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Symmetry of Tetra-*tert*-butyltetrahedrane

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In this paper, the atom centers of tetra-*tert*-butyltetrahedrane molecule using the chemistry package HyperChem is calculated followed by the automorphism group of Euclidean graph of this molecule is computed by Gap System.

Key words: Symmetry of graphs, Tetra-*tert*-butyltetrahedrane, Automorphism, Euclidean graph.

INTRODUCTION

The symmetry of a graph through the automorphism group of the graph has been studied[1–15]. The symmetry group of a molecule depends on the relative positions of atoms in the three-dimensional space, that is, the actual coordinates of the various centres in the three-dimensional space.

As shown by Randic[6], 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 characterized 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.

By symmetry, we mean the automorphism group symmetry of a graph. The symmetry of a graph, also called a topological symmetry, accounts only for the bond relations between atoms and does not fully determine molecular geometry. The symmetry of a graph does not need to be the same as (*i.e.* isomorphic to) the molecular point group symmetry. However, it does represent the maximal symmetry which the geometrical realization of a given topological structure may possess.

In this paper, the automorphism group of weighted graphs is investigated. By definition, a weighted graph is a graph whose edges and vertices are weighted with different weights. The adjacency matrix 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 $i \neq j$ and weight of the vertex i is v_i and $A_{ij} = 0$, otherwise. 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.

Graph theory provides an elegant and natural representation of molecular symmetry and the resulting group expressed in terms of permutations is isomorphic to the permutation-inversion group of Longuet-Higgins. We apply our method to the tetra-*tert*-butyltetrahedrane.

Throughout this paper, all groups considered are assumed to be finite. Our notation is standard and taken mainly from previous studies[16–18]. Darafsheh *et al.*[19] computed the non-rigid group of tetra-*tert*-butyltetrahedrane. So it is natural to ask about automorphism group of the Euclidean graph of this molecule. The aim of this section is solving this problem.

RESULTS AND DISCUSSION

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 automorphismgroups are the same since the latter depends only on which vertices are connected in the graph.

A permutation of the vertices of the Euclidean graph under consideration belongs to the permutation representation of an operation in the point group if and only if the corresponding permutation matrix P satisfies $P^tDP = D$, where P^t is the transpose of permutation matrix P and D is the adjacency matrix of the graph. All such permutations of the nuclei which preserve the connectivity of the Euclidean graph of the molecule form a group which we call the Euclidean distance group.

Consider the tetra-*tert*-butyltetrahedrane molecule to illustrate its automorphism group. It suffices to measure the Euclidean distances and then constructs the Euclidean distance matrix D. 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, Fig. 1, is identical to the automorphism group of the original Euclidean graph. The resulting atom centres are shown in Table-1.

Suppose G is the set of all permutations which preserve the Euclidean connectivity. It is useful to mention that our calculations were done by a GAP program. Using such a program, one can recalculate all the examples of Balasubramanian[7]. For the sake of completeness we write below our GAP-program for computing the automorphism group of the Euclidean graph of the mentioned molecule.

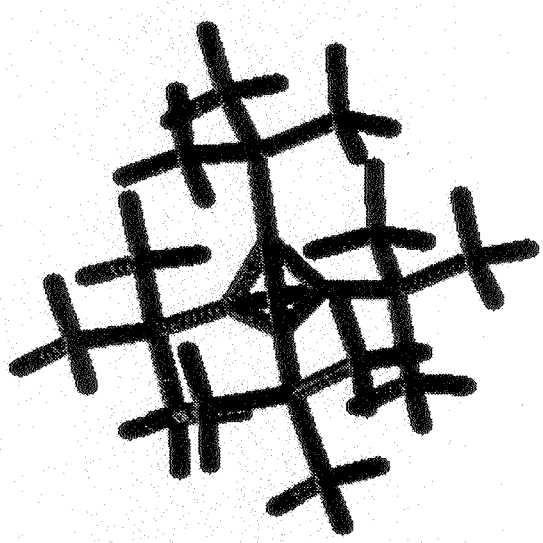

Fig. 1. The structure of tetra-*tert*-butyltetrahedrane

A GAP program for computing the symmetries of tetra-*tert*-butyl tetrahedrane

```
gap> V:=
[[ 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, 27, 28, 29, 30,
31, 32, 33, 34, 35, 36, 37, 38, 39, 43, 41, 42, 40, 44, 45, 52, 47, 48, 49, 50, 51, 46, 53, 54, 55, 56 ],
[ 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 50, 24, 25, 26, 27, 28, 47, 30,
31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 44, 42, 43, 41, 45, 46, 29, 48, 49, 23, 51, 52, 53, 54, 55, 56 ],
[ 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, 27, 28, 29, 30,
31, 32, 33, 34, 35, 36, 37, 38, 42, 40,44, 39, 43, 41, 45, 52, 47, 48, 49, 50, 51, 46, 53, 54, 55, 56 ],
[ 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 48, 22, 23, 24, 25, 26, 27, 28, 47, 30,
31, 32, 33, 34, 35, 36, 37, 38, 39, 43, 44, 42, 40, 41, 45, 46, 29, 21, 49, 50, 51, 52, 53, 54, 55, 56 ],
[ 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 48, 49, 50, 24, 25, 26, 27, 28, 29, 30,
31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 51, 46, 47, 21, 22, 23, 45, 52, 53, 54, 55, 56 ],
[ 2, 1, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30,
31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 44, 42, 43, 41, 51, 52, 47, 48, 49, 50, 45, 46, 53, 54, 55, 56 ],
[ 2, 1, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 50, 24, 25, 26, 27, 28, 47, 30,
31, 32, 33, 34, 35, 36, 37, 38, 39, 43, 41, 42, 40, 44, 51, 52, 29, 48, 49, 23, 45, 46, 53, 54, 55, 56 ],
[2, 1, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 49, 23, 24, 25, 26, 27, 28, 47, 30,
31, 32, 33, 34, 35, 36, 37, 38, 42, 43,41, 39, 40, 44, 51, 52, 29, 48, 22, 50, 45, 46, 53, 54, 55, 56 ],
[ 2, 1, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 48, 22, 23, 24, 25, 26, 27, 28, 29, 30,
31, 32, 33, 34, 35, 36, 37, 38, 42, 43, 44, 39, 40, 41, 51, 52, 47, 21, 49, 50, 45, 46, 53, 54, 55, 56 ],
[ 2, 1, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 48, 49, 23, 24, 25, 26, 27, 28, 29, 30,
31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 44, 42, 43, 41, 45, 46, 47, 21, 22, 50, 51, 52, 53, 54, 55, 56 ],
[ 2, 1, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 48, 49, 50, 24, 25, 26, 27, 28, 47, 30,
31, 32, 33, 34, 35, 36, 37, 38, 39, 43, 41, 42, 40, 44, 45, 46, 29, 21, 22, 23, 51, 52, 53, 54, 55, 56 ]];
gap> T:=[ ];
gap> for i in V do
gap> j:= PermList (i);
gap> Add(T,j);
gap> od;
gap> G:=Group(T);
```

The group G is elementary abelian of order 1024 and its generator set is as follows:

{(40,43)(46,52), (23,50)(29,47)(41,44), (39,42)(41,44)(46,52),
(21,48)(29,47)(40,43)(41,44), (21,48)(22,49)(23,50)(45,51),
(1,2)(41,44)(45,51)(46,52), (1,2)(23,50)(29,47)(40,43)(45,51)(46,52),
(1,2)(22,49)(29,47)(39,42)(40,43)(45,51)(46,52),
(1,2)(21,48)(39,42)(40,43)(41,44)(45,51 X46,52), (1,2)(21,48)(22,49)(41,44),
(1,2)(21,48)(22,49)(23,50)(29,47)(40,43)}

TABLE-1
ATOMS CENTRES OF THE TETRA-*tert*-BUTYL TETRAHEDRANE

C_1	0.000000	0.000000	0.000000	H_9	1.102845	111.101745	55.054712
C_2	1.497596	0.000000	0.000000	H_{10}	1.102571	110.886202	175.530355
C_3	1.497447	60.031080	0.000000	H_{11}	1.102823	111.119549	55.322353
C_4	1.498244	59.963419	–70.504767	H_{12}	1.102478	111.098017	–64.481746
C_5	1.466740	144.630367	–144.273401	H_{13}	1.102434	111.133397	–64.113003
C_6	1.536524	109.388258	–75.245301	H_{14}	1.102569	110.890333	175.882797
C_7	1.536436	109.421080	164.741352	H_{15}	1.102850	111.095881	55.693382
C_8	1.536442	109.389146	44.731065	H_{16}	1.102564	110.898264	175.931568
C_9	1.466763	144.832685	–144.265932	H_{17}	1.102813	111.098089	55.744374
C_{10}	1.536507	109.388202	164.854301	H_{18}	1.102474	111.116391	–64.061870
C_{11}	1.536346	109.420795	44.851509	H_{19}	1.102536	110.912088	175.679699
C_{12}	1.536463	109.391950	–75.166479	H_{20}	1.102820	111.082951	55.489722
C_{13}	1.466747	144.684367	144.965317	H_{21}	1.102464	111.117394	–64.296906
C_{14}	1.536412	109.404208	–74.679909	H_{22}	1.102566	110.884375	175.683124
C_{15}	1.536460	109.393506	165.311105	H_{23}	1.102829	111.098895	55.494364
C_{16}	1.536475	109.383572	45.315541	H_{24}	1.102469	111.111662	–64.314628
C_{17}	1.466663	144.803807	145.230946	H_{25}	1.102426	111.142143	–64.738806
C_{18}	1.536395	109.417637	44.518159	H_{26}	1.102574	110.871357	175.259806
C_{19}	1.536505	109.389817	164.536228	H_{27}	1.102826	111.109740	55.069438
C_{20}	1.536492	109.396930	–75.486755	H_{28}	1.102539	110.889640	175.051160
H_1	1.102552	110.901339	175.044870	H_{29}	1.102870	111.089158	54.876411
H_2	1.102854	111.071985	54.881436	H_{30}	1.102440	111.150143	–64.941823
H_3	1.102464	111.146454	–64.925063	H_{31}	1.102440	111.141671	–64.735715
H_4	1.102465	111.130076	–65.071460	H_{32}	1.102556	110.870805	175.265051
H_5	1.102559	110.882618	174.930639	H_{33}	1.102845	111.104486	55.090515
H_6	1.102873	111.099552	54.744385	H_{34}	1.102524	110.896590	175.398025
H_7	1.102434	111.131429	–64.740187	H_{35}	1.102850	111.093601	55.217382
H_8	1.102548	110.898497	175.247404	H_{36}	1.102460	111.131062	–64.587149

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