Computing the Full Non-Rigid Group of Trimethylborane and Cyclohaxane Using Wreath Product

Enoch Suleiman¹*, M. S. Audu²

¹Department of Mathematics, Federal University Gashua, Gashua, Nigeria
²Department of Mathematics, University of Jos, Jos, Nigeria
Email: *enochsuleiman@gmail.com, audumso2@gmail.com

Abstract

This paper computes the group and character table of Trimethylborane and Cyclohaxane. Results show that the groups are isomorphic to the wreath products $C_3 wr C_2$ and $C_2 wr C_6$ with orders 81 and 384 and with 17 and 28 conjugacy classes respectively, where $C_n$ denotes a cyclic group of order $n$.

Keywords

Non-Rigid Molecule Group, Trimethylborane, Cyclohaxane, Wreath Product, Character Table, Conjugacy Classes

1. Introduction

Symmetry is very important in group theory. The symmetry of non-rigid molecules is a new field in chemistry. Balasubramanian [1] discussed the importance of finite groups which characterize the algebra of the symmetry of discrete structure as useful in predicting many physical and chemical properties. He further reviewed the formulation of symmetry groups of non-rigid molecules as generalized wreath product groups. He formulated the non-rigid hydrazine molecule (N₂H₂). He showed that the molecule is non-rigid in that twisting and inversion operations interconvert all the 16 possible conformations into one another. Considering the permutational subgroup of this molecule, he found out that the permutations operations of the non-rigid molecule can be generated by a group product of much simpler groups, known as wreath product and thus it is a group of order 8. Balasubramanian also used the generating function methods to find the irreducible representation of Boron trimethyl B(CH₃)₃ and also the
non-rigid Deuterion spin species of B(CD$_3$)$_3$ and also that of Butane. Hamadanian and Ashrafi [2] studied the full NRG of trimethylamine N(CH$_3$)$_3$ and prove that is a group of order 1296 with 28 conjugacy classes. Darafsher et al. [3] calculated the irreducible representations and character table of Tetramethylene molecule. They first specify the algebraic structure of the f-NRG of tetramethylethylene molecule with a geometric consideration of dynamic symmetries of the molecule and showed that the f-NRG of the molecule can be specified as $(Z_3) \wr (Z_2 \times Z_2)$. Then using the package GAP, the f-NRG group was computed and is shown to be of order 324 permutations. It is a group of 45 conjugacy classes of elements and contains exactly 45 irreducible characters. Darafsher et al. [4] studied the f-NRG of tetranitrocubane and octanitrocubane and prove that these are groups of order 384 and 12288 respectively. The f-NRG group of tetranitrocubane was shown to be isomorphic to $Z_3 \wr S_4$ while that of octanitrocubane was shown to be isomorphic to $(Z_2) \wr (S_4 \times Z_2)$. The conjugacy classes and the character tables of the two molecules were computed using the GAP package.

Darafsher et al. [5] studied the 2,3-dimethylbutane and found the structure of the full non-rigid group of this molecule to be isomorphic to the semidirect product of four copies of the cyclic group $Z_3$ by the cyclic group $Z_2$, that is, $(Z_3 \times Z_3 \times Z_3 \times Z_3) \times Z_2$, and the complex character table of the group was computed by the package GAP. Moghani et al. [6] studied the non-rigid group of 2,4-dimethylbenzene that is isomorphic to $Z_3 \times (Z_3 \times Z_2)$ with order 36. It was shown that the group has 12 dominant classes and the Markaracter table, the table of all integer-valued characters and the unit subduced cycle index Table of the full non-rigid group of 2,4-dimethyl benzene are derived for the first time. Moghadam et al. [7] computed the f-NRG of fluoro(dimethyl)borane and (difluoromethyl)borane with $C_j$ point group. They proved that the f-NRG of the two molecules is of order 18 and 6 with 6 and 3 conjugacy classes respectively. The conjugacy classes and the character tables were computed using the GAP package. Moghadam et al. [8] studied the symmetry of non-rigid Cis- and trans-dimethyl diborane, trimethyl diborane and tetramethyl diborane with different point groups and the conjugacy classes and the irreducible character tables of the molecules are also calculated.

The character table which is being needed for the classification of wave functions, determination of selection rules, etc. in which were computed for Trimethylborane and Cyclohaxane the groups are found to be isomorphic to the wreath products $C_j \wr C_2$ and $C_j \wr C_6$ with orders 81 and 384 and with 17 and 28 conjugacy classes respectively. We use the GAP package to get the required results.

The next section shows the results that are obtained and some basic definitions while the following section gives the conclusion.

### 2. Results and Computation

Let $\Omega$ be an arbitrary set; we shall often refer to its elements as points. A bijective
A permutation group is just a subgroup of the symmetric group. If $\Gamma$ and $\Delta$ are nonempty sets, then we call $\Delta^\Gamma$ to denote the set of all functions from $\Delta$ to $\Gamma$. In the case that $C$ is a group, we turn $C^\Delta$ into a group by defining product “pointwise” for all $f, g \in C^\Delta$ and $\gamma \in \Delta$ where the product in the right is in $C$.

Let $C$ and $D$ be groups and suppose $D$ acts on the nonempty set $\Delta$. Then the wreath product of $C$ by $D$ is defined with respect to this action is defined to be the semidirect product $C^\Delta \rtimes D = CwrD$ where $D$ acts on the group $C^\Delta$ via

$$f^d(\gamma) := f(\gamma^d)$$

for all $f \in C^\Delta$, $\gamma \in \Delta$ and $d \in D$ and multiplication for all $(f_1, d_1), (f_2, d_2) \in CwrD$ is given by

$$(f_1, d_1)(f_2, d_2) = (f_1f_2^{d_1^{-1}}, d_1d_2)$$

(See [9])

### 2.1. $f$-NRG of Trimethylborane

Consider the trimethylborane compound $\text{B(CH}_3)\text{}_3$ with the structure.

The speediness of the rotation of the methyl group is considered appropriately high that makes the mean time dynamical symmetry of the molecules makes sense. First considering the symmetry of $\text{CH}_3$ which is a cyclic group of order 3 namely $\mathbb{Z}_3$ denoted by $A := \langle (1,2,3) \rangle$ (as shown in Figure 1). Also the remaining 3 corners of the framework are given by: $B_1 := \langle (4,5,6) \rangle$, $B_2 := \langle (7,8,9) \rangle$, $B_3 := \langle (10,11,12) \rangle$ where $B_i$ is the symmetry of the CH$_3$ whose carbon atom is marked as $i, 1 \leq i \leq 3$. Therefore the full symmetry of trimethylborane is: $G = (B_1 \times B_2 \times B_3) \rtimes A$. Which we can write in terms of wreath product as $G := \mathbb{Z}_3 \rtimes \mathbb{Z}_3$. We used GAP package to get the group as follows:

```
    gap> A := Group([1,2,3]);
    Group([1,2,3])
    gap> B := Group([4,5,6]);
    Group([4,5,6])
    gap> G := WreathProduct(A,B);
    Group([ (1,2,3), (4,5,6), (7,8,9), (1,4,7)(2,5,8)(3,6,9) ])
    gap> Elements(G);
    $\mathbb{Z}_3 \rtimes \mathbb{Z}_3$
    gap> Display(CharacterTable(G));
```

(See [10])

From the foregoing Table 1, The Representative of conjugacy classes of the group and Table 2, The Character table obtained gives room for the needed classification of wavefunctions, determination of selection rules, and so on.
Table 1. The representative of conjugacy classes of the group.

| S/N | Representatives | Size | Name |
|-----|-----------------|------|------|
| 1.  | ()              | 1    | 1a   |
| 2.  | (7,8,9)         | 3    | 3a   |
| 3.  | (7,9,8)         | 3    | 3b   |
| 4.  | (4,5,6) (7,8,9)| 3    | 3c   |
| 5.  | (4,5,6) (7,9,8)| 3    | 3d   |
| 6.  | (4,6,5) (7,8,9)| 3    | 3e   |
| 7.  | (4,6,5) (7,9,8)| 3    | 3f   |
| 8.  | (1,4,7) (2,5,8) (3,6,9)| 9 | 3g |
| 9.  | (1,4,7,2,5,8,3,6,9)| 9 | 3h |
| 10. | (1,4,7,3,6,9,2,5,8)| 9 | 3i |
| 11. | (1,7,4) (2,8,5) (3,9,6)| 9 | 3j |
| 12. | (1,4,7) (2,5,8) (3,6,9)| 9 | 3k |
| 13. | (1,4,7,2,5,8,3,6,9)| 9 | 3l |
| 14. | (1,4,7,3,6,9,2,5,8)| 9 | 3m |
| 15. | (1,7,4) (2,8,5) (3,9,6)| 9 | 3n |
| 16. | (1,7,5,2,8,6,3,9,4)| 9 | 3o |
| 17. | (1,7,6,3,9,5,2,8,4)| 9 | 3p |

Table 2. Character Table for Trimethylborane.

|            | 1a | 3a | 3b | 3c | 3d | 3e | 3f | 3g | 3h | 3i | 3j | 9a | 9b | 3l | 9c | 9d |
|------------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 2P         | 1a | 3b | 3a | 3f | 3e | 3d | 3c | 3j | 3i | 3h | 3g | 3l | 9d | 9c | 9b | 9a |
| 3P         | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 3g | 3j | 1a | 3g |
| 5P         | 1a | 3b | 3a | 3f | 3e | 3d | 3c | 3j | 3i | 3h | 3g | 3l | 9d | 9c | 3k | 9b |
| 7P         | 1a | 3a | 3b | 3c | 3d | 3e | 3f | 3g | 3h | 3i | 3j | 3k | 9a | 9b | 3l | 9c |
| \( \chi_1 \) | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  |
| \( \chi_2 \) | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  |
| \( \chi_3 \) | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  | 1  |
| \( \chi_4 \) | 1  | A  | A  | A  | 1  | A  | A  | A  | 1  | A  | A  | A  | A  | A  | A  | A  | A  |
| \( \chi_5 \) | 1  | A  | A  | A  | A  | 1  | A  | A  | A  | 1  | A  | A  | A  | A  | A  | A  | A  |
| \( \chi_6 \) | 1  | A  | A  | A  | 1  | A  | A  | A  | 1  | A  | A  | A  | A  | A  | A  | A  | A  |
| \( \chi_7 \) | 1  | A  | A  | A  | 1  | A  | A  | A  | 1  | A  | A  | A  | A  | A  | A  | A  | A  |
| \( \chi_8 \) | 1  | A  | A  | A  | 1  | A  | A  | A  | 1  | A  | A  | A  | A  | A  | A  | A  | A  |
| \( \chi_9 \) | 1  | A  | A  | A  | 1  | A  | A  | A  | 1  | A  | A  | A  | A  | A  | A  | A  | A  |
| \( \chi_{10} \) | 3  | B  | B  | -C | 0  | 0  | C  | B  | B  | -B | D  | 0  | 0  | 0  | 0  | 0  | 0  |
| \( \chi_{11} \) | 3  | B  | B  | C  | 0  | 0  | -C | D  | -B | B  | B  | 0  | 0  | 0  | 0  | 0  | 0  |

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Continued

\[
\begin{array}{cccccccc}
\chi_{12} & 3 & C & -C & -B & 0 & 0 & -\bar{B} & D & B & \bar{B} & D & 0 & 0 & 0 & 0 & 0 & 0 \\
\chi_{13} & 3 & -C & C & -\bar{B} & 0 & 0 & -B & D & \bar{B} & B & \bar{B} & D & 0 & 0 & 0 & 0 & 0 \\
\chi_{14} & 3 & -B & -\bar{B} & B & 0 & 0 & \bar{B} & D & -C & C & \bar{B} & D & 0 & 0 & 0 & 0 & 0 \\
\chi_{15} & 3 & -\bar{B} & -B & \bar{B} & 0 & 0 & B & \bar{B} & C & -C & D & 0 & 0 & 0 & 0 & 0 & 0 \\
\chi_{16} & 3 & 0 & 0 & 0 & D & \bar{B} & 0 & 3 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\
\chi_{17} & 3 & 0 & 0 & 0 & \bar{B} & D & 0 & 3 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{array}
\]

where: \( A = E(3)^{1/2} = \frac{1 - \sqrt[2]{3}}{2} \); \( B = -E(3) - 2 * E(3)^{1/2} = \frac{3 + \sqrt[2]{3}}{2} \); 
\( C = -E(3) + E(3)^{1/2} = -\sqrt[2]{3} \); \( D = 3 * E(3)^{1/2} = (-3 - 3 * \sqrt[2]{3})/2 \).

\[\text{Figure 1. The structure of trimethylborane.}\]

\subsection*{2.2. f-NRG of Cyclohexane}

Consider the cyclohexane compound \( \text{C}_6\text{H}_{12} \) with the structure.

The speediness of the rotation of the hexane group is considered suitably high that makes the mean time dynamical symmetry of the molecules makes sense. First considering the symmetry of \( \text{C}_6 \) which is a cyclic group of order 6 namely \( \mathbb{Z}_6 \) denoted by \( A := \langle (1,2,3,4,5,6) \rangle \) (as shown in \textbf{Figure 2}). Also the remaining 6 corners of the framework are given by: \( B_1 := \langle (7,8) \rangle, B_2 := \langle (9,10) \rangle, B_3 := \langle (11,12) \rangle, B_4 := \langle (13,14) \rangle, B_5 := \langle (15,16) \rangle \) and \( B_6 := \langle (17,18) \rangle \) where \( B_i \) is the symmetry of the \( \text{H}_2 \) whose carbon atom is marked as \( i, 1 \leq i \leq 6 \). Therefore, the full symmetry of cyclohexane is:

\[ G := (B_1 \times B_2 \times B_3 \times B_4 \times B_5 \times B_6) \times A. \]

Which we can write in terms of wreath product as \( G := \mathbb{Z}_2 \wr \mathbb{Z}_6 \). We used GAP package to get the group as follows:

\begin{verbatim}
gap> A := Group([([1,2])]);
group([([1,2])])
gap> B := Group([([1,2,3,4,5,6])]);
group([([1,2,3,4,5,6])])
gap> G := wreathProduct(A, B);
group([([1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18])])
gap> Elements(G);
group size: 384
gap> Order(G);
384
gap> SizesConjugacyClasses(G);
group size: 384
gap> display(characterTable(G));
group size: 384
\end{verbatim}

(See [10])
From the foregoing Table 3, The Representative of conjugacy classes of the group and Table 4, The Character table obtained gives room for the needed classification of wavefunctions, determination of selection rules, and so on.

![Figure 2. The structure of cyclohexane.](image)

**Table 3.** The conjugacy class table for the group.

| S/N | Representatives     | Size | Name |
|-----|--------------------|------|------|
| 1.  | ()                 | 1    | 1a   |
| 2.  | (11,12)            | 6    | 2a   |
| 3.  | (9,10) (11,12)     | 6    | 2b   |
| 4.  | (7,8) (11,12)      | 6    | 2c   |
| 5.  | (7,8) (9,10) (11,12)| 6 | 2d    |
| 6.  | (5,6) (11,12)      | 6    | 2e   |
| 7.  | (5,6) (9,10) (11,12)| 6 | 2f   |
| 8.  | (5,6) (7,8) (11,12)| 6    | 2g   |
| 9.  | (5,6) (7,8) (9,10) (11,12)| 6 | 2h    |
| 10. | (3,4) (7,8) (11,12)| 6    | 2i   |
| 11. | (3,4) (7,8) (9,10) (11,12)| 6 | 2j   |
| 12. | (3,4) (5,6) (9,10) (11,12)| 6 | 2k   |
| 13. | (3,4) (5,6) (7,8) (9,10) (11,12)| 6 | 2l    |
| 14. | (1,2) (3,4) (5,6) (7,8) (9,10) (11,12)| 1 | 2m  |
| 15. | (1,3,5,7,9,11) (2,4,6,8,10,12)| 32 | 6f |
| 16. | (1,3,5,7,9,11,2,4,6,8,10,12)| 32 | 6g |
| 17. | (1,5,9) (2,6,10) (3,7,11) (4,8,12)| 16 | 3b |
| 18. | (1,5,9) (2,6,10) (3,7,11,4,8,12)| 32 | 6d |
| 19. | (1,5,9,2,6,10) (3,7,11,4,8,12)| 32 | 6e |
| 20. | (1,7) (2,8) (3,9) (4,10) (5,11) (6,12)| 8 | 2n |
| 21. | (1,7) (2,8) (3,9) (4,10) (5,11,6,12)| 24 | 4a |
| 22. | (1,7) (2,8) (3,9,4,10) (5,11,6,12)| 24 | 4b |
| 23. | (1,7,2,8) (3,9,4,10) (5,11,6,12)| 8 | 4c |
| 24. | (1,9,5) (2,10,6) (3,11,7) (4,12,8)| 16 | 3a |
| 25. | (1,9,5) (2,10,6) (3,11,8,4,12,7)| 32 | 6b |
| 26. | (1,9,6,2,10,5) (3,11,8,4,12,7)| 16 | 6c |
| 27. | (1,11,9,7,5,3) (2,12,10,8,6,4)| 32 | 6a |
| 28. | (1,11,10,8,6,4,2,12,9,7,5,3)| 32 | 12a |
Table 4. Character table for Cyclohexane molecule.

| 1a | 2a | 2b | 2c | 2d | 2e | 2f | 2g | 2h | 2i | 2j | 2k | 2l | 2m | 6a | 12a | 3a | 6b | 6c | 2n | 4a | 4b | 4c | 3b | 6d | 6e | 6f | 12b |
|-----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 3P  | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 1a | 6c | 3b | 3b | 3b | 3b | 3b | 3b | 3b | 3b | 6e | 6e | 6b | 6e |
| 5P  | 1a | 2a | 2b | 2c | 2d | 2e | 2f | 2g | 2h | 2i | 2j | 2k | 2l | 2m | 6a | 12a | 3a | 6b | 6c | 2n | 4a | 4b | 4c | 3b | 6d | 6e | 6f | 12b |
| 7P  | 1a | 2a | 2b | 2c | 2d | 2e | 2f | 2g | 2h | 2i | 2j | 2k | 2l | 2m | 6a | 12a | 3a | 6b | 6c | 2n | 4a | 4b | 4c | 3b | 6d | 6e | 6f | 12b |
| 11P | 1a | 2a | 2b | 2c | 2d | 2e | 2f | 2g | 2h | 2i | 2j | 2k | 2l | 2m | 6a | 12a | 3a | 6b | 6c | 2n | 4a | 4b | 4c | 3b | 6d | 6e | 6f | 12b |

Where:

- \( A = E(3) = \frac{1 - \sqrt{-3}}{2} \)
- \( B = 2 \times E(3) = -1 + \sqrt{-3} \)
3. Conclusion

In this paper, we computed the group, the conjugacy classes and character tables of Trimethylborane and Cyclohexane as seen in Tables 1-4. We found that the groups are isomorphic to the wreath products $C_3 \wr C_2$ and $C_3 \wr C_6$ with orders 81 and 384 and with 17 and 28 conjugacy classes respectively, where $C_n$ is cyclic group of order $n$. We used the GAP package for our calculations. The character tables obtained give room for the needed classification of wavefunctions, determination of selection rules, and so on.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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