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Computing the Order, Conjugacy Classes and Character Table of the Full Non-Rigid Group of Cyclopentane Chemical Compound using Wreath Product of Cyclic groups

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ABSTRACT

The theory of full non-rigid molecular groups (f.NRG) proves useful in exploring the internal dynamics of these molecules. In this study, we determined the group order of Cyclopentane and identified its conjugacy classes. Using computational methods, we calculated the group order, its character table, conjugacy classes and the point group of Cyclopentane was analyzed. Our results showed that the point groups were found to be isomorphic to the Wreath Product 〖Z〗_5 wrZ_2, where Z_n represents a cyclic group of size n, with order 160 and 16 conjugacy classes. All calculations were performed using GAP 4.11.1.

1. Introduction

The use of Group theory in studying fully non-rigid molecules is gaining significant attention in research, as highlighted in Ezra, (1982) and (Maruani, *et al.,* 1992). Although symmetry is primarily a mathematical concept, its application in chemistry is crucial. The mathematical foundations of symmetry and group theory play a vital role in addressing various chemical problems. These concepts are particularly useful in tasks such as classifying molecular and crystal structures, analyzing chemical bonding, predicting vibrational spectra, and determining the optical activity of compounds. Cyclopentane is a chemical compound with the molecular formula C_5H_{10}. While the symmetry properties of fully non-rigid molecules are well-established, exploring these properties remains a growing area of interest in chemistry (Alan V.,2001) and (Istvan *et al.,* 2009). The main objectives of this study are to determine the group order of Cyclopentane, identified its conjugacy classes and irreducible character tables of the molecule and finally to show that the point group of Cyclopentane is isomorphic to a Wreath Product $\mathbb{Z}_5 wr \mathbb{Z}_2$ corresponding to cyclic groups $\mathbb{Z}_n$ of size n. In Smeyers (1992), the authors presented several papers on character tables for restricted non-rigid molecular groups (r-NRG) of specific molecules. For instance, the r-NRG of the triple-equivalent methyl rotation in pyramidal trimethylamine, including inversion, was computed in (Smeyers, *et al.*,2000). They demonstrated that the r-NRG of this molecule forms a group with 648 elements, comprised of two subgroups of order 324 without inversion. Further studies, such as those in Balasubramanian, (2004a) and Balasubramanian, (2004b), carried out similar computations on the full non-rigid groups of other molecules. In a similar context, (Ashrafi, *et al.,* 2003) computed the full non-rigid groups for compounds like tetra-ammine platinum (II) and trimethylamine, which are examples of C2v and C4v point groups, point groups are classifications of molecular symmetry. The C_{2v} point group has the following symmetry elements: A principal C_2 rotation axis and two vertical mirror planes (σv). While The C_{4v} point group has: A principal C_4 rotation axis and four vertical mirror planes (σv).

Additionally, (Ashrafi, *et al.,* 2004) and (Darafsheh, *et al.,* 2005) demonstrated that the molecular structure of tetra-ammine platinum (II) is isomorphic to a Wreath Product of a certain degree. Work on other molecules, such as hexamethylbenzene by (Darafsheh, *et al.,* 2005b) and melamine by (Darafsheh, *et al.,* 2006 and Ashrafi, *et al.,* 2005), also expanded on these findings. Wreath products help in understanding certain subgroup structures within symmetric groups.

2. Preliminaries

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We here give some basic definitions that are relevant to our work:

2.1 Permutation group

A permutation group is a group G whose elements are permutations of a given set X and whose group operation is the composition of functions in G which are a bijection from the set X to itself.

2.2 Character Table

A character table is a two-dimensional table whose rows correspond to irreducible representations, and whose columns correspond to conjugacy classes of group elements.

2.3 Conjugate Elements and Conjugacy Classes

Let G be a group and a, b ∈ G. a and b in G are conjugate if there exists a g ∈ G such that $g^{-1}ag = b$.
Recall that for $H \leq G$, the conjugate subgroup of H by a fixed g ∈ G is
$gHg^{-1} = \{ghg^{-1} \mid h \in H\}$. Additionally, H is normal iff $gHg^{-1} = H$ for all g ∈ G.
We can also fix the element we are conjugating. Given x ∈ G, we may ask: "which elements can be written as gxg^{-1} for some g ∈ G?" The set of all such elements in G is called the conjugacy class of x, denoted clG (x). Formally, this is the set $clG(x) = \{ gxg^{-1} \mid g \in G\}$.

2.4 Symmetric group

The symmetric groups S_n is the group of permutations on a set with n elements. The symmetric group of degree n on a finite set is define to be the group whose elements are all bijective functions from X to X and whose group operation is that of function composition. Permutations and bijection are two the same operation meaning rearrangement.

2.5 Orbitals

Orbital is a region of space around the nucleus of an atom where there is a high probability of finding an electron. Orbitals are mathematical functions derived from solutions to the Schrödinger equation and describe the behavior and distribution of electrons within an atom.

2.6 Cyclic group

If G is a group and a∈G, it may happen that every element of G is a power of a in other words, G may consist of all the powers of a, that is $G = \{a^n : n \in Z\}$. In that case, G is called a cyclic group, and a is called its generator. We write G = ⟨a⟩ and say that G is the cyclic group generated by a. If G = ⟨a⟩ is the cyclic group generated by a, and a has order n, we say that G is a cyclic group of order n.

2.7 A point group

A point group describes all the symmetry operations that can be performed on a molecule that results in a conformation indistinguishable from the original. Examples point groups are used in Group Theory, the mathematical analysis of groups to determine properties such as a molecule's molecular orbitals

2.8 Wreath Products

The wreath product of C by D denoted by W=CwrD is the semi-direct product of P by D, so that, $W = \{(f, d) \mid f \in P, d \in D\}$ with multiplication in W defines as $(f_1 d_1)(f_2 d_2) = (\left(f_1 f_2^{d_1^{-1}}\right), (d_1 d_2))$ for all $f_1 f_2 \in P$ *and* $d_1, d_2 \in D$.. Henceforth, we write fd instead of (fd) for elements of W.

Note; we wish to henceforth notice that

(a) If C and D are finite groups then a wreath product W determines by an action of D on a finite group of order $|W| = |C|^{\Delta}.|D|$.

(b) P is normal subgroup of W and D is a subgroup of W.

(c) The action of W on $\Gamma \times \Delta$ is given by $(\alpha, \beta)fd = (\alpha f(\beta), \beta d)$ where $\alpha \in \Gamma$ and $\beta \in \Delta$.

3. Methodology

Let Ω represent a nonempty set. A permutation of Ω is defined as a bijection from Ω to itself. We denote the collection of all such permutations as S_Ω . When Ω is finite, denoted as $\Omega = \{1,2, \ldots, n\}$, we use to represent the symmetric group of degree n with $|S_n| = n!$ instead of S_Ω, which refers to the number of elements in S_Ω and is called the order of the group S_n (Enoch, et'al., 2020). Joseph-Louis Lagrange during his time observed permutation as arrangements, that is, as a list $i_1, i_2, \ldots, i_n$ with no repetition of any of the elements of Ω. Given an arrangement, $i_1, i_2, \ldots, i_n$, define a function $\alpha: \Omega \to \Omega$ by $\alpha(j) = i$ for all $j \in \Omega$. Thus, every rearrangement gives a bijection (Burness, et'al.,2016). The Wreath product of two permutation groups C and 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 $(f_1,d_1)(f_2,d_2) = ((f_1,f_2d_1^{-1})\ (d_1,d_2))\ \ \forall\ \ f_1,f_2 \in P\ and\ d_1,d_2 \in D$. 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 focus on computational analysis of Cyclopentane. First, we outline the algebraic structure of the non-rigid group associated with these molecules. In applying this, we observed that the permutation group of degree 2p (p=5) through the wreath product (Samuel *et al.,* 2023), analyzed the symmetry operations of non-rigid Cyclopentane. Based on the group's structure, we employ a specialized programming language known as "Groups, Algorithms, and Programming" (GAP) to perform computations of character tables. GAP, a tool within computational group theory, provides insights into many properties of these groups, as shown by (Karimi, *et al.,* 2011) and (Moghani, *et al.,* 2010). We compute the order of the f-NRG of the group and its conjugacy classes. Finally, we use GAP to compute the Conjugacy Classes and irreducible character tables of these molecules.

4. Results

Cyclopentane C_5H_{10} is in the family of Alkane. The general formula of Cyclopentane is C_nH_{2n} when n=5. Thus, C_5H_{10} is the single molecular formula of Cyclopentane. The single bonds connect to five carbon atoms in cyclic form of Cyclopentane.

Cyclopentane **(**C_5H_{10}**)** ion also belongs to the Dihedral point group, which includes n additional C_2 axes positioned perpendicular to the principal axis of symmetry (order n). As no other symmetry elements are present, the point group classification is D_{5h}.

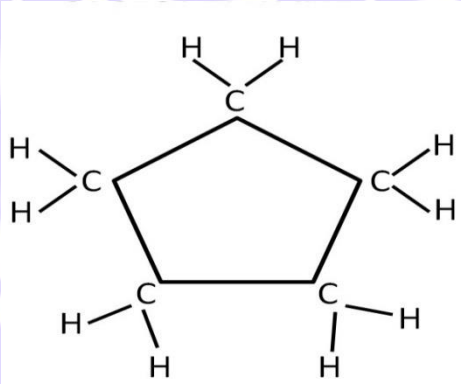

Figure 1 Cyclopentane Structure A

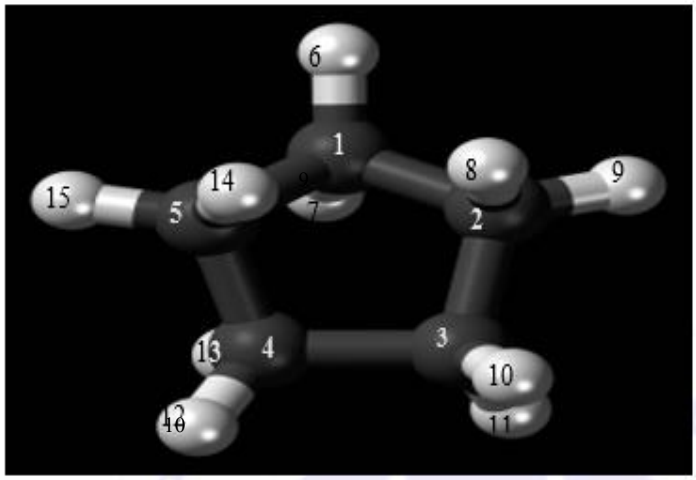

Figure 2 Cyclopentane Structure B
where A represents the chemical structure of **Cyclopentane**
B represents its geometry

As seen in Figure 1, Cyclopentane (C_5H_{10}) typically exhibits two key symmetry axes in its molecular structure. In its most stable conformation, Cyclopentane adopts a puckered or envelope shape to minimize angle strain. The primary symmetry axes are outlined as follows:
Cyclopentane has a C_5 principal axis, along with five C_2 axes, with no additional symmetry elements. The C_5 axis is perpendicular to the plane of the ring, and each C_2 axis passes through the midpoint of one C-C bond and its opposite bond, across the ring. This arrangement gives the molecule its characteristic non-planar shape, compared to a flat pentagon.
Therefore, the symmetry of C_5H_{10} has a puckered or envelope shape (compared to a planar pentagon Shape). The C_5 axis goes through the centre of the atom of the C molecules, and the five C_2 axes go through the five equatorial H atoms. The C_5H_{10} symmetry elements, namely C_5 and C_2 axes, are denoted by $C_5 \coloneqq \langle(1,2,3,4,5)\rangle$ (as shown in figure 2) Also the remaining 5 corners of the framework are given by: $C_{21} \coloneqq \langle(6,7)\rangle$, $C_{22} \coloneqq \langle(8,9)\rangle$, $C_{23} \coloneqq \langle(10,11)\rangle$, $C_{24} \coloneqq \langle(12,13)\rangle$ and $C_{25} \coloneqq \langle(14,15)\rangle$ respectively. Where C_i is the symmetry of the H_2 whose carbon atom are marked as i , $i \leq 1 \leq 5$. Therefore, the full symmetry of Cyclopentane as can be viewed clearly from figure 2, is: $G = (C_{21} \times C_{22} \times C_{23} \times C_{24} \times C_{25}) \rtimes C_5$, which we can write in terms of wreath product as $G \coloneqq \mathbb{Z}_5 wr \mathbb{Z}_2$.

We used GAP package to get the group as follows:

```
gap> Z2 :=Group((1,2));
Group([ (1,2) ])
gap> Z5 :=Group((3,4,5,6,7));
Group([ (3,4,5,6,7) ])
gap> G :=WreathProduct(Z2,Z5);
Group([(1,2),(3,4),(5,6),(7,8),(9,10),(1,3,5,7,9)(2,4,6,8,10)])
gap> Order(G);
160
gap> Elements(G);;
gap> CC :=ConjugacyClasses(G);
[()^G,(9,10)^G,(7,8)(9,10)^G,(5,6)(9,10)^G,(5,6)(7,8)(9,10)^G,(3,4)(7,8)(9,10)^G,(3,4)(5,6)(7,8)(9,10)^G,(1,2
)(3,4)(5,6)(7,8)(9,10)^G,(1,3,5,7,9)(2,4,6,8,10)^G,(1,3,5,7,9,2,4,6,8,10)^G,(1,5,9,3,7)(2,6,10,4,8)^G,(1,5,9,4,8,
2,6,10,3,7)^G,(1,7,3,9,5)(2,8,4,10,6)^G,(1,7,3,9,6,2,8,4,10,5)^G,(1,9,7,5,3)(2,10,8,6,4)^G,(1,9,8,6,4,2,10,7,5,3
)^G ]
```

```
gap> List(CC,x->Order(Representative(x)));
[ 1, 2, 2, 2, 2, 2, 2, 2, 5, 10, 5, 10, 5, 10, 5, 10 ]
gap> Display(CharacterTable(G));
CT2
```

Table 1: Cyclopentane Representation of Conjugacy Classes

S/N	Rpresentative	Size	Name
1	( )	1	1a
2	(9,10)	2	2a
3	(7,8)(9,10)	2	2b
4	(5,6)(9,10)	2	2c
5	(5,6)(7,8)(9,10)	2	2d
6	(3,4)(7,8)(9,10)	2	2e
7	(3,4)(7,8)(9,10)	2	2f
8	(1,2)(3,4)(5,6)(9,8)(9,10)	2	2g
9	(1,3,5,7,9)(2,4,6,8,10)	5	5a
10	(1,3,5,7,9,2,4,6,8,10)	10	10a
11	(1,5,9,3,7)(2,6,10,4,8)	5	5b
12	(1,5,9,4,8,2,6,10,4,3,7)	10	10b
13	(1,7,3,9,5)(2,8,4,10,6)	5	5c
14	(1,7,3,9,,6,2,8,4,10,5)	10	10c
15	(1,9,7,5,3)(2,10,8,6,4)	5	5d
16	(1,9,8,6,4,2,10,7,5,3)	10	10d

Table 2: Character Table for Cyclopentane

	1a	2a	2b	2c	2d	2e	2f	2g	5a	10a	5b	10b	5c	10c	5d	10d
2P	1a	1a	1a	1a	1a	1a	1a	1a	5b	5b	5d	5d	5a	5a	5c	5c
3P	1a	2a	2b	2c	2d	2e	2f	2g	5c	10c	5a	10a	5d	10d	5b	10b
5P	1a	2a	2b	2c	2d	2e	2f	2g	1a	2g	1a	2g	1a	2g	1a	2g
7P	1a	2a	2b	2c	2d	2e	2f	2g	5b	10b	5d	10d	5a	10a	5c	10c
χ_1	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	-1
χ_3	1	-1	1	1	-1	-1	1	-1	A	-A	B	-B	/B	-/B	/A	-/A
χ_4	1	-1	1	1	-1	-1	1	-1	B	-B	/A	-/A	A	-A	/B	-/B
χ_5	1	-1	1	1	-1	-1	1	-1	/B	-/B	A	-A	/A	-/A	B	-B
χ_6	1	-1	1	1	-1	-1	1	-1	/A	-/A	/B	-/B	B	-B	A	-A
χ_7	1	1	1	1	1	1	1	1	A	A	B	B	/B	/B	/A	/A
χ_8	1	1	1	1	1	1	1	1	B	B	/A	/A	A	A	/B	/B
χ_9	1	1	1	1	1	1	1	1	/B	/B	A	A	/A	/A	B	B
χ_{10}	1	1	1	1	1	1	1	1	/A	/A	/B	/B	B	B	A	A
χ_{11}	5	-3	1	1	1	1	-3	5	0	0	0	0	0	0	0	0
χ_{12}	5	3	1	1	-1	-1	-3	-5	0	0	0	0	0	0	0	0
χ_{13}	5	-1	-3	1	3	-1	1	-5	0	0	0	0	0	0	0	0

χ_{14}	5	-1	1	-3	-1	3	1	-5	0	0	0	0	0	0	0	0
χ_{15}	5	1	-3	1	-3	1	1	5	0	0	0	0	0	0	0	0
χ_{16}	5	1	1	-3	1	-3	1	5	0	0	0	0	0	0	0	0

A = E(5)^4
B = E(5)^3

5. Discussions

The character table and conjugacy classes of cyclopentane provide a systematic way to understand its symmetry properties, molecular vibrations, and other group-theoretical aspects. Let's break this down:

1. Conjugacy Classes of Cyclopentane

The conjugacy classes group symmetry operations into sets that are equivalent under the group. These are key to constructing the character table and understanding symmetry. Conjugacy Classes Depend on Cyclopentane's Conformation: Planar Cyclopentane (Idealized, D_5h):
Conjugacy classes: Operations like identity (E), rotations (C_5, C_5^2, C_2), mirror reflections (σv, σh), and improper rotations (S_5). These operations classify the molecule into symmetry sets and allow us to describe how molecular orbitals or vibrations transform.
Envelope Conformation (C_s): There are only two conjugacy classes: Identity (E) and Reflection plane (σ). This simplicity reflects the lower symmetry of the puckered structure.

2. Character Table of Cyclopentane

The character table summarizes how symmetry operations affect molecular orbitals, vibrations, or any other property under the symmetry group.
Planar Cyclopentane (D_5h): The D_5h point group has a more complex character table that includes: Symmetry species (A_1', A_2', E_1', E_2', A_1'', A_2'', E_1'', E_2'') corresponding to different molecular properties. Characters under operations like C_5, C_2, and reflections.

Applications:
IR and Raman Spectroscopy: Vibrational modes are classified as IR or Raman active.
Molecular Orbitals: Orbitals are labeled by their symmetry properties, e.g., bonding or antibonding combinations.

Used to classify vibrational modes, molecular orbitals, and transitions.

3. Dynamics of Cyclopentane Symmetry

Cyclopentane is non-rigid, undergoing rapid interconversion between conformations (e.g., envelope, twist forms). This dynamic behavior: Averages the symmetry over time, often approximating a higher-symmetry group like D_5.

Vibrational analysis and spectroscopy may reflect this averaged symmetry rather than a static conformation.

4. Importance of the Character Table and Conjugacy Classes

i. Vibrational Spectroscopy: The character table allows classification of vibrational modes as IR or Raman active.
Example: For envelope conformation (C_s), only A' vibrations are Raman active.
ii. Electronic Transitions: Molecular orbitals are classified using the symmetry species from the table, aiding in predicting electronic spectra.
iii. Chemical Reactivity: Symmetry considerations (e.g., conservation of symmetry species) help explain reaction mechanisms.
iv. Theoretical Chemistry: Understanding symmetry helps simplify quantum mechanical calculations (e.g., molecular orbital theory, Huckel theory).

Cyclopentane can be described as a group in terms of its symmetry properties, which vary based on its conformation. Here's a detailed explanation:

1. Symmetry Elements in Different Conformations:
Planar Cyclopentane (Idealized): In the theoretical planar conformation, cyclopentane is symmetric and can be associated with the D_5h point group. Group elements: Identity (E), rotations (C_5, C_5^2, C_2), mirror planes (σv, σh), and improper rotations (S_5).
Envelope Conformation (Most Common): In the envelope conformation (where one carbon is out of the plane), the molecule has much lower symmetry, described by the C_s point group.
Group elements: Identity (E) and one reflection plane (σ).
Twist Conformation: The twist conformation has no symmetry elements beyond identity (E) and is classified under the C_1 point group.

2. Cyclopentane as a Set of Transformations (Mathematical Group): A point group is a mathematical group because it satisfies the following:
Closure: Combining any two symmetry operations results in another symmetry operation in the group.
Associativity: The order of applying operations does not matter.
Identity: The identity operation (E) leaves the molecule unchanged.
Inverses: Each symmetry operation has an inverse.

3. Conformational Flexibility and Dynamic Symmetry:
Cyclopentane is not rigid; it undergoes rapid interconversion between conformations (e.g., envelope and twist forms). This dynamic behavior is better represented by its time-averaged symmetry, which may approximate a higher-symmetry group like D_5 under certain conditions.
Cyclopentane does not belong to a single fixed symmetry group due to its flexibility. However, in theoretical planar form, it belongs to D_5h, in envelope form, it belongs to C_s., if distorted further (twist), it may reduce to C_1. This illustrates how group theory applies to both idealized structures and realistic, flexible molecules.

6. Conclusion

In applying the permutation group of degree 2p (p=5) through the wreath product (Samuel, et'al., 2023), we analyzed the symmetry operations of non-rigid Cyclopentane. The conjugacy classes and irreducible character tables of the molecule were determined, as presented in Tables 1 and 2, using computational group theory. Our findings shows that the point groups of Cyclopentane is isomorphic to a Wreath Product $\mathbb{Z}_5 wr \mathbb{Z}_2$, corresponding to cyclic groups $\mathbb{Z}_n$ of size n with an order of 160 and 16 conjugacy classes. All calculations were performed using GAP 4.11.1.

Innovative Contributions of the work

The resulting character tables describe the molecule's symmetry properties, crucial for interpreting molecular vibrations and predicting outcomes for infrared (IR) and Raman spectroscopy, both of which are key to identifying chemical compounds and understanding molecular structures. Symmetry considerations are also essential for determining molecular orbital overlap more efficiently, as orbitals with matching irreducible representations possess the correct symmetry for overlap and molecular orbital formation. Representations labeled A and B denote non-degenerate orbitals. Below Table 2, mathematical functions are provided for assigning orbitals to their respective irreducible representations.
In summary, Conjugacy classes define the fundamental symmetry operations of cyclopentane, grouping them into equivalence sets. The character table encodes how molecular properties transform under these symmetry operations.
For cyclopentane, the symmetry depends on the conformation (planar vs. envelope). These tools are crucial for analyzing spectroscopic, electronic, and chemical properties.

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Conflicts of Interest

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

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