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AUTOMORPHISM GROUPS OF SOME NON-TRANSITIVE GRAPHS

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Abstract. An Euclidean graph associated with a molecule is defined by a weighted graph with adjacency matrix $M = [dij]$, where for ij, 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. Balaban introduced some monster graphs and then Randic computed complexity indices of them (1973, 2001). In this paper, with a simple method, we calculate the automorphism group of some weighted graphs

Keywords: Weighted graph, Euclidean graph, Automorphism group.

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1. Introduction

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. Structural symmetry is related to the automorphism group of the vertex is a subgroup of the vertex permutation group. By symmetry we mean the automorphism group symmetry of a graph. The symmetry of a graph, also called topological symmetry, which need not be the same as (i.e. isomorphic to) the molecular point group symmetry. However, it dose represent the maximal symmetry which the topological structure may passes.

Randic[1, 2]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[3] that the two symmetries are connected. 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 [3] showed that the automorphism group of Euclidean graph of a molecule is the Permutation-Inversion group of the molecule. The second author, in Ref. 19 showed that for each finite group H, there exists a finite regular completed weighted graph G such that $Aut(G)$ contains a copy of H. This shows that the order of $Aut(G)$ can be arbitrarily large. He also proved an algorithm to compute the automorphism group of weighted graphs. In this paper, using this algorithm and a GAP program [20, 21], we calculate the automorphism group of some graphs of Balaban's paper [12].

A simple graph G is called a weighted graph if each edge e is assigned a nonnegative 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 xX such that $X = \{(x)| \in Aut(G)\}$. G is called vertex transitive or simply transitive, if it has a unique orbit.

A permutation of the vertices of a graph belongs to its automorphism group if it satisfies

$$P^t AP = A, \qquad (1)$$

where Pt 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).

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 Refs. 22-25, in the next section, we calculate the automorphism group of two weighted graphs.

2. Results and Discuttions

The adjacency matrix $A = [wij]$ of a weighted graph is defined as: $A_{ij} = w_{ij}$, if ij and vertices i and j are connected by an edge with weight w_{ij}; $Aij = v_i$, if $i = j$ and the weight of the vertex i is v_i, and, $Aij = 0$, 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.

Balaban [12] introduced the monster graphs G_{14} and G_{16}, Figures 1 and 2. We calculate Euclidean edges of G_{14} and G_{16} in Tables 1 and 2.

It should be mentioned that one does not have to work with exact Euclidean distances in that a mapping of weights into a set of integers would suffice as long as different weights are identified with different integers. In fact the automorphism group of the integer-weighted graph is identical to the automorphism group of the original Euclidean graph .To illustrate let us map the Euclidean edge weighted for G_{14} as: $0.30 \rightarrow 1$, $0.58 \rightarrow 2$, $0.80 \rightarrow 3$, $0.95 \rightarrow 4$. Also, we map the Euclidean edge weighted for G_{16} as: $0.20 \rightarrow 1$, $0.40 \rightarrow 2$, $0.58 \rightarrow 3$ and $0.74 \rightarrow 4$ and $0.86 \rightarrow 5$, $0.95 \rightarrow 6$ and $0.99 \rightarrow 7$.

Therefore we got the distance matrices A and B for G_{14} and G_{16}, respectively. We now write a GAP program for calculating the symmetries of graph G_{14} and G_{16} .

3. A GAP program for symmetries of G_{14} and G_{16}

A GAP program for calculating the symmetries of graph G_{14} is:

$$P := [[0,1,2,3,0,0,0,3,2,1],[1,0,1,0,3,4,0,4,3,0],[2,1,0,1,2,3,0,0,0,3],$$
$$[3,0,1,0,1,0,3,4,0,4],[0,3,2,1,0,1,2,3,0,0],[0,4,3,0,1,0,1,0,3,4],$$
$$[0,0,0,3,2,1,0,1,2,3],[3,4,0,4,3,0,1,0,1,0],[2,3,0,0,0,3,2,1,0,1]$$
$$[1,0,3,4,0,4,3,0,1,0]]$$

$$n := 10; i := 0; H := [\ ];$$
$$t := SymmetricGroup(n);$$
$$tt := Elements(t);$$

for a in tt do

$$x1 := PermutationMat(a, n);$$
$$x := TransposedMat(x1);$$
$$y := x * P * x1;$$
$$\text{if } y = P \text{ then } AddSet(H, a); fi;$$
$$od;$$
$$G := Group(H);$$

And a GAP program for calculating the symmetries of graph G_{16} is also as follows:

$$\begin{aligned} T := [&[0,1,2,0,0,5,0,0,0,0,5,0,,0,2,1],[1,0,1,0,3,0,5,0,7,0,0,5,0,0,0]\\ &[2,1,0,1,0,0,0,5,0,7,0,0,5,0,0],[0,0,1,0,1,2,0,0,0,6,0,7,0,0,4]\\ &[0,3,0,1,0,1,0,0,4,0,0,0,7,6,4],[5,0,0,2,1,0,1,2,0,0,5,0,0,0,0]\\ &[0,5,0,0,0,1,0,1,0,3,0,5,0,7,0],[0,0,5,0,0,2,1,0,1,0,0,0,5,0,7]\\ &[0,7,0,0,4,0,0,1,0,1,2,0,0,0,6],[0,0,7,6,0,0,3,0,1,0,1,0,0,4,0]\\ &[5,0,0,0,0,5,0,0,2,1,0,1,2,0,0],[0,5,0,7,0,0,5,0,0,0,1,0,1,0,3]\\ &[0,0,5,0,7,0,0,5,0,0,2,1,0,1,0],[2,0,0,0,6,0,7,0,0,4,0,0,1,0,1]\\ &[1,0,0,4,0,0,0,7,6,0,0,3,0,1,0]] \end{aligned}$$

$$n := 15; i := 0; K := [];$$
$$t := SymmetricGroup(n);$$
$$tt := Elements(t);$$

for a in tt do

$$x1 := PermutationMat(a, n);$$
$$x := TransposedMat(x1);$$
$$y := x * T * x1;$$
$$\text{if } y = T \text{ then AddSet } (K, a); fi;$$
$$od;$$
$$G := Group(K);$$

The program does not miss any permutation since it checks the candidate of the given automorphism group in lexiogarphical order. The output of this program is the automorphism group of the weighted graph G_{14} and G_{16} respectively. After running this program for the weighted graphs G_{14} and G_{16}, we calculate

$Aut(G_{14})$ and $Aut(G_{16})$ as follows:

$$\begin{aligned} Aut(G_{14}) = \{&(1), (2,10)(3,9)(4,8)(5,7), (1,3)(4,10)(5,9)(6,8), (1,9,7,5,3)(2,10,8,6,4),\\ &(1,5)(2,4)(6,10)(7,9), (1,7,3,9,5)(2,8,4,10,6),\\ &(1,7)(2,6)(3,5)(8,10), (1,5,9,3,7)(2,6,10,4,8),\\ &(1,9)(2,8)(3,7)(4,6), (1,3,5,7,9)(2,4,6,8,10)\} \end{aligned}$$

$$\begin{aligned} Aut(G_{16}) = \{&(1), (1,11,6)(2,12,7)(3,13,8)(4,14,9)(5,15,10),\\ &(1,6,11)(2,7,12)(3,8,13)(4,9,14)(5,10,15)\} \end{aligned}$$

Using these calculations, we can see that G_{14} and G_{16}, as the weighted graphs, are not vertex transitive. In fact, G_{14} and G_{16} have exactly two and five orbits, respectively. These orbits are as follows:

$$\begin{aligned} &\mathbf{O}_{14}(1) = \{1,3,5,7,9\},\\ &\mathbf{O}_{14}(2) = \{2,4,6,8,10\},\\ &\mathbf{O}_{16}(1) = \{1,6,11\},\\ &\mathbf{O}_{16}(2) = \{2,7,12\},\\ &\mathbf{O}_{16}(3) = \{3,8,13\},\\ &\mathbf{O}_{16}(4) = \{4,9,14\},\\ &\mathbf{O}_{16}(6) = \{5,10,15\}. \end{aligned}$$

$$A = \begin{bmatrix} 0 & 1 & 2 & 3 & 0 & 0 & 0 & 3 & 2 & 1 \\ 1 & 0 & 1 & 0 & 3 & 4 & 0 & 4 & 3 & 0 \\ 2 & 1 & 0 & 1 & 2 & 3 & 0 & 0 & 0 & 3 \\ 3 & 0 & 1 & 0 & 1 & 0 & 3 & 4 & 0 & 4 \\ 0 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 0 & 0 \\ 0 & 4 & 3 & 0 & 1 & 0 & 1 & 0 & 3 & 4 \\ 0 & 0 & 0 & 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 4 & 0 & 4 & 3 & 0 & 1 & 0 & 1 & 0 \\ 2 & 3 & 0 & 0 & 0 & 3 & 2 & 1 & 0 & 1 \\ 1 & 0 & 3 & 4 & 0 & 4 & 3 & 0 & 1 & 0 \end{bmatrix}$$

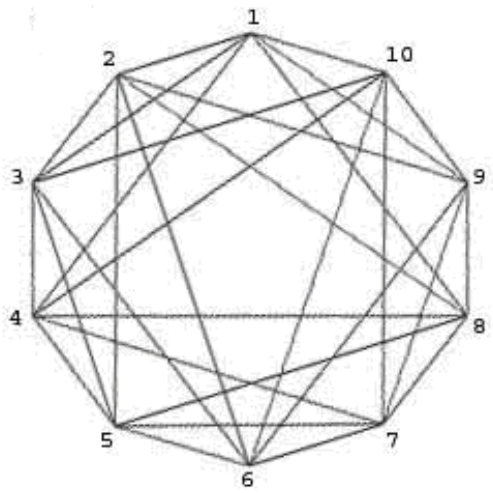

FIGURE 1. Topoligical representation of isomerizations of G_{14}.

$$B = \begin{bmatrix}
0 & 1 & 2 & 0 & 0 & 5 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 2 & 1 \\
1 & 0 & 1 & 0 & 3 & 0 & 5 & 0 & 7 & 0 & 0 & 5 & 0 & 0 & 0 \\
2 & 1 & 0 & 1 & 0 & 0 & 0 & 5 & 0 & 7 & 0 & 0 & 5 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & 2 & 0 & 0 & 0 & 6 & 0 & 7 & 0 & 0 & 4 \\
0 & 3 & 0 & 1 & 0 & 1 & 0 & 0 & 4 & 0 & 0 & 0 & 7 & 6 & 0 \\
5 & 0 & 0 & 2 & 1 & 0 & 1 & 2 & 0 & 0 & 5 & 0 & 0 & 0 & 0 \\
0 & 5 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 3 & 0 & 5 & 0 & 7 & 0 \\
0 & 0 & 5 & 0 & 0 & 2 & 1 & 0 & 1 & 0 & 0 & 0 & 5 & 0 & 7 \\
0 & 7 & 0 & 0 & 4 & 0 & 0 & 1 & 0 & 1 & 2 & 0 & 0 & 0 & 6 \\
0 & 0 & 7 & 6 & 0 & 0 & 3 & 0 & 1 & 0 & 1 & 0 & 0 & 4 & 0 \\
5 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 2 & 1 & 0 & 1 & 2 & 0 & 0 \\
0 & 5 & 0 & 7 & 0 & 0 & 5 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 3 \\
0 & 0 & 5 & 0 & 7 & 0 & 0 & 5 & 0 & 0 & 2 & 1 & 0 & 1 & 0 \\
2 & 0 & 0 & 0 & 6 & 0 & 7 & 0 & 0 & 4 & 0 & 0 & 1 & 0 & 1 \\
1 & 0 & 0 & 4 & 0 & 0 & 0 & 7 & 6 & 0 & 0 & 3 & 0 & 1 & 0
\end{bmatrix}$$

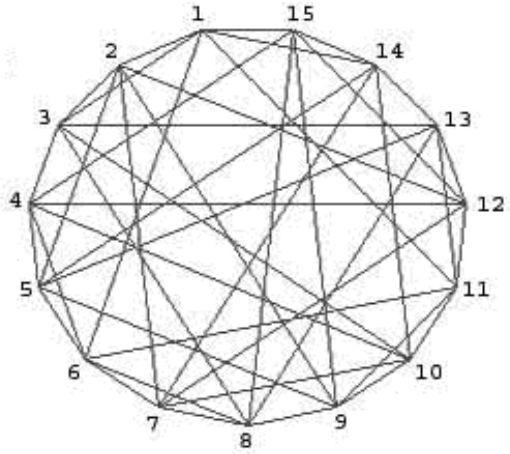

FIGURE 2. Topoligical representation of rearrangement mode of intramolecular isomerizations of tringonal bipyramidal structure (G_{16})

TABLE 1. Euclidean edge weights for G_{14}

0	0.3090	0.5878	0.8090	0	0	0	0.8090	0.5878	0.3090
0.3090	0	0.3090	0	0.8090	0.9511	0	0.9511	0.8090	0
0.5878	0.3090	0	0.3090	0.5878	0.8090	0	0	0	0.8090
0.8090	0	0.3090	0	0.3090	0	0.8090	0.9511	0	0.9511
0	0.8090	0.5878	0.3090	0	0.3090	0.5878	0.8090	0	0
0	0.9511	0.8090	0	0.3090	0	0.3090	0	0.8090	0.9511
0	0	0	0.8090	0.5878	0.3090	0	0.3090	0.5878	0.8090
0.8090	0.9511	0	0.9511	0.8090	0	0.3090	0	0.3090	0
0.5878	0.8090	0	0	0	0.8090	0.5878	0.3090	0	0.3090
0.3090	0	0.8090	0.9511	0	0.9511	0.8090	0	0.3090	0

TABLE 2. Euclidean edge weights for G_{16}

0	0.20	0.40	0	0	0.86	0	0	0	0	0.86	0	0	0.40	0.20
0.20	0	0.20	0	0.58	0	0.86	0	0.99	0	0	0.86	0	0	0
0.40	0.20	0	0.20	0	0	0	0.86	0	0.99	0	0	0.86	0	0.20
0	0	0.20	0	0.20	0.40	0	0	0	0.95	0	0.99	0	0	0.74
0	0.58	0	0.20	0	0.20	0	0	0.74	0	0	0	0.99	0.95	0
0.86	0	0	0.40	0.20	0	0.20	0.40	0	0	0.86	0	0	0	0
0	0.86	0	0	0	0.20	0	0.20	0	0.58	0	0.86	0	0.99	0
0	0	0.86	0	0	0.40	0.20	0	0.20	0	0	0	0.86	0	0.99
0	0.99	0	0	0.74	0	0	0.20	0	0.20	0.40	0	0	0	0.95
0	0	0.99	0.95	0	0	0.58	0	0.20	0	0.20	0	0	0.74	0
0.86	0	0	0	0	0.86	0	0	0.40	0.20	0	0.20	0.40	0	0
0	0.86	0	0.99	0	0	0.86	0	0	0	0.20	0	0.20	0	0.58
0	0	0.86	0	0.99	0	0	0.86	0	0	0.40	0.20	0	0.20	0
0.40	0	0	0	0.95	0	0.99	0	0	0.74	0	0	0.20	0	0.20
0.20	0	0	0.74	0	0	0	0.99	0.95	0	0	0.58	0	0.20	0

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