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On Symmetry of Some Nano Structures

MODJTABA GHORBANI[1,*], ALI ZAEEMBASHI[1], MOHSEN SHAHREZAEI[2] AND AMIR TABATABAEI ADNANI[3]

[1]Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785-136, I. R. Iran
[2]Department of Mathematics, Faculty of Science, Imam Hossein University, Tehran, I.R. Iran
[3]Department of Statistics, Tehran North Branch, Islamic Azad University, Tehran, I. R. Iran

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ABSTRACT

It is necessary to generate the automorphism group of a chemical graph in computer-aided structure elucidation. An Euclidean graph associated with a molecule is defined by a weighted graph with adjacency matrix M = [*dij*], where for *i≠j*, dij is the Euclidean distance between the nuclei i and j. In this matrix *dii* can be taken as zero if all the nuclei are equivalent. Otherwise, one may introduce different weights for distinct nuclei. A.T. Balaban introduced some monster graphs and then M. Randic computed complexity indices of them (see A.T. Balaban, Rev. Roum. Chim. 18(1973) 841-853 and M. Randic, Croat. Chem. Acta 74(3)(2001) 683-705). In this paper, we describe a simple method, by means of which it is possible to calculate the automorphism group of weighted graphs.

Keywords: Weighted graph, euclidean graph.

1. INTRODUCTION

Diamondoid was first discovered and isolated from a Czechoslovakian petroleum in 1933. The isolated substance was named adamantane, from the Greek for diamond. This name was chosen because it has the same structure as the diamond lattice, highly symmetrical and strain free. It is generally accompanied by small amounts of alkylated adamantanes, 2-methyl, 1-ethyl, and probably 1-methyl, 1, 3-dimethyl and others.

The carbon skeleton of adamantane comprises a small cage structure. Because of this, adamantane and diamondoids in general are commonly known as cage hydrocarbons.

*Author correspondence should be addressed. (E-mail: mghorbani@srttu.edu)

In a broader sense they may be described as saturated, polycyclic, cage-like hydrocarbons that are present in some reservoir fluids. The diamond-like term arises from the fact that their carbon atom structure can be superimposed upon a diamond lattice. The simplest of these polycyclic diamondoids is adamantane, followed by its homologues diamantane, tria-, tetra-, penta- and hexamantane. The homologous polymantane series has the general molecular formula $C_{4n+6}H_{4n+12}$ where n=1, 2, 3, ...(n=1 for adamantane).

Graph theory is a branch of discrete mathematics concerned with relation, between objects. From the point of the graph theory, all organic molecular structures can be drawn as graphs in which atoms and bonds are represented by vertices and edges, respectively. By symmetry we mean the automorphism group symmetry of a graph which is a subgroup of its vertex permutation group. The symmetry of a graph, also called topological symmetry, which need not be the isomorphic to the molecular point group symmetry. However, it dose represent the maximal symmetry of its topological structure.

Randic [1, 2] showed a graph can be depicted in different ways such that its point group symmetry or three dimensional preception may differ, but the underlying connectivity symmetry is still the same as characterised by the automorphism group of the graph which by definition comprises permutations of the vertices of the graph that leave the adjacency matrix invariant. However, the molecular symmetry depends on the coordinates of the various nuclei which relate directly to their three dimensional geometry.

Automorphisms have other advantages such as in generation nuclear spin species, NMR spectra, nuclear spin statistics in molecular spectroscopy, chirality and chemical isomerism. There is also another important application of the automorphism group of weighted graphs to fullerenes. The reader is encouraged to consult the leading papers by Balasubramanian [3 - 11] and [12 - 17] for background materials as well as basic computational techniques.

Longuet-Higgins [18] showed that a more desirable representation of molecular symmetry is to use nuclear permutation and inversion operations resulting in a group called Permutation-Inversion (PI) group. Balasubramanian showed that the automorphism group of Euclidean graph of a molecule is the Permutation-Inversion group of the molecule.

A. Ashrafi [19] proved a result that is useful for computing symmetry of molecules. Using this result, Lemma 1 and its Corollary, and a MATLAB program that is presented in [22] for computing a solution matrix for the automorphism group of Euclidean graphs. Finally we use GAP [20, 21] to compute the full automorphism group of some graphs which is defined by Balaban [12]. Here, we report on the automorphism group of Structure of Higher Diamondoids. Herein, our notation is standard and taken from the standard book of graph theory [16, 22-28].

2. EXPRIMENTAL

A simple graph G is called a weighted graph if each edge e is assigned a non-negative number $w(e)$, called the weight of e. An automorphism of a weighted graph $G = (V, E)$ is a permutation g of V with the following properties: (i) for any u,v in V, $g(u)$ and $g(v)$ are adjacent if and only if u is adjacent to v. (ii) for each e in E, $w(g(e)) = w(e)$. The set of all automorphism of a weighted graph G, with the operation of composition of permutations, is a permutation group on $V(G)$, denoted Aut(G). A non-empty subset X of $V(G)$ is called an orbit of G under the action of Aut(G), if there exists $x \in X$ such that $X = \{\alpha(x) \mid \alpha \in \mathrm{Aut}(G)\}$,. G is called vertex transitive or simply transitive, if it has a unique orbit.

It is a well-known fact that a permutation of the vertices of a graph belongs to its automorphism group if it satisfies $P^tAP = A$ (1), where P^t is the transpose of permutation matrix P and A is the adjacency matrix of the graph under consideration. There are $n!$ possible permutation matrices for a graph with n vertices. However, all of them may not satisfy the relation (1). Set $\mathrm{Aut}(G) = \{\sigma_1, \sigma_2, \cdots, \sigma_m\}$. 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 [23]

We would like to bring to attention of the spectroscopy community a free software package for group theory named GAP [21], which greatly facilitates the following calculations. For a given adjacency matrix A, we can write a simple GAP program to calculate all the permutation matrices with $P^tAP = A$. Using this program and a similar approach as in [22], in the next section, we calculate the automorphism group of two weighted graphs.

3. MAIN RESULTS

The adjacency matrix $A = [w_{ij}]$ of a weighted graph is defined as: $A_{ij}=w_{ij}$, if $i \neq j$ and vertices i and j are connected by an edge with weight w_{ij}; $A_{ij}=v_i$, if i=j and the weight of the vertex i is v_i, and, $A_{ij}=0$, in the case that $i \neq j$ and i, j are not adjacent. Note that v_i can be taken as zero if all the nuclei are equivalent. Otherwise, one may introduce different weights for nuclei in different equivalence classes and the same weight for the nuclei in the same equivalence classes. Symmetry operations on a graph are called graph automorphisms. They affect only the labels of vertices by permuting them so that the adjacency matrix of the graph remains unchanged. The graph symmetry is completely determined by all the automorphisms it has, i.e. by specifying all the permutations which leave the adjacency matrix intact. The automorphism group of a graph depends only on the connectivity of the graph and does not depend on how the graph is represented in three dimensions. That is, a graph, in general, can be represented in different ways in three dimensions such that two representations could yield different three-dimensional symmetries and yet their automorphism groups are

the same since the latter depends only on which vertices are connected in the graph. Balasubramanian [7] calculated the automorphism group of the Euclidean graph of benzene molecule. By his result, this is a group of order 12. We continue Balasubramanian's result to compute the automorphism group of the Euclidean graph of Structure of Higher Diamondoids Figure 1. now by using GAP program following we calculate the symmetries of graph of Higher Diamondoids as follows:

The output of this program is matrix which its rows represent the automorphisms of the graph. To complete our calculation we can compute the automorphism group of the adjacency graph of Higher Diamondoids. After running this program for the adjacency graph of Higher Diamondoids, we calculate Automorphism graph as follows:

Aut(G_1) = Aut(G_5) = {()},

Aut(G_2) = {(),(1,3)(5,7)(8,12)(9,11)(13,17)(14,16)(18,25)(19,23)(20,24)},

Aut(G_3)={(),(1,3)(5,7)(8,10)(11,15)(16,18)(19,22),(1,19)(2,20)(3,22)(4,21)(5,16) (6,17) (7,18)(8,11)(9,13)(10,15),(12,14),(1,22)(2,20)(3,19)(4,21)(5,18)(6,17)(7,16) (8,15)(9,13)(10,11)(12,14)},

Aut(G_4) = {(),(3,7)(4,9)(6,8)(13,14),(1,3)(4,5)(8,10)(11,14),(1,3,7)(4,9,5)(6,10,8) (11,14,13) (1,7,3) (4,5,9)(6,8,10)(11,13,14),(1,7)(5,9)(6,10)(11,13),(1,11) (2,12) (3,13) (4,6) (5,10)(7,14) (8,9)},

Aut(G_5) = {(1,11)(2,12)(3,14)(4,8)(5,10)(6,9)(7,13),(1,13,3,11,7,14)(2,12) (1,13) (4,10,9,8,5,6) (2,12)(3,14)(4,8)(5,6)(7,11)(9,10),(1,14)(2,12)(3,11)(4,10)(5,8)(6,9) (7,13)(1,14,7,11,3,13)(2,12)(4,6,5,8,9,10)},

Aut(G_6) = {(),(1,4)(5,15)(6,16)(9,10)(11,17),(1,9)(2,8)(3,18)(4,10)(5,11)(6,16) (12,14) (15,17),(1,10)(2,8)(3,1)(4,9)(5,17)(11,15)(12,14)},

Aut(G_7) = {(),(1,3)(4,6)(9,10)(11,13)(17,26)(19,24)(20,23),(1,20)(2,21)(3,23)(4,24) (5,22) (6,19)(7,25)(8,16)(9,1)(10,26)(11,13)(15,18),(1,23)(2,21)(3,20)(4,19)(5,22) (6,24)(7,25)(8,16)(9,26) (10,17)(15,18)},

Aut(G_8) = {(),(1,3)(5,7)(8,2)(9,11)(13,17)(14,16)(18,25)(19,23)(20,24)}.

Using these calculations, we can see that G_1 – G_8, as the weighted graphs, are not vertex transitive. These orbits are as follows:

$\Delta_{G_1} = \Delta_{G_5} = \{\{1\},\{2\},\{3\},\{4\},\{5\},\{6\},\{7\},\{8\},\{9\},\{10\},\{11\},\{12\},\{13\},\{14\},\{15\},\{16\},\{17\},$

$\{18\},\{19\},\{20\},\{21\},\{22\},\{23\},\{24\},\{25\},\{26\}\}.$

$\Delta_{G_2} = \{\{1,5,11\},\{2,\ 4,7\},\{3,6,8\},\{9,12,21\},\{10,15,18\},\{13,14,17,19,20,22\},\{16\}\}.$

$\Delta_{G_3} = \{\{1,3,19,22\},\{2,20\},\{4,21\},\{5,7,16,18\},\{6,17\},\{8,10,11,5\},\{9,\ 3\},\{12,14\}\}.$

$\Delta_{G_4} = \{\{1,3,7,11,13,14\},\{2,12\},\{4,5,6,8,9,10\}\}.$

$\Delta_{G_6} = \{\{1,4,9,10\},\{2,8\},\{3,18\},\{5,11,15,17\},\{6,16\},\{7\},\{12,14\},\{13\}\}.$

$\Delta_{G_7} = \{\{1,3,20,23\},\{2,21\},\{4,6,19,24\},\{5,22\},\{7,25\},\{8,16\},\{9,10,17,26\},\{11,13\},\{12\},$

$\{14\ \},\{15,18\}\}.$

$\Delta_{G_8} = \{\{1,3\},\{2\},\{4\},\{5,7\},\{6\},\{8,12\},\{9,11\},\{10\},\{13,17\},\{14,16\},\{15\},\{18,25\},\{19,23\},$

$\{20,24\},\{21\},\{22\},\{26\}\}.$

Here, group G_1, …, G_8 are $C_{14}H_{20}$, $C_{18}H_{24}$, $C_{22}H_{28}$ [121], $C_{26}H_{32}$[1212], $C_{26}H_{32}$[1213], $C_{26}H_{32}$[1(2,3)4], $C_{26}H_{3.2}$[12(3)4] and $C_{26}H_{32}$[12(1)3], respectively.

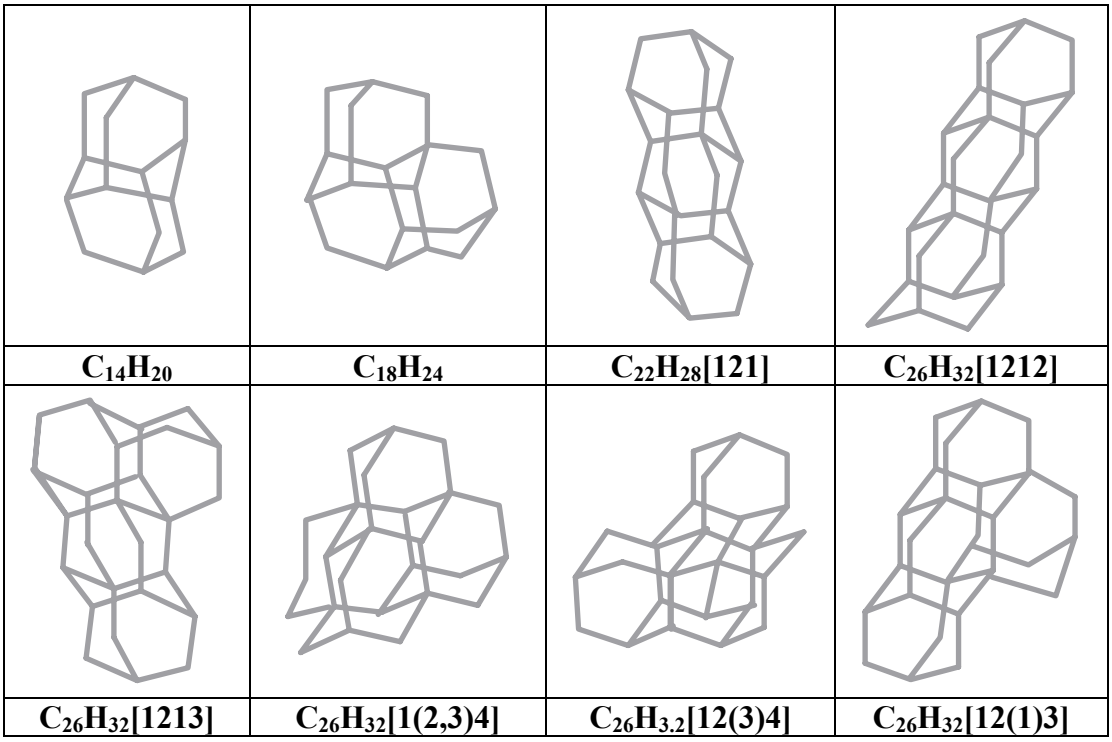

Figure 1. Structure of Higher Diamondoids.

A GAP Program for Computing the Symmetries of Structure of Higher Diamondoids

```
f:=function(G,n);
 local H,i,a,d,g,dd;
 H=[];
                              for i in 1..n] do
 Add(a,i);
                              od;
 for i in G do
          Add(H,PermListList(a,i));
   od;
    d:=]; dd:=];
  for i in 1..n] do
      for g in H do
       AddSet(d,i^g);
                        od ;    AddSet(dd,d);  d:=];
           od;
       HH:=Elements(Group(H));
                           Print("Group=",HH,"\n");
         Print("Orbits=",dd,"\n");
 return;end;
```

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