number of common properties.

A fullerene is any molecule composed entirely of carbon and its era was started in 1985 with the discovery of a stable C_{60} cluster^{1,2}. Let F be a fullerene graph with exactly p , h , n and m pentagons, hexagons, carbon atoms and bonds between them, respectively. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is $n = (5p+6h)/3$, the number of edges is $m = (5p+6h)/2 = 3/2n$ and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $(5p+6h)/3 - (5p+6h)/2 + p + h = 2$, and therefore $p = 12$, $v = 2h + 20$ and $e = 3h + 30$. This implies that such molecules made up entirely of n carbon atoms and having 12 pentagonal and $(n/2 - 10)$ hexagonal faces, where $n \neq 22$ is a natural number equal or greater than 20.

An Euclidean graph is a weighted graph related to a molecule 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. Otherwise, one may introduce different weights for different nuclei. By symmetry we mean the automorphism group symmetry of Euclidean graph of molecule under consideration. Here, an automorphism of a weighted graph G is a permutation g of the vertex set of G with the property that: (i) for any vertices u and v , $g(u)$ and $g(v)$ are adjacent if and only if u is adjacent to v ; (ii) for every vertex v and edge e , $w(g(v)) = w(v)$. The set of all

automorphisms of a graph G , with the operation of composition of permutations, is a permutation group on $V(G)$, denoted $\text{Aut}(G)$, see for more details [3-15].

Balasubramanian [16-23] considered the Euclidean matrix of a chemical graph to find its symmetry. He proved that for computing the symmetry of a molecule, it is sufficient to solve the matrix equation $P^tEP = E$, where E is the Euclidean matrix of the molecule under consideration and P varies on the set of all permutation matrices with the same dimension as E . He computed the Euclidean graphs and automorphism group for benzene, eclipsed and staggered forms of ethane and eclipsed and staggered forms of ferrocene.

2. Results and discussion

If K is any subset in a group G , we designate by $\langle K \rangle$ the subgroup consisting of all finite products $x_1x_2 \dots x_n$, where each x_i is an element of K or the inverse of an element of K . We say that $\langle K \rangle$ is generated by K . It is easy to see that $\langle K \rangle$ is contained in any subgroup of G which contains K . The dihedral group D_n is the symmetry group of an n -sided regular polygon for $n > 1$. These groups are one of the most important classes of finite groups currently applicable in chemistry. For example D_3 , D_4 , D_5 and D_6 point groups are dihedral groups. One group presentation for D_n is $\langle x, y \mid x^n = y^2 = e, yxy = x^{-1} \rangle$. This means that D_n is generated by a two elements set $\{x, y\}$ with the condition $x^n = y^2 = 1$ and $yxy = x^{-1}$. The computations of the symmetry properties of molecules we carried out by the aid of GAP [11]. GAP stands for Groups, Algorithms and Programming. The name was chosen to reflect the aim of the system, which is a group theoretical software for solving computational problems in computational group theory. This software was constructed by GAP's team in Aachen. GAP is a free and extendable software package. The term extendable means

that you can write your own programs in the GAP language, and use them in just the same way as the programs which form part of the system (the "library"). More information on the motivation and development of GAP to date can be found on GAP web page on <http://www.gap-system.org>. GAP contains a large library of functions, which are important for the calculations of this paper. In this paper the GAP functions for computing permutation matrices from permutations and vice versa are crucial for our calculations.

For a permutation σ on n objects, the corresponding permutation matrix is an $n \times n$ matrix P_σ given by $P_\sigma = [x_{ij}]$, $x_{ij} = 1$ if $i = \sigma(j)$ and 0 otherwise. It is easy to see that $P_\sigma P_\tau = P_{\sigma\tau}$, for any two permutations σ and τ on n objects, and so the set of all $n \times n$ permutation matrices is a group isomorphic to the symmetric group S_n on n symbols. It is a well-known fact that a permutation σ of the vertices of a graph G belongs to its automorphism group if it satisfies $P_\sigma^t A P_\sigma = A$, where A is the adjacency matrix of G .

In mathematics, groups are often used to describe symmetries of objects. Here our notations are standard and mainly taken from [24-34].

The isolated pentagon rule (IPR) is now widely accepted as a general rule for determining the stability of all-carbon fullerene cages composed of hexagons and pentagons. The graph of fullerene C_{80} , depicted in figure 1 is non-IPR and in the following theorem we compute its symmetry group.

Theorem. The symmetry group G of fullerene C_{80} is isomorphic to dihedral group D_{20} .

Proof. By using concept of symmetry one can see that the generators of fullerene graph C_{80} are as follows:

$X = (2,16)(4,14)(5,18)(6,17)(7,20)(8,19)(9,36)(10,35)(11,34)(12,33)(13,49)(15,51)(21,24)(22,23)(25,37)(26,52)(27,39)(28,50)(29,54)(30,53)(31,56)(32,55)(38,40)(41,42)(43,44)(45,60)(46,59)(47,58)(48,57)(62,67)(63,66)(65,77)(68,80)(69,73)(70,79)(71,78)(72,76)(74,75);$

$Y = (1,65)(2,66)(3,68)(4,67)(5,48)(6,45)(7,46)(8,47)(9,42)(10,43)(11,44)(12,41)(13,69)(14,70)(15,72)(16,71)(17,36)(18,33)(19,34)(20,35)(21,30)(22,31)(23,32)(24,29)(25,73)(26,74)(27,76)(28,75)(37,77)(38,78)(39,80)(40,79)(49,61)(50,62)(51,64)(52,63)(53,60)(54,57)(55,58)(56,59);$

By using GAP program one can see that $X^2 = Y^2 = (XY)^{10} = 1$ and $X^{-1}(XY)X = (XY)^{-1}$ and so this symmetry group is isomorphic with a dihedral group of order 20, namely D_{20} .

A GAP program for computing symmetry group of fullerene C_{180}

```
f:=function(x,y)
local g,d,r,t;
g:= Group(x,y);
d:=Elements(g);
t:=ConjugacyClassesSubgroup(g);
r:=Length(d);
return;
end;
```

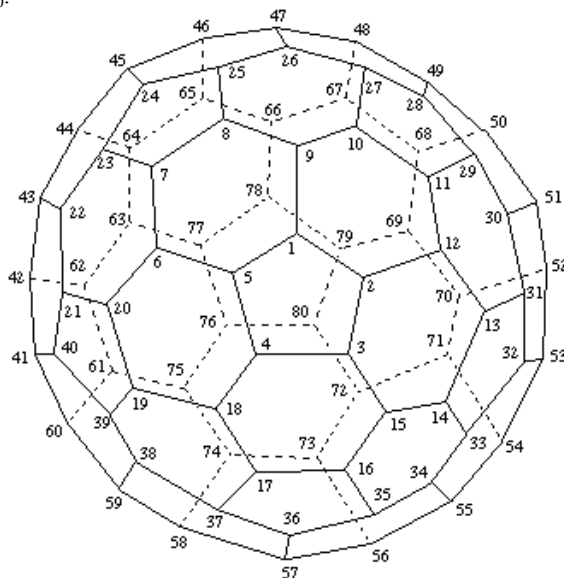


Fig. 1. Fullerene graph C_{80} .

References

- [1] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R.E. Smalley *Nature* **318**, 162 (1985).
- [2] H. W. Kroto, J. E. Fichier, D. E Cox, *The Fullerene*, Pergamon Press, New York, 1993.
- [3] M. Damnjanović, I. Milošević, T. Vuković, R. Sredanović, *J. Phys. A: Math. Gen.* **32**, 4097 (1999).
- [4] I. Milošević, R. Živanović, M. Damnjanović **38**, 4445 (1997).

- [5] G. S. Ezra, Symmetry Properties of Molecules, Lecture Notes in Chemistry **28**, Springer, 1982.
- [6] J. S. Lomont, Applications of Finite Groups, Academic Press Inc., New York, **1959**.
- [7] M. V. Diudea, Bull. Chem. Soc. Japan **75**, 487 (2002).
- [8] M. V. Diudea, MATCH Commun. Math. Comput. Chem. **45**, 109 (2002).
- [9] M. V. Diudea, P.E. John, MATCH Commun. Math. Comput. Chem. **44**, 103 (2001).
- [10] D. J. Higham, N. J. Higham, MATLAB Guide, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA **2000**.
- [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, MATCH Commun. Math. Comput. Chem. **53**, 161 (2005).
- [13] M. Randic, J. Chem. Phys. **60**, 3920 (1974).
- [14] M. Randic, Chem. Phys. Letters **42**, 283 (1976).
- [15] M. Randic, M. I. Davis, Int. J. Quant. Chem. **26**, 69 (1984).
- [16] K. Balasubramanian, J. Chem. Phys. **72**, 665 (1980).
- [17] K. Balasubramanian, J. Chem. Phys. **75**, 4572 (1981).
- [18] K. Balasubramanian, Int. J. Quant. Chem. **21**, 411 (1982).
- [19] K. Balasubramanian, Studies Phys. Theor. Chem. **23**, 149 (1983).
- [20] K. Balasubramanian, Chem. Rev. **85**, 599 (1985).
- [21] K. Balasubramanian, Chem. Phys. Letters **232**, 415 (1995).
- [22] K. Balasubramanian, J. Phys. Chem. **108**, 5527 (2004).
- [23] K. Balasubramanian, Chem. Phys. Letters **391**, 69 (2004).
- [24] A. R. Ashrafi, Chem. Phys. Letters **406**, 75 (2005).
- [25] A. R. Ashrafi, M.R. Ahmadi, Cent. Eur. J. Chem. **3**, 647 (2005).
- [26] M. Ghorbani, A. R. Ashrafi, M. Hemmasi, Optoelectron. Adv. Mater. – Rapid Comm. **3**(12), 1306 (2009).
- [27] A. R. Ashrafi, M. Ghorbani, Fullerenes, Nanotubes and Carbon Nanostructures, 2009 Accepted.
- [28] A. R. Ashrafi, M. Ghorbani, M. Jalali, Optoelectron. Adv. Mater. – Rapid Comm. **3**(8), 823 (2009).
- [29] A. R. Ashrafi, M. Ghorbani, Optoelectron. Adv. Mater. – Rapid Comm. **3**(6), 596 (2009).
- [30] M. A. Hosseinzadeh, M. Ghorbani, J. Optoelectron. Adv. Mater. **11**(11), 1671 (2009).
- [31] A. R. Ashrafi, M. Ghorbani, M. Jalali, Ind. J. Chem. **47A**, 535 (2008).
- [32] M. Ghorbani, A. R. Ashrafi, J. Comput. Theor. Nanosci. **3**, 803 (2006).
- [33] A. R. Ashrafi, M. Jalali, M. Ghorbani, M. V. Diudea, MATCH Commun. Math. Comput. Chem. **60**(3), 905 (2008).
- [34] M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures **3**(4), 269 (2008).
- [35] A. R. Ashrafi, M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures **3**(4), 245 (2008).

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