OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 4, No. 9, September 2010, p. 1423 - 1426

Computing symmetry of fullerene molecule C_{84}

D. SALMANI[a], A. TAATIAN[a], M. FAGHANI[b], M. GHORBANI[c,*]
[a]*School of Management, University of Tehran, Tehran, I. R. Iran*
[b]*Department of Mathematics, Payam-e-Noor University, Tehran, I. R. Iran*
[c]*Department of Mathematics, Faculty of Science, Shahid Rajaee, Teacher Training University, Tehran, 16785-136, I. R. Iran*

Suppose M is a molecule and G is its molecular graph with atoms labeled by numbers 1, 2, … n. Define the adjacency matrix A = [a_{ij}] of G to be a 0-1 matrix with this property that a_{ij} = 1 if and only if the there is a bond connecting atoms i and j. An Euclidean graph associated to 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 simple method is described, by means of which it is possible to calculate the automorphism group of weighted graphs. We apply this method to compute the symmetry of the fullerenes molecule C_{84}.

(Received July 22, 2010; accepted September 15, 2010)

Keywords: Topological symmetry, C_{84} fullerene

1. Introduction

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 = (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 ≠ 22 is a natural number equal or greater than 20 [1,2].

In mathematics, groups are often used to describe symmetries of objects. To explain, we introduce some algebraic notion. A group is a tuple (S,o), where S is a set and ◦ is a closed binary operation over S such that:

- o acts associatively: a o b o c = a o (b o c), for every a, b, c ∈ S;
- there is a neutral element e such that a o e = e o a, for every element of of S;
- each element has an inverse.

In algebra and geometry ,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. 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

- the permutation of *X* assigned to the identity element of *G* is the identity transformation of *X*;
- 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*.

Since each element of *G* is represented as a permutation, a group action is also known as a permutation representation.

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

Detecting topological symmetry of molecules is a well-studied problem with applications in a large number of areas. The Euclidean matrix of a molecular graph G is a matrix D(G) = [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. In this paper a new algorithm for computing topological symmetry of fullerene molecules is presented. We apply our algorithm on a fullerene molecule C_{84} with point group symmetry D_{6h}.

A MATLAB Program for computing the symmetries of molecules

```
n=length(a);
  for i=1:n-1
        for j=i+1:n
              b(i,j)=norm(a(i,:)-a(j,:));
        end
  end
b(n,n)=0;
b=b+b';

function y=halat(s,a)
  t=1:length(a);
  m=length(s);
  t(s)=[];
  j=0;
        for i=t
              if min(min(a(1:m+1,1:m+1)==a([s,i],[s,i])))==1
                    j=j+1;
                    y(j)=i;
              end
        end

function s=hazf(s)
  m=size(s);
        for i=m(1):-1:1
              if min(s(i,:))==0
                    s(i,:)=[];
              end
        end

function s=jaigasht(a)
  m=length(a);
        for i=1:m
              s(i,1)=i;
        end
        for j=2:m
              n=size(s);
              k=0;
                    for i=1:n(1)
                          y=[halat(s(i,:),a)];
                                for r=1:length(y)
                                      b(r+k,1:n(2)+1)=[s(i,:),y(r)];
                                end
                          k=k+length(y);
                    end
              s=b;
              s=hazf(s);
        end
  b=0;
  n=size(s);
        for i=1:n(1)
              for j=1:n(2)
                    b(i,s(i,j))=j;
              end
        end
  s=b;
```

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. For the sake of completeness, we describe some of these functions which are useful throughout. Let $a_1, a_2, \ldots, a_r$ are permutations of $\{1,2,\ldots,n\}$. The command "Group(a_1,a_2,…,a_r)" computes the group generated by permutations $a_1, a_2, \ldots, a_r$. For two groups A and B, the commands "Size(A)", "GeneratorsOfGroup(A)" and "Intersection(A,B)" compute the cardinality of the set A, a generator set for A and intersection of A and B, respectively. Finally the command "IsSimple(A)" determines whether or not A has a non-trivial proper normal subgroup. 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 encourage the readers to consult papers [17-24] 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. In what follows we present a MATLAB program for computing a solution matrix for the automorphism group of Euclidean graphs.

Our program needs the Cartesian coordinates of the atoms to determine the Euclidean distances in the molecule under consideration. If we calculate these distances by HyperChem [17] then for computing the symmetry of molecule under consideration, it is enough to delete the first eight lines of the program and load the distance matrix of the molecule under consideration. In Table 1, the Cartesian coordinates of the fullerene molecule C_{84} is given.

Table 1. Cartesian coordinates of C_{84} molecule.

No	x	y	z
1	1.909410	0.460660	-3.935100
2	2.245510	-0.934470	-3.667500
3	0.620070	0.805210	-4.279330
4	1.273670	-1.907830	-3.758730
5	1.213120	-2.936670	-2.759810
6	-0.545580	4.129060	0.587030
7	0.368610	3.850820	-0.450370
8	0.029040	1.979650	-3.703430
9	2.633900	1.283200	-3.008210
10	2.030860	2.362860	-2.329810
11	0.670560	2.726640	-2.693000
12	-0.163310	3.473420	-1.750360
13	3.552730	0.402130	-2.325110
14	2.566560	2.743120	-1.021820
15	1.738120	3.484910	-0.084970
16	4.050840	0.755460	-1.109800
17	3.657380	2.009630	-0.509910
18	3.177090	-0.970270	-2.576140
19	3.055950	-1.890540	-1.514130
20	2.030380	-2.917250	-1.610020
21	-1.391320	1.723450	-1.610020
22	-1.564070	3.405840	-3.643810
23	-2.166250	2.417110	-1.902710
24	-1.957920	3.921380	-2.767480
25	-2.462100	3.563550	0.437760
26	-3.647380	-1.241250	-0.794370
27	-3.960680	0.058550	1.857900
28	-3.491340	2.532500	1.608220
29	-2.453280	3.269050	-0.890200
30	-3.425480	2.295980	1.646290
31	-3.959360	1.917060	1.555780
32	-3.309990	1.109720	0.251120
33	1.039060	3.449460	2.355660
34	-0.233410	3.789340	2.296040
35	-1.345950	3.075130	1.956390
36	-1.142080	1.863920	2.538680
37	-2.167690	0.837720	3.232910
38	2.070650	3.429800	3.137540
39	3.889070	1.866110	1.284790
40	3.103490	2.568890	0.899100
41	-3.226820	1.740310	-2.057330
42	-4.172500	0.497610	0.248210
43	-3.795560	-0.317510	-0.839580
44	-3.301860	0.331380	-2.043410
45	-2.468080	-0.414930	-2.986620
46	-1.634240	0.315100	-3.859010
47	-0.409280	-0.225380	-4.375630
48	-2.133350	-1.805170	-2.719850
49	-0.993150	-2.347820	-3.348180
50	-0.091960	-1.543050	-4.122890
51	-3.528680	-2.174470	0.761450
52	-2.630270	-2.458190	-1.507990
53	-3.458780	-1.716570	-0.570950
54	-0.174520	-3.329290	-2.673870
55	-0.636250	-3.936090	-1.547670
56	-1.942410	-3.594720	-1.033150
57	-2.179730	-2.874020	2.548810
58	-2.713970	-3.253050	1.244140
59	-1.928710	-3.956110	0.355830
60	-0.890120	-3.218990	2.892910
61	1.269560	2.376750	3.236420
62	0.227180	1.498070	3.598200
63	0.562340	0.108230	3.865250
64	-0.470050	-0.924810	3.769150
65	-1.830700	-0.561030	3.406510
66	-2.666320	-1.562210	2.869000
67	-0.060550	-2.258930	3.563910
68	2.925320	0.599350	3.248600
69	2.607580	1.916950	2.995680
70	2.257060	-1.603320	3.265820
71	1.911540	-0.285590	3.747760
72	1.297560	-2.563240	3.176210
73	4.225200	0.470660	1.166690
74	3.255270	-1.487190	2.227940
75	3.757250	-0.144730	2.307900
76	-0.562770	-4.320800	0.719920
77	0.264100	-4.183850	-0.445170
78	1.533600	-3.570400	-0.398310
79	-0.058320	-3.962920	1.951950
80	1.283130	-3.460660	2.043970
81	2.065740	-3.192710	0.901360
82	3.098130	-2.159500	0.997740
83	3.591740	-1.510430	-0.206130
84	4.200420	-0.244230	-0.077670

Using these coordinates and our MATLAB program given above, one can see that the symmetry group of the C_{84} fullerene is isomorphic to the group S_4. Suppose G is the symmetry group of this fullerene. Then $G = \langle X, Y \rangle$, where X and Y are the following permutations:

X = (1, 2)(3, 4)(5, 8)(6,80)(7,81)(9,18)(10,19)(11,20)(12,78)(14,83)(15,82)
(17,84)(21,54)(22,77)(23,55)(24,79)(25,76)(26,27)(28,59)(29,60)(30,57)
(31,58)(32,66)(33,70)(34,72)(35,67)(36,64)(37,65)(38,74)(39,73)(40,75)
(41,56)(42,51)(43,53)(44,52)(45,48)(46,49)(47,50)(61,71)(62,63)(68,69),

Y = (1,76,31,69)(2,59,30,40)(3,79,28,68)(4,58,29,39)(5,51,35,17)
(6,84,49,66)(7,83,48,65)(8,80,41,71)(9,77,42,61)(10,78,43,62)
(11,81,44,63)(12,82,45,64)(13,55,27,33)(14,20,53,36)(15,19,52,37)
(16,54,26,34)(18,56,32,38)(21,72,23,70)(22,74,46,67)(24,73,50,57) (25,75,47,60).

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**, 221 (2008).

[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).

*Corresponding author: mghorbani@srttu.edu