Full Length Research Paper

Full non-rigid group theory and symmetry of some diborane derivatives

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The full non-rigid (f.NRG) molecules group theory is seen to be used advantageously to study the internal dynamics of such molecules. In this work, a computational method is applied to study the f.NRG of cis- and trans- dimethyl diborane, trimethyl diborane and tetramethyl diborane with different point groups. We considered the point groups of them and computed the other, conjugacy classes and the corresponding symmetry for each permutation. Also the irreducible character tables of them are calculated.

Key words: Non-rigid group, character table, cis- and trans-dimethyl diborane, trimethyl diborane, tetramethyl diborane.

INTRODUCTION

Group theory for non-rigid molecules is becoming increasingly relevant and its numerous applications to vibrational spectroscopy of small molecules are appearing in the literatures (Bunker, 1979; Altmann, 1977; Ezra, 1982; Maruani and Serre, 1983; Smeyers et al., 1993, 1998; Vivier-Bunge et al., 1998). As it is well known, group theory for non-rigid molecules was essentially developed for two points of view: 1) The molecular symmetry group theory (MSG) of permutation inversion groups constructed by permutations and permutation-inversions of identical particles (the MSG group is formed by all feasible permutations); 2) the full and restricted non-rigid group theory built up with physical operations, expressed in terms of internal coordinates that transform one conformation into another iso-energetic one (Longuet-Higgins, 1963).

As a classical electron-deficient molecule with unique hydrogen bridge bonding, diborane has created considerable interest in the structural chemistry (Shriver and Atkins, 2001). Diborane exists as the molecule B_2H_6 and the molecular formulas of the compounds of intermediate compositions are observed to be $B_2H_5(CH_3)$, $B_2H_4(CH_3)_2$, $B_2H_3(CH_3)_3$ and $B_2H_2(CH_3)_4$. In addition, it has been documented that diborane can undergo polymerization into higher boron hydrides, which makes borane chemistry an intriguing area for both experimental and theoretical studies. The symmetry properties of rigid molecules are well known and so it is natural to investigate non-rigid molecules. The non-rigid molecule group (NRG) theory in which the dynamic symmetry operations are defined as physical operations is a new field in chemistry.

Smeyers (1992) in a series of papers, applied this notion to determine the character table of restricted NRG of some molecules. For example, Smeyers and Villa (2000) computed the r-NRG of the triple equivalent methyl rotation in pyramidal trimethyl amine with inversion and proved that the r-NRG of this molecule is a group of order 648, containing two subgroups of order 324 without inversion.

Also, Balasubramanian (2004a, b) has computed full non-rigid group of some molecules. For example, he computed the full non-rigid group for water pentamer and extended aromatic $C_{48}N_{12}$ azafullerene. In a series of paper, some authors computed full non-rigid group of some molecules such as tetraammine platinum(II) (Ashrafi

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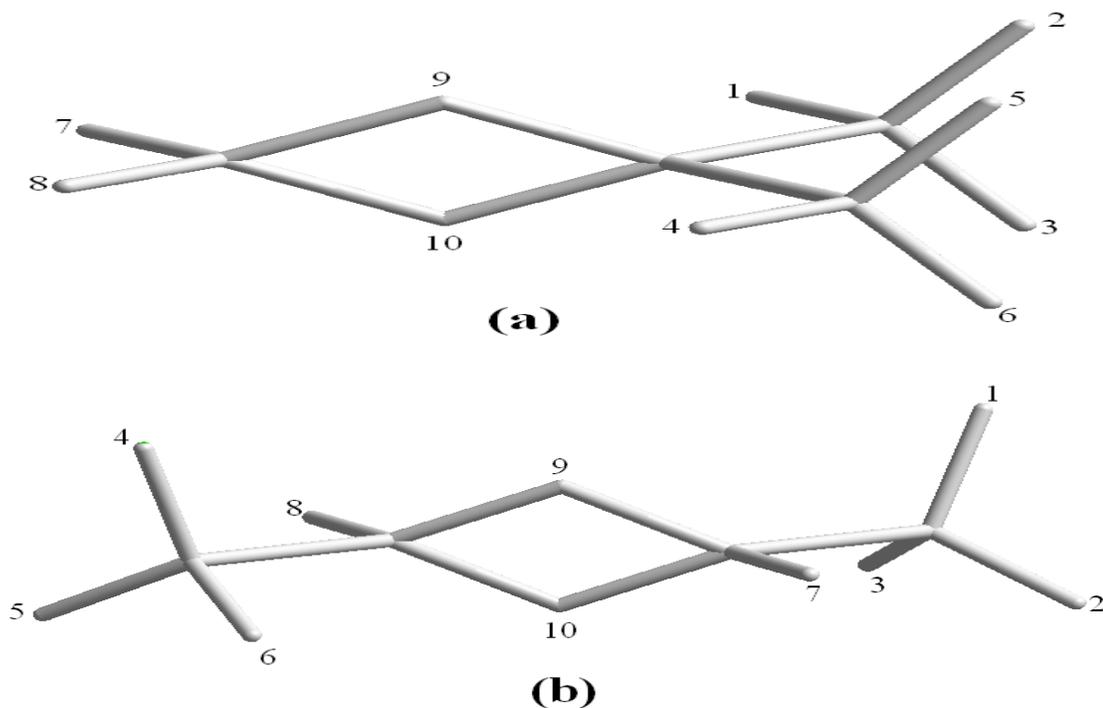
Figure 1. The structure of cis- dimethyl diborane (a), with CS symmetry and trans- dimethyl diborane; (b), with C2 symmetry.

and Hamadanian, 2003), cis- and trans-dichloro-diammine platinum(II) and trimethylamine (Hamadanian and Ashrafi, 2003), tetraammine platinum(II) with C_{2v} and C_{4v} point group (Ashrafi and Hamadanian, 2004; Darafsheh et al., 2005a), tetraamine platinum(II) as wreath product (Darafsheh et al., 2005b), hexamethylbenzene (Darafsheh et al., 2006) and melamine (Ashrafi and Hamadanian, 2005).

MATERIALS AND METHODS

In this paper, the full non-rigid groups of tetramethyldiborane, trimethyl diborane and cis- and trans-dimethyl diborane are computed. Firstly, the algebraic structures of the full non-rigid group of these molecules are specified. Then, based on the structure of the group, a useful programming language, namely, "Groups, Algorithms and Programming" (GAP) (The GAP Group, 2008) is applied and the character Tables of full non-rigid molecules group theory (f-NRG) of these molecules are computed. The GAP package is used to find many properties of the groups (Karimi et al., 2011; Ashrafi and Ghorbani, 2010; Moghani et al., 2010). We determine the order of the f-NRG of these diborane derivative and conjugacy classes of the molecules. Finally, we calculate the character tables of the molecules.

Our computations were carried out using the GAP system. GAP is a free and extensible software package for computation in discrete abstract algebra, in which you can write your own programs in the GAP language and use them in the same way the programs which form part of the system are used. More information on the motivation and development of GAP to date can be found on the GAP web page (http://www.gapsystem.org/).

MAIN RESULT AND DISCUSSION

Theoretical method of determining conjugacy classes and character tables

First of all, we consider the point group of cis- and trans-dimethyl diborane, trimethyl diborane and tetramethyl diborane in the case of rigid state and determine the point groups of f.NRG of these molecules with symmetry groups Cs, C_2, Cs and D_{2h}, which denoted by H, K, L and G, respectively. Then, we apply H, K, L and G to compute their conjugacy classes and character tables.

Cis- and trans- dimethyl diborane

Now, we consider the point groups H and K of the f-NRG of cis- and trans-dimethyl diborane. From the Figures 1a and b, it follows that the elements $\alpha_1 = (1, 2, 3)$ and $\alpha_2 = (4, 5, 6)$ in the groups H and K permuting hydrogens in either of CH_3 cases together with the element α_1 and α_2. Also, $(1,4)(2,5)(3,6)(7,8)$ corresponding to σ reflection (β_1) and C_2 rotation (α_3) in the cis- and trans- dimethyl diboranes, respectively generate the groups H and K. In particular, K=H and it is easy to see that these groups have order 18 with 9 conjugacy classes. The representatives for conjugacy classes of H and K are given in Table 1. Also the character table of H and K can

Table 1. The representatives of conjugacy classes of the groups H and K.

No.	Representative	Size	Name	Symmetry Cs	Symmetry C$_2$
1	()	1	1a	E	E
2	(4,5,6)	2	3a	α_2	α_2
3	(4,6,5)	2	3b	α_2^{-1}	α_2^{-1}
4	(1,2,3)(4,5,6)	1	3c	$\alpha_1\alpha_2$	$\alpha_1\alpha_2$
5	(1,2,3)(4,6,5)	2	3d	$\alpha_1\alpha_2^{-1}$	$\alpha_1\alpha_2^{-1}$
6	(1,3,2)(4,6,5)	1	3e	$\alpha_1^{-1}\alpha_2^{-1}$	$\alpha_1^{-1}\alpha_2^{-1}$
7	(1,4)(2,5)(3,6)(7,8)	3	2a	β_1	α_3
8	(1,4,2,5,3,6)(7,8)	3	6a	$\alpha_1\beta_1$	$\alpha_1\alpha_3$
9	(1,4,3,6,2,5)(7,8)	3	6b	$\alpha_1^{-1}\beta_1$	$\alpha_1^{-1}\alpha_3$

Table 2. The character table of the groups H and K.

C$_2$ or Cs (non-rigid)	1a	3a	3b	3c	3d	3e	2a	6a	6b
χ_1	1	1	1	1	1	1	1	1	1
χ_2	1	1	1	1	1	1	-1	-1	-1
χ_3	1	ρ	σ	σ	1	ρ	-1	$-\rho$	$-\sigma$
χ_4	1	σ	ρ	ρ	1	σ	-1	$-\sigma$	$-\rho$
χ_5	1	ρ	σ	σ	1	ρ	1	ρ	σ
χ_6	1	σ	ρ	ρ	1	σ	1	σ	ρ
χ_7	2	-1	-1	2	-1	2	0	0	0
χ_8	2	$-\sigma$	$-\rho$	2ρ	-1	2σ	0	0	0
χ_9	2	$-\rho$	$-\sigma$	2σ	-1	2ρ	0	0	0

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

be easily computed using GAP function Irr (G).

From conjugacy classes of the groups H and K, we were able to compute the irreducible character table of the molecules. The values of the irreducible character $\chi_i (1 \le i \le 9)$ for Cs and C$_2$ symmetries is shown in Table 2.

We know the rigid configuration of cis- and trans-dimethyl diborane have 14 atoms and 3N-6=42-6=36 degrees of internal freedom according to the Cs and C$_2$ symmetries and it can be classified as: $\Gamma_{vib} = 17A' + 2A''$ for Cs symmetry and $\Gamma_{vib} = 7A + 7B$ for C$_2$ symmetry. But the configuration with Cs (non-rigid) and C$_2$ (non-rigid) symmetries possess some rotations of methyl groups with the symmetry representations:

Cs (Non-rigid)	1(1a)	2(3a)	2(3b)	1(3c)	2(3d)	1(3e)
	3(2a)	3(6a)	3(6b)			
Γ_σ	14	11	11	8	8	8
	4	4	4			

$$\Gamma_\sigma = 7\chi_1 + 3\chi_2 + \chi_8 + \chi_9$$

C$_2$ (Non-rigid)	1(1a)	2(3a)	2(3b)	1(3c)	2(3d)	1(3e)
	3(2a)	3(6a)	3(6b)			
Γ_σ	14	11	11	8	8	8
	0	0	0			

$$\Gamma_\sigma = 5\chi_1 + 5\chi_2 + \chi_8 + \chi_9$$

Figure 2. The structure of trimethyl diborane with C_S symmetry.

Table 3. The representatives of conjugacy classes of the group L.

No.	Representative	Size	Name	Symmetry
1	()	1	1a	E
2	(7,8,9)	2	3a	α_3
3	(4,5,6)	2	3b	α_2
4	(4,5,6)(7,8,9)	2	3c	$\alpha_2\alpha_3$
5	(4,5,6)(7,9,8)	2	3d	$\alpha_2\alpha_3^{-1}$
6	(2,3)(5,6)(8,9)(10,11)	27	2a	β_1^{-1}
7	(1,2,3)	2	3e	α_1
8	(1,2,3)(7,8,9)	2	3f	$\alpha_1\alpha_3$
9	(1,2,3)(7,9,8)	2	3g	$\alpha_1\alpha_3^{-1}$
10	(1,2,3)(4,5,6)	2	3h	$\alpha_1\alpha_2$
11	(1,2,3)(4,5,6)(7,8,9)	2	3i	$\alpha_1\alpha_2\alpha_3$
12	(1,2,3)(4,5,6)(7,9,8)	2	3j	$\alpha_1\alpha_2\alpha_3^{-1}$
13	(1,2,3)(4,6,5)	2	3k	$\alpha_1\alpha_2^{-1}$
14	(1,2,3)(4,6,5)(7,8,9)	2	3l	$\alpha_1\alpha_2^{-1}\alpha_3$
15	(1,2,3)(4,6,5)(7,9,8)	2	3m	$\alpha_1\alpha_2^{-1}\alpha_3^{-1}$

Trimethyl diborane with Cs point group

Similar mentioned method, by Figure 2 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 reflection, β_1 = (2,3)(5,6)(8,9)(10,11)

for Cs point group. The permutations ($\alpha_1, \alpha_2, \alpha_3$ and β_1) generate the group L and a simple GAP program shows that L is group of order 54 with 15 conjugacy classes. The representative for conjugacy classes and character table of L are shown in Tables 3 and 4.

We know the rigid configuration of trimethyl diborane have 17 atoms and 3N-6=51-6=45 degrees of internal

Table 4. The character table of the group L.

Cs (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
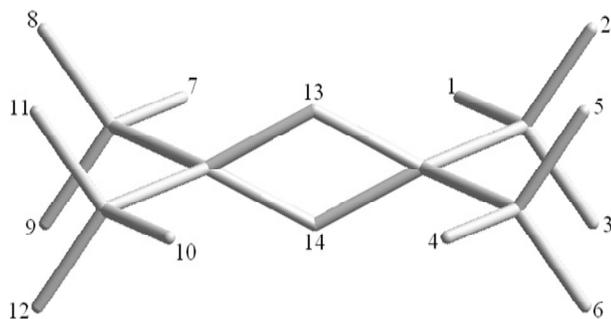
Figure 3. The structure of tetramethyl diborane with D_{2h} symmetry.

freedom according to the Cs symmetry and it can be classified as: $\Gamma_{vib} = 12A' + 5A''$. But the configuration with Cs (non-rigid) symmetry possesses possible rotations of methyl groups with the symmetry representations:

Cs (Non-rigid) $|$ 1(1a) 2(3a) 2(3b) 2(3c) 2(3d) 27(2a) 2(3e) 2(3f) 3(3g) 2(3h) 2(3i) 2(3j) 2(3k) 2(3l) 3(3m)

Γ_σ $|$ 17   14   14   11   11   7 14 11 11   11   8   8   11 8 8

$\Gamma_\sigma = 9\chi_1 + 2\chi_2 + \chi_3 + \chi_5 + \chi_{11}$

Tetramethyl diborane with D_{2h}

Finally, we consider the point group G of the f-NRG of tetramethyl diborane. Figure 3 illustrates that, there are four elements $\alpha_1 = (1,2,3)$, $\alpha_2 = (4,5,6)$, $\alpha_3 = (7,8,9)$ and

$\alpha_4 = (10,11,12)$ in the group G, which permutes hydrogens in either of CH_3 cases. Also, there are seven elements:

$\alpha_5 = (1,10)(2,11)(3,12)(4,7)(5,8)(6,9),$

$\alpha_6 = (1,7)(2,9)(3,8)(4,10)(5,12)(6,11),$

$\alpha_7 = (1,4)(2,6)(3,5)(7,10)(8,12)(9,11)(13,14),$

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

$\beta_2 = (1,4)(2,5)(3,6)(7,10)(8,11)(9,12),$

$\beta_3 = (2,3)(5,6)(8,9)(11,12)(13,14),$

$\gamma = (1,10)(2,12)(3,11)(4,7)(5,9)(6,8)(13,14)$

which correspond to $C_2(z)$, $C_2(y)$, $C_2(x)$, $\sigma(yz)$, $\sigma(xz)$, $\sigma(xy)$ and i, respectively. These eleven permutations generate the group G and a simple GAP program shows that G is a group of order 1296 with 84 conjugacy classes. The conjugacy classes of G can be computed.

Symmetry of tetramethyl diborane

By definition, a weighted graph is a graph whose edges and vertices are weighed 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 $i=j$ 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.

Now, consider the tetramethyl diborane (Figure 3) with
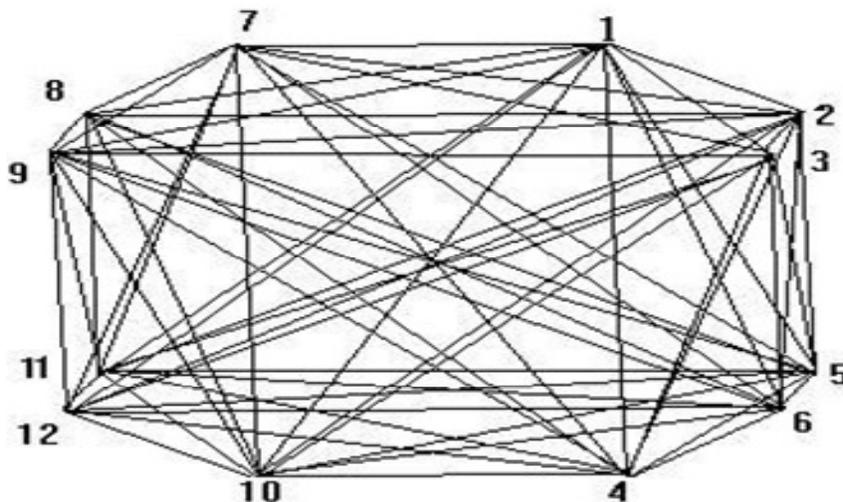
Figure 4. The Euclidean graph of tetramethyl diborane with D_{2h} point group.

Table 5. Euclidean edges for tetramethyldiborane with D_{2h} point group.

No.	1	2	3	4	5	6	7	8	9	10	11	12
1	0	1.78	1.78	4.376	3.812	3.812	2.602	4.060	4.060	5.091	5.277	5.277
2	1.78	0	1.78	3.812	2.596	3.148	4.060	5.119	5.42	5.277	5.740	6.009
3	1.78	1.78	0	3.812	3.142	2.596	4.060	5.42	5.1194	5.277	6.009	5.740
4	4.376	3.812	3.812	0	1.78	1.78	5.091	5.277	5.277	2.602	4.060	4.060
5	3.812	2.596	3.148	1.78	0	1.78	5.277	5.740	6.009	4.060	5.119	5.42
6	3.812	3.142	2.596	1.78	1.78	0	5.277	6.009	5.740	4.060	5.42	5.1194
7	2.602	4.060	4.060	5.091	5.277	5.277	0	1.78	1.78	4.376	3.812	3.812
8	4.060	5.119	5.42	5.277	5.740	6.009	1.78	0	1.78	3.812	2.596	3.148
9	4.060	5.42	5.1194	5.277	6.009	5.740	1.78	1.78	0	3.812	3.142	2.596
10	5.091	5.277	5.277	2.602	4.060	4.060	4.376	3.812	3.812	0	1.78	1.78
11	5.277	5.740	6.009	4.060	5.119	5.42	3.812	2.596	3.148	1.78	0	1.78
12	5.277	6.009	5.740	4.060	5.42	5.1194	3.812	3.142	2.596	1.78	1.78	0

D_{2h} point group to illustrate the Euclidean graph (Figure 4) and its automorphism group. It suffices to measure the Euclidean distances (Table 5) in terms of the H-H bond lengths 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 is identical to the automorphism group of the original Euclidean graph.

To illustrate, let us map the Euclidean edge weighed for this molecule with D_{2h} point group as 1.78→1, 4.376→2, 3.812→3, 2.596→4, 3.148→5, 2.602→6, 4.060→7, 5.119→8, 5.42→9, 5.091→10, 5.277→11, 5.704→12 and 6.009→13 where the weights are calculated using PM3 method of the chemistry package Hyperchem

(Hyperchem, 2009). The distance matrix D for tetramethyl diborane with D_{2h} is computed as follows:

$$A = \begin{bmatrix}
0 & 1 & 1 & 2 & 3 & 3 & 6 & 7 & 7 & 10 & 11 & 11 \\
1 & 0 & 1 & 3 & 4 & 5 & 7 & 8 & 9 & 11 & 12 & 13 \\
1 & 1 & 0 & 3 & 5 & 4 & 7 & 9 & 8 & 11 & 13 & 12 \\
2 & 3 & 3 & 0 & 1 & 1 & 10 & 11 & 11 & 6 & 7 & 7 \\
3 & 4 & 5 & 1 & 0 & 1 & 11 & 12 & 13 & 7 & 8 & 9 \\
3 & 5 & 4 & 1 & 1 & 0 & 11 & 13 & 12 & 7 & 9 & 8 \\
6 & 7 & 7 & 10 & 11 & 11 & 0 & 1 & 1 & 2 & 3 & 3 \\
7 & 8 & 9 & 11 & 12 & 13 & 1 & 0 & 1 & 3 & 4 & 5 \\
7 & 9 & 8 & 11 & 13 & 12 & 1 & 1 & 0 & 3 & 5 & 4 \\
10 & 11 & 11 & 6 & 7 & 7 & 2 & 3 & 3 & 0 & 1 & 1 \\
11 & 12 & 13 & 7 & 8 & 9 & 3 & 4 & 5 & 1 & 0 & 1 \\
11 & 13 & 12 & 7 & 9 & 8 & 3 & 5 & 4 & 1 & 1 & 0
\end{bmatrix}$$

The symmetry group of tetramethyl diborane can be computed using the following GAP programs.

```
PermutationGroup:=function(A)
local
list,dimension,counter,row,perviousrow,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
  perviousrow:=StructuralCopy(A[list[listcounter][1]]);
  Sort(perviousrow);
  if row=perviousrow 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),Gen
eratorsOfGroup)));
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;
```

Note: use only the function SymmetryGroup() with symmetric group of degree n, instead of our PermutationGroup() function, to begin with the possible permutation as automorphism of A. Clearly, this is time consuming when n, the dimension of A, is large. Hence we wrote the first function, PermutationGroup(), to decrease such permutations. In our investigation, the number of possible permutations decreases from 12!=479001600 to 967680, which illustrates a remarkable difference.

Using our GAP programs, the group G of symmetries of tetramethyl diborane is computed as follows:

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

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

It can be easily seen that this group is isomorphic to $C_2 \times C_2 \times C_2$ and is generated by a rotation $(1,10)(2,11)(3,12)(4,7)(5,8)(6,9)$ and two reflections $(1,4)(2,5)(3,6)(7,10)(8,11)(9,12)$ and $(1,7)(2,8)(3,9)(4,10)(5,11)(6,12)$.

CONCLUSIONS

The method described in this paper appears to be more efficient in dealing with the construction of the character table of symmetry group of the molecule. The structure of the group of full symmetries of a non-rigid molecule, which is denoted by f-NRG, is determined by examining various concepts and construction in group theory. First, all the permutations and inversions which do not change the whole framework of the molecule should be examined. Then using the GAP package, the character table of the f-NRG group is computed. The symmetry groups of the non-rigid cis- and trans- di methyl diborane, trimethyl diborane and tetramethyl diborane with different point groups are studied and the conjugacy classes and the irreducible character tables of the molecules are calculated.

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