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DETERMINATION OF THE CONJUGACY CLASSES AND CHARACTER TABLE OF THE FULL NON-RIGID GROUP OF HEXACHLOROCYCLOPROPANE CHEMICAL COMPOUND VIA WREATH PRODUCT OF PAIR OF PERMUTATION GROUPS

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ABSTRACT: *The use of full non-rigid (f.NRG) molecules group theory to study the internal dynamics of molecular structures of chemical compounds is trending in the research space. In this paper, we use computational method to compute the group elements and group table of the Hexachlorocyclopropane molecular (algebraic) structure and thereafter determine the order and conjugacy classes of the group and finally the corresponding symmetry for each permutation group. We considered the point group of the compound which turns out to be isomorphic to the Wreath Products $C_3 wr C_2$, where C_n denotes a cyclic group of order n. We found that the group has order 18 and 9 conjugacy classes. Investigating the solubility of the components of Hexachlorocyclopropane chemical compound can be considered for further study.*

KEYWORDS: Non-Rigid Group, Hexachlorocyclopropane, Wreath Product, Character Table, Conjugacy Classes, Permutation Group

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INTRODUCTION

The application of Group theory concepts to full non-rigid molecules is becoming increasingly relevant and is dense in the research space; see [10] and [12]. Symmetry as a concept is more of mathematics subject and not chemistry. However, the underlying mathematical theory for symmetry and group theory are of great importance in chemistry because they can be used to solve quite plenty of chemistry problems. For example it can be applied when it comes to the classification of the structures of molecules and crystals, understanding chemical bonding, predicting vibrational spectra and determining the optical activity of compounds.

Hexachlorocyclopropane exists as a chemical compound with molecular formula as C_3Cl_6. Full rigid molecules' symmetry properties are well known and so investigating them is a natural thing to do, though study in this research area is new in chemistry. [14] presented a number of papers on the determination of character tables of restricted f-NRG of some chemical molecules. For example, Computation of the r-NRG of the triple equivalent methyl rotation in pyramidal trimethylamine with inversion was done by [15]. The authors proved that the r-NRG of this molecule is a group has 648 elements, consists two subgroups of order 324 without inversion. We also have in [4] and [5] where computation of full non-rigid group of some other molecules were carried out. In the same vein, [1] computed full non-rigid group of tetra-ammine platinum (II), trimethylamine, tetraammine platinum (II), etc which are all examples of C2v and C4v point groups. Authors such as [2] and [7] proved that molecular structure tetra-amine platinum (II) is isomorphic to the Wreath Product of certain degree. [8] worked on hexamethylbenzene while [9] and [3] studied melamine.

MATERIALS AND METHODS

Let Ω be a nonempty set, a permutation of Ω is a bijection $\alpha: \Omega \to \Omega$. We denote the set of all permutations of Ω by S_Ω. When Ω is finite, that is, $\Omega = \{1,2,\dots,n\}$, we write S_n (the symmetric group of degree n) instead of S_Ω where $|S_n| = n!$ is the number of elements in S_n referred to as the order of the group S_n. Joseph-Louis Lagrange during his time observed permutation as arrangements, that is, as a list $i_1,\ i_2,\ \dots,\ i_n$ with no repetition of any of the elements of Ω. Given an arrangement, $i_1,\ i_2,\ \dots,\ i_n$, define a function $\alpha: \Omega \to \Omega$ by $\alpha(j) = i$ for all $j \in \Omega$. Thus, every rearrangement gives a bijection ([6]). The Wreath product of two permutation groups C by D denoted by $W = C\ wr\ D$ is the semi-direct product of P (a set of mappings) by D, so that, $W = \{(f,d) | f \in P, d \in D\}$, with multiplication in W defined as $(f_1,d_1)(f_2,d_2) = ((f_1, f_2 d_1^{-1})\ (d_1,d_2))\ \ \forall\ \ f_1,f_2 \in P\ and\ d_1,d_2 \in D$. W is a special form of permutation group. Understanding the nature of the Wreath products facilitates comprehension of certain types of subgroups of the symmetric groups.

In this paper, we carry out computation of Hexachlorocyclopropane. We start by first, specifying the algebraic structure of the non-rigid group of these molecules. Then, on the bases of the structure of the group, a useful programming language, namely, "Groups, Algorithms and Programming" (GAP) is applied and the character Tables is computed. The use of this computational group theory package (GAP) is capable of revealing many properties of the groups according to [11] and [13]. We determine the order of the f-NRG of

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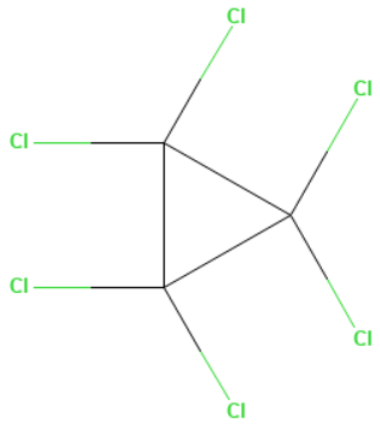
the group and it's conjugacy classes. Finally, we compute the character tables of the molecules with the aid of the computational group theory (GAP}.

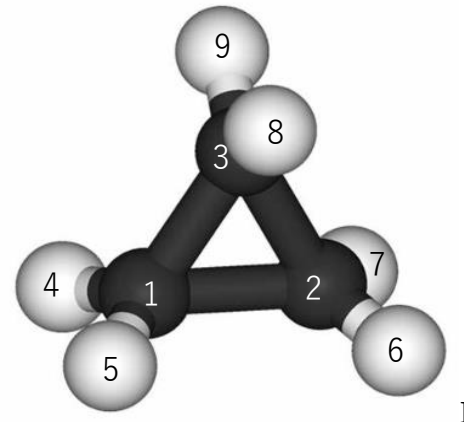
RESULTS AND DISCUSSIONS

The Hexachlorocyclopropane **(**C_3Cl_6**)** ion belongs to the Dihedral groups which are point groups that have n additional C_2 axes that stand perpendicular to the principal axis of the order 3. Since there are no other symmetry elements, the point group is of the type D_{3h}.



A

Figure 1: Hexachlorocyclopropane Structure.



B

Figure 2: Hexachlorocyclopropane Geometry.

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Where A = Chemical structure of Hexachlorocyclopropane

B = Geometry of Hexachlorocyclopropane

From figure 1 we have a C_3 principal axis, and three additional C_2 axes, but no other symmetry element. The C_3 axis stands perpendicular to the paper plane, and there are three C_2 axes in the paper plane. Therefore the symmetry of C_3Cl_6 has a trigonal bipyramidal shape. The C_3 axis goes through the centre of the atom of the C molecules, and the three C_2 axes go through the three equatorial Cl atoms. The C_3Cl_6 symmetry elements, namely C_3 and C_2 axes, are denoted by $C_3 := \langle(1,2,3)\rangle$ and $C_{21} := \langle(4,5)\rangle$, $C_{22} := \langle(6,7)\rangle$, $C_{23} := \langle(8,9)\rangle$ respectively.

Therefore the full symmetry of Hexachlorocyclopropane as can be viewed clearly from figure 2, is: $G = (C_{21} \times C_{22} \times C_{23}) \rtimes C_3$, which we can write in terms of wreath product as $:= \mathbb{Z}_2 \; wr \; \mathbb{Z}_3$. We used GAP package to get the group as follows:

```
gap>

gap> C3 := Group((1,2,3));

Group([ (1,2,3) ])

gap> C2 := Group((4,5));

Group([ (4,5) ])

gap> G := WreathProduct(C3,C2);

Group([ (1,2,3), (4,5,6), (1,4)(2,5)(3,6) ])

gap> Order(G);

18

gap> CC := ConjugacyClasses(G);

[ ()^G, (4,5,6)^G, (4,6,5)^G, (1,2,3)(4,5,6)^G, (1,2,3)(4,6,5)^G, (1,3,2)(4,6,5)^G,

  (1,4)(2,5)(3,6)^G, (1,4,2,5,3,6)^G, (1,4,3,6,2,5)^G ]

gap> List(CC, x -> Order(Representative(x)));

[ 1, 3, 3, 3, 3, 3, 2, 6, 6 ]

gap> Display(CharacterTable(G));
```


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Table 1: The Representatives of Conjugacy Classes for Hexachlorocyclopropane

S/N	Representatives	Size	Name
1.	(1)	1	$1a$
2.	(4,5,6)	3	$3a$
3.	(4,6,5)	3	$3b$
4.	(1,2,3)(4,5,6)	3	$3c$
5.	(1,2,3)(4,6,5)	3	$3d$
6.	(1,3,2)(4,6,5)	3	$3e$
7.	(1,4)(2,5)(3,6)	2	$2a$
8.	(1,4,2,5,3,6)	6	$6a$
9.	(1,4,3,6,2,5)	6	$6b$

Table 2: Character Table for Hexachlorocyclopropane

	$1a$	$3a$	$3b$	$3c$	$3d$	$3e$	$2a$	$6a$	$6b$
$2P$	$1a$	$3b$	$3a$	$3e$	$3d$	$3c$	$1a$	$3c$	$3e$
$3P$	$1a$	$1a$	$1a$	$1a$	$1a$	$1a$	$2a$	$2a$	$2a$
$5P$	1a	3b	3a	3e	3d	3c	2a	6b	6a
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	A	$\bar{A}$	$\bar{A}$	1	A	-1	$-A$	$\overline{-A}$
χ_4	1	$\bar{A}$	A	A	1	$\bar{A}$	-1	$\overline{-A}$	$-A$
χ_5	1	A	$\bar{A}$	$\bar{A}$	1	A	1	A	$\bar{A}$
χ_6	1	$\bar{A}$	-1	A	1	$\bar{A}$	1	$\bar{A}$	A
χ_7	2	-1	A	2	-1	2	0	0	0
χ_8	2	$\bar{A}$	$-A$	B	-1	$\bar{B}$	0	0	0
χ_9	2	$-A$	$\overline{-A}$	$\bar{B}$	-1	B	0	0	0

Where:

$A = E(3)^2 = (-1 - Sqrt(-3))/2$ = -1 - b3

$B = 2 * E(3)^2 = -1 - Sqrt(-3)$ = -1 + i3

Note: Table 1 provides the Representatives of the conjugacy classes of the group while Table 2 gives the Character table. Across the top of the character table is a list of all the symmetry operations in the point group. Down the left side of the character table is a list of irreducible

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representations. An irreducible representation describes how in this case the atoms changes when the different symmetry operations are performed. It could stay the same (1), become inverted (-1), or change completely (0). Representations with A and B labels indicate non-degeneracy. Just below the Table 2 are mathematical functions which can be used to assign orbitals to the irreducible representations.

CONCLUSIONS

In this work, the symmetry operations of the non-rigid Hexachlorocyclopropane were studied. The conjugacy classes and the irreducible character tables of the molecules were computed as seen in table 1 and 2 using computational group theory. We found that the group is isomorphic to the Wreath Products $\mathbb{Z}_2 wr \mathbb{Z}_3$ and has order 18 and 9 conjugacy classes. We used GAP 4.11.1 for our calculations. Clearly, the character table makes it easy to classify the wave functions, determine selection rules, and so on. Thus, symmetry can be applied in the determination of orbital overlap for molecular orbitals more quickly and easily. Note, only orbitals that have the same irreducible representation have the correct symmetry to overlap and form a molecular orbital. It is natural to follow this study with the investigation of the solubility of the components of Hexachlorocyclopropane chemical compound.

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