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THE FULL NON-RIGID GROUP THEORY FOR TRIMETHYLBORANE WITH C_{3v}, C_{3h} AND C_S POINT GROUPS.

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Abstract

The full non-rigid molecule group theory in which the dynamical symmetry operations are defined as physical operations is a new field in chemistry. According to H. C. Longuet Higgins's paper in 1963, many types of non rigid molecules, such as trimethylborane, have very rapid effective symmetry, which increases with their number of internal rotation. In this work, we study the full non-rigid groups (f-NRG) of trimethylborane with C_{3v}, C_{3h} and C_S points groups and prove that they are the groups of order 162, with 13 conjugacy classes for C_{3h} and C_{3v} point groups and order 54, with 15 conjugacy classes for C_S point group. We apply a simple method to compute the character tables of these groups.

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Key words: trimethylborane; non-rigid group; character table; groups algorithms and programming (GAP)

Resumen

La teoría de grupos de moléculas totalmente no rígidas en la que se definen las operaciones de simetría dinámica como operaciones físicas es un nuevo campo de la química. Según el trabajo de H. C. Longuet Higgins en 1963, muchos tipos de moléculas no rígidos, como el trimetillborano, tienen una muy rápida simetría efectiva, la cual aumenta con su número de rotación interna. En este trabajo estudiamos los grupos totalmente no rígidos (f-NRG) del trimetillborano con grupos puntuales C_{3v}, C_{3h} y C_S y demostramos que los grupos son de orden 162, con 13 clases de conjugación para los grupos puntuales C_{3h} y C_{3v} y orden 54, con 15 clases de conjugación para el grupo puntual C_S. Aplicamos un método sencillo para calcular las tablas de caracteres de estos grupos.

Palabras clave: trimetilborano; grupo no rígido; tabla de caracteres; grupos algoritmos y promagración (GAP)

Introduction

The mathematical tools of group theory have been used extensively for the analysis of the symmetry properties of physical systems. Group theory is the mathematics of symmetries and plays an important role in the study of molecules, crystals, and clusters in chemistry although applications have usually been restricted to small or moderately sized systems due to computational limitations. To be practical for large systems, finite group theory requires both computer calculation and the advanced computational methods. Otherwise, the symmetry properties of rigid molecules are well known and so it is natural to investigate non-rigid molecules.

Large nuclear shifts arise when periodic internal rearrangements of individual atoms or whole molecular fragments take place in the molecule. The transition of the system of nuclei from one steric configuration to another constitutes the high-amplitude motion and the molecules where such transitions occur are referred to as stereochemically non-rigid!

In principle any molecules with identical nuclei can have several steric configurations differing from one another as a result of nuclear transpositions, provided that these transpositions are not equivalent to the rotation of the molecules as a whole. When the rotational barrier in low and rotation is essentially free, such as in the case of CH_3BF_2 and $(CH_3)_3B$, the interpretation of the IR spectra of the C-H stretching region in the partially deuterated compounds is more complicated [1]. Group theory for these non-rigid molecules is more relevant to large amplitude motion of these molecules that its applications have appeared in the literature [2-9].

Lomont [10] has given two methods for calculating character tables. These are satisfactory for small groups, but both of them require knowledge of the class constant and hence of the group multiplication table and they become very unwieldy as soon as the order of the group becomes even moderately large. For non-rigid molecules, whose symmetry groups may have several thousand elements, they are usually quite impracticable.

In a series of paper Ashrafi and coauthors computed full non-rigid groups of some molecules such as tetraammine platinum(II) [11], cis- and transdichlorodiammine platinum(II) and trimethylamine [12], tetraammine platinum(II) with C_{2v} and C_{4v} point group [13,14], tetraamine platinum(II) as a wreath product [15], tetra-tertbutyltetrahedrane [16], tetramethylethylene [17], hexamethylbenzene [18] and melanine [19].

In [20], Longuet-Higgins investigated the symmetry groups of non-rigid molecules, where changes from one conformation to another can occur easily. In many cases, these symmetry groups are not isomorphic with any of the familiar symmetry groups of rigid molecules and their character tables are not known. It is therefore of some interest and importance to develop simple methods of

calculating these character tables, which are needed for classification of wave functions, determination of selection rules, and so on.

A flexible molecule may show more than one conformer and the stable structures can lie far away on the potential energy surface [21]. So, in this paper, we investigate the f-NRG of trimethylborane with C_{3v}, C_{3h} and C_S point groups. Using the chemistry package Hyperchem and the group theory package GAP, we calculate the conjugacy classes and character tables of these geometries for $B(CH_3)_3$. Throughout this note, all considered groups are assumed to be finite. Our notation is standard and is taken mainly from [22,23].

Theoretical method and results

Determination of conjugacy classes

First of all, we consider the point group of trimethylborane in the case of non-rigid state. The aim of this section is to calculate the conjugacy classes of full non-rigid group of this molecule with different symmetry groups C_{3h}, C_{3v} and C_S, which denoted by G, H and K, respectively. By Figure 1(a, b and c), we have three rotations α_1=(1,2,3), α_2=(4,5,6) and α_3=(7,8,9) for three methyl groups. We assume that these operations are all feasible, that barrier to rotation of the methyl group is low. Also, we have a C_3 rotation,

$$\alpha_4=(10,11,12)(1,4,7)(2,5,8)(3,6,9),$$

for C_{3h} and C_{3v} point groups. Now let β_1 be the permutation in correspondence to σh for C_{3h} and C_S point groups and γ_1, γ_2 and γ_3 be permutations in correspondence to σv, $\sigma'v$ and $\sigma''v$ for C_{3v} point group. Then, we have

$$\beta_1=(1,3)(4,6)(7,9),$$
$$\gamma_1=(2,3)(5,9)(6,8)(4,7)(11,12),$$
$$\gamma_2=(5,6)(1,7)(2,9)(3,8)(10,12),$$
$$\gamma_3=(8,9)(1,4)(3,5)(2,6)(10,11).$$

The permutations (α_1, α_2, α_3, α_4, β_1), (α_1, α_2, α_3, α_4, γ_1, γ_2, γ_3) and (α_1, α_2, α_3, β_1) generate the groups G, H and K, respectively, and a simple GAP program shows that G and H are groups of order 162 with 13 conjugacy classes and K is group of order 54 with 15 conjugacy classes. Note that the groups G and H are not isomorphic (in fact $G'=\langle\alpha_1, \alpha_2, \alpha_3\rangle$, $H'=\langle\alpha_1, \alpha_2, \alpha_3, \alpha_4\rangle$, where G' and H' are derived subgroups of G and H, respectively [24]. The representative for conjugacy classes of G, H and K are shown in Tables 1, 2 and 3, respectively.

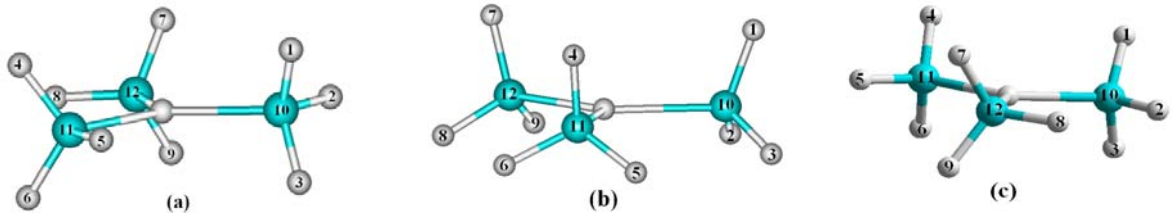

Figure 1. The structures of trimethylborane with (a) C_{3h}, (b) C_{3v} and (c) C_S symmetries.

Table 1. The representatives of conjugacy classes of the group G (C_{3h}).

No.	Representative	Size	Name	Symmetry
1	()	1	1a	1
2	(7,8,9)	6	3a	α_3
3	(4,5,6)(7,8,9)	6	3b	$\alpha_2\alpha_3$
4	(4,5,6)(7,9,8)	6	3c	$\alpha_2\alpha_3^{-1}$
5	(2,3)(5,6)(8,9)	27	2a	$\beta_1\alpha_1\alpha_2\alpha_3$
6	(1,2,3)(4,5,6)(7,8,9)	2	3d	$\alpha_1\alpha_2\alpha_3$
7	(1,2,3)(4,5,6)(7,9,8)	6	3e	$\alpha_1\alpha_2\alpha_3^{-1}$
8	(1,4,7)(2,5,8)(3,6,9)(10,11,12)	9	3f	α_4
9	(1,4,7,2,5,8,3,6,9)(10,11,12)	18	9a	$\alpha_4\alpha_1$
10	(1,4,7)(2,6,8,3,5,9)(10,11,12)	27	6a	$\alpha_4\alpha_3^{-1}\alpha_2^{-1}\alpha_1^{-1}\beta_1$
11	(1,7,4)(2,8,5)(3,9,6)(10,12,11)	9	3g	α_4^{-1}
12	(1,7,5,2,8,6,3,9,4)(10,12,11)	18	9b	$\alpha_3\alpha_4^{-1}$
13	(1,7,4)(2,9,5,3,8,6)(10,12,11)	27	6b	$\beta_1\alpha_1\alpha_2\alpha_3\alpha_4^{-1}$

Table 2. The representatives of conjugacy classes of the group H (C_{3v}).

No.	Representative	Size	Name	symmetry
1	()	1	1a	1
2	(7,8,9)	6	3a	α_3
3	(4,5,6)(7,8,9)	3	3b	$\alpha_2\alpha_3$
4	(4,5,6)(7,9,8)	6	3c	$\alpha_2\alpha_3^{-1}$
5	(4,6,5)(7,8,9)	3	3d	$\alpha_2^{-1}\alpha_3$
6	(2,3)(4,7)(5,9)(6,8)(11,12)	27	2a	γ_1
7	(2,3)(4,7,5,9,6,8)(11,12)	27	6a	$\alpha_3^{-1}\gamma_1^{-1}$
8	(2,3)(4,7,6,8,5,9)(11,12)	27	6b	$\gamma_3^{-1}\alpha_3^{-1}\alpha_4^{-1}$
9	(1,2,3)(4,5,6)(7,8,9)	6	3e	$\alpha_1\alpha_2\alpha_3$
10	(1,2,3)(4,5,6)(7,9,8)	2	3f	$\alpha_1\alpha_2\alpha_3^{-1}$
11	(1,4,7)(2,5,8)(3,6,9)(10,11,12)	18	3g	α_4
12	(1,4,7,2,5,8,3,6,9)(10,11,12)	18	9a	$\alpha_4\alpha_1$
13	(1,4,7,3,6,9,2,5,8)(10,11,12)	18	9b	$\alpha_4\alpha_1^{-1}$

Table 3. The representatives of conjugacy classes of the group K (C_S).

No.	Representative	Size	Name	Symmetry
1	()	1	1a	1
2	(7,8,9)	2	3a	α_3
3	(4,5,6)	2	3b	α_2
4	(7,8,9)(4,5,6)	2	3c	$\alpha_2\alpha_3$
5	(7,9,8)(4,5,6)	2	3d	$\alpha_2\alpha_3^{-1}$
6	(8,9)(5,6)(2,3)	27	2a	$\beta_1^{-1}\alpha_1\alpha_2\alpha_3$
7	(1,2,3)	2	3e	α_1
8	(7,8,9)(1,2,3)	2	3f	$\alpha_1\alpha_3$
9	(7,9,8)(1,2,3)	2	3g	$\alpha_1\alpha_3^{-1}$
10	(4,5,6)(1,2,3)	2	3h	$\alpha_1\alpha_2$
11	(7,8,9)(4,5,6)(1,2,3)	2	3i	$\alpha_1\alpha_2\alpha_3$
12	(7,9,8)(4,5,6)(1,2,3)	2	3j	$\alpha_1\alpha_2\alpha_3^{-1}$
13	(4,6,5)(1,2,3)	2	3k	$\alpha_1\alpha_2^{-1}$
14	(7,8,9)(4,6,5)(1,2,3)	2	3l	$\alpha_1\alpha_2^{-1}\alpha_3$
15	(7,9,8)(4,6,5)(1,2,3)	2	3m	$\alpha_1\alpha_2^{-1}\alpha_3^{-1}$

Determination of character table

From the conjugacy classes of the groups G, H and K in the last section, we are able to compute the whole irreducible character table for them, separately. The values of the irreducible characters χ_i ($1 \le i \le 13$ for C_{3h} and C_{3v} symmetries and $1 \le i \le 15$ for C_S symmetry) at each class occupies the rest of Tables 4, 5 and 6, respectively.

We know the rigid configuration of trimethylborane has 13 atoms and 3N-6=39-6=33 degrees of internal freedom, according to the C_{3h} symmetry (the most stable configuration of this molecule [25]) and it can be classified as:

$$\Gamma_{vib} = 6A' + 5A'' + 7E' + 4E''$$

But the configuration with C_{3h} (non-rigid) symmetry possesses 3N-6-n=39-6-26=7 [26] (where n=27-1 is the number of all possible rotations of methyl groups) normal modes with the symmetry representations:

C_{3h}	1(1a)	6(3a)	6(3b)	6(3c)	27(2a)	2(3d)	6(3e)	9(3f)	18(9a)	27(6a)	9(3g)	18(9b)	27(6b)
Γ_σ	12	9	6	6	3	3	3	0	0	0	0	0	0

$$\Gamma_\sigma = \frac{3}{2}\chi_1 + \frac{1}{2}\chi_2 + \frac{1}{2}\chi_3 + \frac{1}{2}\chi_4 + \frac{3}{2}\chi_5 + \frac{3}{2}\chi_6 + \chi_{11}$$

Table 4. The character table and power map of group G (C_{3h}).

C_{3h} (non-rigid)	1a	3a	3b	3c	2a	3d	3e	3f	9a	6a	3g	9b	6b
χ_1	1	1	1	1	1	1	1	1	1	1	1	1	1
χ_2	1	1	1	1	-1	1	1	1	1	-1	1	1	-1
χ_3	1	1	1	1	-1	1	1	σ	σ	-σ	ρ	ρ	-ρ
χ_4	1	1	1	1	-1	1	1	ρ	ρ	-ρ	σ	σ	-σ
χ_5	1	1	1	1	1	1	1	σ	σ	σ	ρ	ρ	ρ
χ_6	1	1	1	1	1	1	1	ρ	ρ	ρ	σ	σ	σ
χ_7	2	-1	-1	2	0	2	-1	2	-1	0	2	-1	0
χ_8	2	-1	-1	2	0	2	-1	2σ	-σ	0	2ρ	-ρ	0
χ_9	2	-1	-1	2	0	2	-1	2ρ	-ρ	0	2σ	-σ	0
χ_{10}	6	0	-3	0	0	-3	3	0	0	0	0	0	0
χ_{11}	6	3	0	0	0	-3	-3	0	0	0	0	0	0
χ_{12}	6	-3	3	0	0	-3	0	0	0	0	0	0	0
χ_{13}	6	0	0	-3	0	6	0	0	0	0	0	0	0

$$\rho = e^{\frac{2\pi i}{3}} = -\frac{1}{2} + i\frac{\sqrt{3}}{2}, \sigma = e^{\frac{4\pi i}{3}} = -\frac{1}{2} - i\frac{\sqrt{3}}{2}, i = \sqrt{-1}$$

Table 5. The character table and power map of group H (C_{3v}).

C_{3v} (non-rigid)	1a	3a	3b	3c	3d	2a	6a	6b	3e	3f	3g	9a	9b
χ_1	1	1	1	1	1	1	1	1	1	1	1	1	1
χ_2	1	1	1	1	1	-1	-1	-1	1	1	1	1	1
χ_3	2	2	2	2	2	0	0	0	2	2	-1	-1	-1
χ_4	2	-1	-1	2	2	0	0	0	2	-1	2	-1	-1
χ_5	2	-1	-1	2	2	0	0	0	2	-1	-1	-1	2
χ_6	2	-1	-1	2	2	0	0	0	2	-1	-1	2	-1
χ_7	3	0	0	3σ	3ρ	-1	-ρ	-σ	3	0	0	0	0
χ_8	3	0	0	3ρ	3σ	-1	-σ	-ρ	3	0	0	0	0
χ_9	3	0	0	3σ	3ρ	1	ρ	σ	3	0	0	0	0
χ_{10}	3	0	0	3ρ	3σ	1	σ	ρ	3	0	0	0	0
χ_{11}	6	0	-3	0	0	0	0	0	-3	3	0	0	0
χ_{12}	6	3	0	0	0	0	0	0	-3	-3	0	0	0
χ_{13}	6	-3	3	0	0	0	0	0	-3	0	0	0	0

$$\rho = e^{\frac{2\pi i}{3}} = -\frac{1}{2} + i\frac{\sqrt{3}}{2}, \sigma = e^{\frac{4\pi i}{3}} = -\frac{1}{2} - i\frac{\sqrt{3}}{2}, i = \sqrt{-1}$$

Table 6. The character table and power map of group K (C_S).

C_S (non-rigid)	1a	3a	3b	3c	3d	2a	3e	3f	3g	3h	3i	3j	3k	3l	3m
χ_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
χ_2	1	1	1	1	1	-1	1	1	1	1	1	1	1	1	1
χ_3	2	2	2	2	2	0	-1	-1	-1	-1	-1	-1	-1	-1	-1
χ_4	2	2	-1	-1	-1	0	-1	-1	-1	2	2	2	-1	-1	-1
χ_5	2	-1	2	-1	-1	0	2	-1	-1	2	-1	-1	2	-1	-1
χ_6	2	-1	-1	-1	2	0	-1	2	-1	2	-1	-1	-1	-1	2
χ_7	2	-1	-1	2	-1	0	-1	-1	2	2	-1	-1	-1	2	-1
χ_8	2	-1	2	-1	-1	0	-1	-1	2	-1	-1	2	-1	-1	2
χ_9	2	-1	2	-1	-1	0	-1	2	-1	-1	2	-1	-1	2	-1
χ_{10}	2	2	-1	-1	-1	0	-1	-1	-1	-1	-1	-1	2	2	2
χ_{11}	2	2	-1	-1	-1	0	2	2	2	-1	-1	-1	-1	-1	-1
χ_{12}	2	-1	-1	-1	2	0	-1	-1	2	-1	2	-1	2	-1	-1
χ_{13}	2	-1	-1	-1	2	0	2	-1	-1	-1	-1	2	-1	2	-1
χ_{14}	2	-1	-1	2	-1	0	-1	2	-1	-1	-1	2	2	-1	-1
χ_{15}	2	-1	-1	2	-1	0	2	-1	-1	-1	2	-1	-1	-1	2

Symmetry of trimethylborane

Symmetry operations on a graph, graph automorphisms, affect only on the label of vertices by permuting them such that the adjacency matrix of the graph remains unchanged. The graph symmetry is completely determined by all its automorphisms, i.e., by specifying all the permutations which leave the adjacency matrix invariant.

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 trimethylborane (Figures 1) with C_{3h}, C_{3v} and C_S point groups to illustrate the Euclidean graphs (Figures 2) and their automorphism groups. It suffices to measure the Euclidean distances (Table 7) in terms of the H−H bond lengths and then constructs the Euclidean distance matrix A. It should be mentioned that one does not have to work with exact Euclidean distances in which 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. For the molecule under consideration, we map the Euclidean edge weighted for trimethylborane with C_{3h} point group as 1.747→1, 3.583→2, 2.889→3, 3.987→4, 4.343→5, 3.890→6, 1.07→7, 3.538→8, 2.862→9,

3.104→10, 3.736→11 and 2.858→12 where the weights are calculated using PM3 method of the chemistry package Hyperchem [27]. Note that all permutations of the vertices do not belong to the automorphism group of the weighted graph since the weights of all the edges are not the same. For example, the permutation (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12) does not belong to the automorphism group since the resulting graph shown in Figure 2 does not preserve connectivity.

We computed below the distance matrix A for trimethylborane with C_{3h} point group.

$$A=\begin{bmatrix} 0 & 1 & 1 & 2 & 3 & 4 & 2 & 5 & 4 & 7 & 10 & 8 \\ 1 & 0 & 1 & 5 & 6 & 5 & 3 & 6 & 3 & 7 & 11 & 9 \\ 1 & 1 & 0 & 4 & 3 & 2 & 4 & 5 & 2 & 7 & 10 & 8 \\ 2 & 5 & 4 & 0 & 1 & 1 & 2 & 3 & 4 & 8 & 7 & 10 \\ 3 & 6 & 3 & 1 & 0 & 1 & 5 & 6 & 5 & 9 & 7 & 11 \\ 4 & 5 & 2 & 1 & 1 & 0 & 4 & 3 & 2 & 8 & 7 & 10 \\ 2 & 3 & 4 & 2 & 5 & 4 & 0 & 1 & 1 & 10 & 8 & 7 \\ 5 & 6 & 5 & 3 & 6 & 3 & 1 & 0 & 1 & 11 & 9 & 7 \\ 4 & 3 & 2 & 4 & 5 & 2 & 1 & 1 & 0 & 10 & 8 & 7 \\ 7 & 7 & 7 & 8 & 9 & 8 & 10 & 11 & 10 & 0 & 12 & 12 \\ 10 & 11 & 10 & 7 & 7 & 7 & 8 & 9 & 8 & 12 & 0 & 12 \\ 8 & 9 & 8 & 10 & 11 & 10 & 7 & 7 & 7 & 12 & 12 & 0 \end{bmatrix}$$

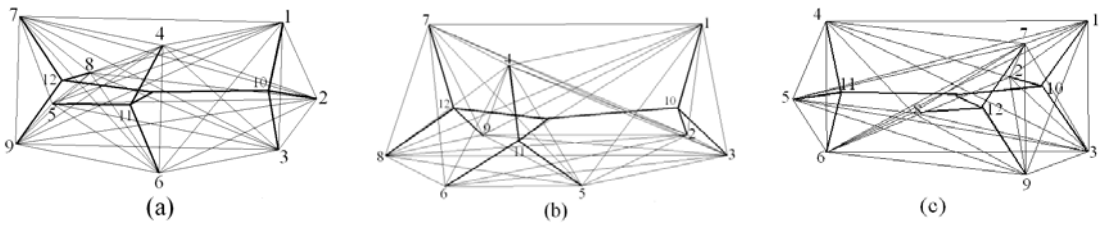

Figure 2. The Euclidean graph of Trimethylborane with (a) C_{3h}, (b) C_{3v} and (c) C_S point groups.

Table 7. Euclidean edges for trimethylborane with C_{3h} point group.

No.	1	2	3	4	5	6	7	8	9	10	11	12
1	0	1.747	1.747	3.583	2.889	3.987	3.583	4.343	3.987	1.07	3.104	3.538
2	1.747	0	1.747	4.343	3.890	4.343	2.889	3.89	2.889	1.07	3.736	2.862
3	1.747	1.747	0	3.987	2.889	3.583	3.987	4.343	3.583	1.07	3.104	3.538
4	3.583	4.343	3.987	0	1.747	1.747	3.583	2.889	3.987	3.538	1.07	3.104
5	2.889	3.890	2.889	1.747	0	1.747	4.343	3.890	4.343	2.862	1.07	3.736
6	3.987	4.343	3.583	1.747	1.747	0	3.987	2.889	3.583	3.538	1.07	3.104
7	3.583	2.889	3.987	3.583	4.343	3.987	0	1.747	1.747	3.104	3.538	1.07
8	4.343	3.890	4.343	2.889	3.890	2.889	1.747	0	1.747	3.736	2.862	1.07
9	3.987	2.889	3.583	3.987	4.343	3.583	1.747	1.747	0	3.104	3.538	1.07
10	1.07	1.07	1.07	3.538	2.862	3.538	3.104	3.736	3.104	0	2.858	2.858
11	3.104	3.736	3.104	1.07	1.07	1.07	3.538	2.862	3.538	2.858	0	2.858
12	3.538	2.862	3.538	3.104	3.736	3.104	1.07	1.07	1.07	2.858	2.858	0

GAP Program

The symmetry group of trimethylborane can be computed using the following GAP [28] programs for each point group. In the programs below the function PermutationGroup() optimizes the underlying permutation group by omitting all permutations which do not left invariant the set of vertices with different weight set of incident edges. Also the function SymmetryGroup() determine the symmetry group of the rigid point group of the molecule with given distance matrix.

```
PermutationGroup:=function(A)
local list,dimension,counter,row,previousrow,isnew,listcounter;
list:=[[1]];
dimension:=DimensionsMat(A)[1];
counter:=2;
while counter<=dimension do
row:=StructuralCopy(A[counter]);
Sort(row);
 isnew:=true;
 for listcounter in [1..Number(list)] do
 previousrow:=StructuralCopy(A[list[listcounter][1]]);
 Sort(previousrow);
 if row=previousrow then
 Add(list[listcounter],counter);
 isnew:=false;
 fi;
 od;
 if isnew=true then
 Add(list,[counter]);
  fi;
  counter:=counter+1;
 od;
 return Group(Concatenation(List(List(list,SymmetricGroup),GeneratorsOfGroup)));
 end;

SymmetryGroup:=function(A)
  local n,S,list,element,X,Y,counter;
  n:=DimensionsMat(A)[1];
  S:=PermutationGroup(A);
  List:=[];
  counter:=1;
  for element in S do
  X:=PermutationMat(element,n);
  Y:=TransposedMat(X);
  if Y*A*X=A then
```

```
  Add(list,element);
  fi;
  counter:=counter+1;
  od;
  return Group(list);
end;
```

Utilizing the SymmetryGroup() function for matrix A, we obtain the following group

G_A={(), (1,7,4)(2,8,5)(3,9,6)(10,12,11), (1,3)(4,6)(7,9),
(1,9,4,3,7,6)(2,8,5)(10,12,11), (1,4,7)(2,5,8)(3,6,9)(10,11,12),
(1,6,7,3,4,9)(2,5,8)(10,11,12)}

for the rigid trimethylborane with C_{3h} point group (where the elements of G_A are in correspondence with the symmetries, α_4^{-1}, β_1^{-1}, $\beta_1^{-1}\alpha_4^{-1}$, α_4 and β_1 respectively).

With the same method, we can show that

H_B={(), (1,7,4)(2,8,5)(3,9,6), (1,4,7)(2,5,8)(3,6,9),
(1,4)(2,6)(3,5)(8,9), (2,3)(4,7)(5,9)(6,8), (1,7)(2,9)(3,8)(5,6)}
K_C={(), (1,3)(4,6)(7,9)}

for the rigid trimethylborane with C_{3v} and C_S point groups (where the elements of H_B and K_C are in correspondence to the symmetries $\{\alpha_4^{-1}, \alpha_4, \gamma_3, \gamma_1 \text{ and } \gamma_2\}$ and $\{\beta_1\}$, respectively). It is straightforward to verify that the $G_A \cong C_6$ is a cyclic group, $H_B \cong S_3$ is the full symmetry group on three letters and $K_C \cong C_2$ is a cyclic group.

Conclusions

If G and H comprise of all symmetries of the full non-rigid group of trimethylborane with C_{3h} and C_{3v} point groups, then we have shown that G and H are non-isomorphic groups of order 162 with 13 conjugacy classes and K is group of order 54 with 15 conjugacy classes. Also we computed the character table of G, H and K using GAP small group library.

Finally suppose G_A, H_B and K_C denote the set of all permutations, which preserves the Euclidean connectivity for trimethylborane with C_{3h}, C_{3v} and C_S point groups, respectively. Then using our GAP program "SymmetryGroup()", we have G_A, H_B and K_C are isomorphic to the cyclic group C_6 , the symmetric group on three letters S_3, and the cyclic group C_2, respectively.

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