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A New Method for Computing The Symmetry of Big Fullerene C_{180}

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It is well known that the symmetry operators in the point group of a molecule always commute with its Hamiltonian operator. So the group H of molecular graph must contain the point group H of the graph. It is also well-known fact that the set of all permutation matrices fixed by Hamiltonian constitute the full automorphism group of the molecular graph under consideration. These facts were used and some new algorithm to compute the symmetry of fullerene C_{180}.

Key Words: Symmetry, Fullerene C_{180}.

INTRODUCTION

One of the main branch of chemistry, the organic chemistry is devoted to the study of C-C bonds and different molecules originating from them. Carbon is only tetravalent element able to produce long homoatomic stable chains or different four-regular nets. The discovery of buckyballs, C_{60}, which has a nanometer scale hollow spherical structure in 1985 by Kroto *et al.*[1] revealed a new form of existence of carbon element other than graphite, diamond and amorphous carbon. Fullerenes with a wide range of numbers of carbon atoms have been produced[2]. Isomers with 60, 70, 76, 78 and 84 atoms have been produced in sufficient quantity to be characterized by NMR spectroscopy.

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.

Balasubramanian[3-7] in some leading papers considered the Euclidean matrix of a chemical graph to find its symmetry. He proved that for computing the symmetry of a molecule, it is enough to solve the matrix equation P^tEP

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= 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 its automorphism group for benzene, eclipsed and staggered forms of ethane and eclipsed and staggered forms of ferrocene[3].

COMPUTATIONAL DETAILS

The present computations of the symmetry properties of molecules were carried out with the use of GAP[8]. 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. The motivation for this study is outlined[9] and the reader is encouraged to consult this paper for background material as well as basic computational techniques.

The techniques discussed here are useful in finding symmetry of molecules. We begin with two important results that, in certain situations, are very effective at establishing automorphisms of Euclidean graphs[10].

Lemma 1: Suppose $A = [a_{ij}]$ and $B = [b_{ij}]$ are two matrices and P is a permutation matrix related to the permutation σ. If $B = PAP^t$, $\sigma(i) = r$ and $\sigma(j) = s$, then $a_{rs} = b_{ij}$.

Lemma 2: Let $A = [a_{ij}]$ be the adjacency matrix of a weighted graph and σ be a permutation such that $A = PAP^t$ and σ maps $i_1 \rightarrow j_1$, $i_2 \rightarrow j_2, \ldots, i_t \rightarrow j_t$. Then, we have:

$$\begin{bmatrix} a_{i_1 i_1} & \cdots & a_{i_1 i_t} \\ \vdots & & \vdots \\ a_{i_t i_1} & \cdots & a_{i_t i_t} \end{bmatrix} = \begin{bmatrix} a_{j_1 j_1} & \cdots & a_{j_1 j_t} \\ \vdots & & \vdots \\ a_{j_t j_1} & \cdots & a_{j_t j_t} \end{bmatrix}$$

Lemma 3: Let G be an Euclidean graph, $A = \mathrm{Aut}(G)$ and $O_1, O_2, \ldots, O_t$ are orbits of the action of A on the vertices of G. Then for every $\alpha \in A$ and every positive integer i, $1 \leq i \leq t$, $\alpha(O_i) = O_i$.

RESULTS AND DISCUSSION

Using the above mentioned results, Lemmas 1-3, a MATLAB program for computing the symmetry of big fullerene C_{180} is prepared*.

*The Cartesian coordinates of these fullerenes is taken from the homepage of Dr. Steffen Weber at http://jcrystal.com/steffenweber/. This program is available upon the request from authors.

A MATLAB Program is applied to compute the symmetry of fullerenes C_{180}. Suppose A is a solution matrix computed by present program. To compute the automorphism group of Euclidean graph of fullerenes under consideration, we need a GAP program as follows:

```
B:=[];
N:=Size(A);
        for i in [1,2..N] do
           d:=PermListList(A[1],A[i]);
            Add(B,d);
        od;
  G:=AsGroup(B);
  GeneratorsOfGroup(G);
```

Using these programs, a generating set calculated for the automorphism group of fullerenes C_{180}. Suppose {X, Y, Z} is a generating set for the automorphism group C_{180}. The present calculations give the following permutations as a generating set for the symmetry group of this fullerene:

X_{180}: (2,5) (3,4) (6,14) (7,13) (8,12) (9,11) (10,15) (16,29) (17,28) (18,27) (19,26) (20,30) (21,24) (22,23) (32,35) (33,34) (36,56) (37,60) (38,59) (39,58) (40,57) (41,51) (42,55) (43,54) (44,53) (45,52) (47,50) (48,49) (61,63) (64,66) (67,85) (68,86) (69,87) (70,88) (71,89) (72,90) (73,81) (74,80) (75,79) (76,84) (77,83) (78,82) (92,93) (94,95) (97,111) (98,110) (99,109) (100,114) (101,113) (102,112) (103,117) (104,116) (105,115) (106,120) (107,119) (108,118) (121,133) (122,135) (123,134) (124,137) (125,136) (126,138) (127,147) (128,146) (129,145) (130,150) (131,149) (132,148) (139,141) (142,144) (151,153) (154,156) (157,177) (158,176) (159,175) (160,180) (161,179) (162,178) (163,171) (164,170) (165,169) (166,174) (167,173) (168,172).

Y_{180}: (1,2) (3,5) (6,19) (7,18) (8,17) (9,16) (10,20) (11,14) (12,13) (21,29) (22,28) (23,27) (24,26) (25,30) (31,35) (32,34) (36,51) (37,55) (38,54) (39,53) (40,52) (41,46) (42,50) (43,49) (44,48) (45,47) (57,60) (58,59) (61,67) (62,68) (63,69) (64,70) (65,71) (66,72) (73,85) (74,86) (75,87) (76,88) (77,89) (78,90) (79,81) (82,84) (91,109) (92,111) (93,110) (94,113) (95,112) (96,114) (97,123) (98,122) (99,121) (100,126) (101,125) (102,124) (103,129) (104,128) (105,127) (106,132) (107,131) (108,130) (115,117) (118,120) (134,135) (136,137) (139,145) (140,146) (141,147) (142,148) (143,149) (144,150) (151,175) (152,176) (153,177) (154,178) (155,179) (156,180) (157,171) (158,170) (159,169) (160,174) (161,173) (162,172) (163,165) (166,168).

Z_{180}: (1,6,50,41,18) (2,7,46,42,19) (3,8,47,43,20) (4,9,48,44,16) (5,10,49,45, 17) (11,12,13,14,15) (21,30,53,31,40) (22,26,54,32,36) (23,27, 55,33,37) (24,28,51,34,38) (25,29,52,35,39) (56,60,59,58,57) (61,91,117, 111,68) (62,92,115,109,67) (63,93,116,110,69) (64,94,119,113,70) (65,95,

120,114,72) (66,96,118,112,71) (73,85,103,164,129) (74,87,105,165,128) (75,86,104,163,127) (76,89,107,168,132) (77,88,106,166,131) (78,90, 108,167,130) (79,99,170,159,123) (80,98,171,157,122) (81,97,169, 158,121) (82,102,174,161,126) (83,101,172,162,125) (84,100,173,160,124) (133,145,175,151,139) (134,146,177,152,141) (135,147,176,153,140) (136,148,179,154,143) (137,149,178,155,142) (138,150,180,156,144).

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