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Exploring Structural Dynamics: Characterization of the Non-Rigid Group of Diethyl Ether Compound $(C_2H_5)_2O$ *

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ABSTRACT: This research paper unveils the character table of the non-rigid diethyl ether compound $(C_2H_5)_2O$. The associated symmetry group is determined to be of order 36, consisting of 36 symmetry operations classified into 18 conjugacy classes and 18 irreducible representations. To the best of our knowledge, this investigation is carried out for the first time and provides novel insights into the structural dynamics of diethyl ether, highlighting its non-rigid characteristics.

Key Words: Non-Rigid molecule group, diethyl ether, wreath product, character table, conjugacy classes.

Contents

1. Introduction

Symmetry occupies a central position in group theory and plays a fundamental role in chemical applications. In particular, the study of symmetry in non-rigid molecules has attracted sustained interest due to its significance in understanding molecular motion and spectroscopic behavior. Balasubramanian [1] emphasized the importance of finite groups in describing algebraic symmetries of discrete structures and demonstrated their effectiveness in predicting physical and chemical properties.

Darafsheh *et al.* [2] employed group-theoretical techniques to investigate the symmetry structure of tetramethylethylene, computing its character table via wreath products. Subsequently, Ashrafi and Hamadanian [3] conducted a detailed analysis of the full non-rigid group of tetraammine platinum(II) associated with the C_{2v} point group, establishing that it is a group of order 216 with 27 conjugacy classes and explicitly determining its character table.

Further progress was achieved by Darafsheh and Moghani [4], who derived the $\mathbb{Q}$-conjugacy character table for the previously unexplored full non-rigid group of 2, 3-dimethylbutane. In a related study, Karimi and Aghaei [5] examined the complete non-rigid group of triethylborane with point group C_{3h}, proving that it has order 648 and 88 conjugacy classes, along with a full characterization of its irreducible representations. Moghadam *et al.* [6] further showed that the full non-rigid groups of dimethylborane and difluoromethyl possess orders 18 and 6, with 6 and 3 conjugacy classes, respectively.

More recently, Suleiman and Mshelia [7] constructed the character table for the full non-rigid molecular group of dirhenium decacarbonyl. Suleiman and Audu [10] extended this framework by computing the full non-rigid groups of trimethylborane and cyclohexane using wreath product techniques. Related developments in symmetry and mathematical modeling continue to appear in the literature, including applications to fluid dynamics and graph-theoretical structures [8,9,11].

Despite these substantial contributions, the conjugacy classes and character table necessary for the classification of wave functions, determination of selection rules, and detailed symmetry analysis of diethyl

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ether remain unexplored. The present study addresses this gap by providing a comprehensive investigation of the non-rigid symmetry group associated with diethyl ether.

The novelty of this work lies in presenting, for the first time, the character table of the non-rigid diethyl ether molecule $(C_2H_5)_2O$. The associated symmetry group is shown to be of order 36, consisting of 36 symmetry operations distributed among 18 conjugacy classes and 18 irreducible representations. These results provide new insights into the non-rigid structural dynamics of diethyl ether and contribute to a deeper understanding of its molecular symmetry.

2. Main Results

Let Ω be an arbitrary set whose elements are called *points*. A bijective mapping from Ω onto itself is called a *permutation* of Ω. The collection of all permutations of Ω forms a group under the operation of composition of mappings. This group is known as the *symmetric group* on Ω and is denoted by $\mathrm{Sym}(\Omega)$ or S_Ω.

In the special case where $\Omega = \{1, 2, \ldots, n\}$, the symmetric group is denoted by S_n, where n is a positive integer. A *permutation group* is any subgroup of a symmetric group.

For a finite group G, the number of elements in G, denoted by $|G|$, is called the *order* of G. If G is infinite, its order is written as $|G| = \infty$. For an element $x \in G$, the *order of* x is defined as the order of the cyclic subgroup generated by x, denoted by

$$\langle x \rangle = \{e, x, x^2, x^3, \ldots, x^{-1}, x^{-2}, x^{-3}, \ldots\},$$

where e is the identity element of G. If $\langle x \rangle$ is finite, then

$$\langle x \rangle = \{e, x, x^2, \ldots, x^k\},$$

and the order of x is the smallest positive integer k such that $x^k = e$. These definitions provide the fundamental concepts required for the study of permutations, symmetric groups, and subgroup orders.

2.1. The f-NRG of Diethyl Ether

Consider the diethyl ether molecule $(C_2H_5)_2O$ with the molecular structure shown in Figure 1.

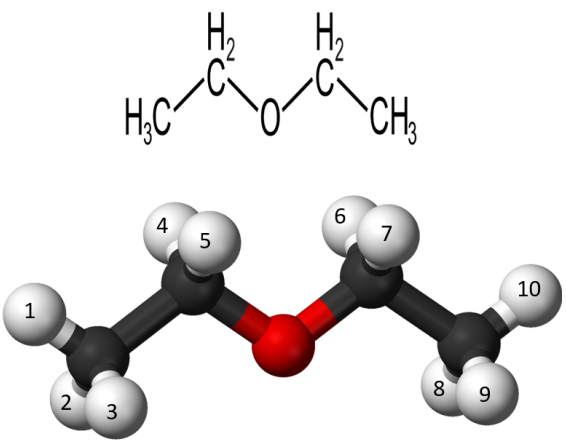

Figure 1: Structure of Diethyl ether.

The rapid rotational motion of the methyl group exhibits a high degree of mobility, which plays a crucial role in generating the dynamical symmetry of molecular systems. This fast internal rotation motivates a detailed investigation of the dynamical symmetry properties associated with such non-rigid molecules. As an initial step in this analysis, special attention is given to the labeling of hydrogen atoms, with emphasis on identifying the fundamental vertices of the molecular framework.

We begin by renaming the hydrogen atoms corresponding to the corners of the molecular skeleton. Using the GAP software package, the full non-rigid group associated with the diethyl ether molecule is computed. The group is generated by the following permutations:

```
gap>
G := Group(
(1,2,3)(8,9,10)(4,5)(6,7),
(1,10)(2,8)(3,9)(4,6)(5,7),
(1,9)(2,10)(3,8)(4,6)(5,7),
(1,8)(2,9)(3,10)(4,6)(5,7),
(1,10)(2,8)(3,9)(4,7)(5,6),
(1,9)(2,10)(3,8)(4,7)(5,6),
(1,8)(2,9)(3,10)(4,7)(5,6)
);

Group([
(1,2,3)(4,5)(6,7)(8,9,10),
(1,10)(2,8)(3,9)(4,6)(5,7),
(1,9)(2,10)(3,8)(4,6)(5,7),
(1,8)(2,9)(3,10)(4,6)(5,7),
(1,10)(2,8)(3,9)(4,7)(5,6),
(1,9)(2,10)(3,8)(4,7)(5,6),
(1,8)(2,9)(3,10)(4,7)(5,6)
])
```

The complete set of elements of the group is obtained using the command:

```
gap> Elements(G);
```

which yields all 36 distinct permutations of the group. Furthermore, the order of the group is verified by:

```
gap> Order(G);
36
```

confirming that the computed full non-rigid group of diethyl ether is of order 36. Finally, the character table of the group is generated using:

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

The resulting character table reveals that the group consists of 18 conjugacy classes and, consequently, 18 irreducible representations. These computations provide a rigorous algebraic foundation for analyzing the dynamical symmetry and non-rigid behavior of the diethyl ether molecule.

$$A = E(3)^2 = \frac{-1-\sqrt{-3}}{2}, \qquad B = 2E(3)^2 = -1-\sqrt{-3},$$

The symmetry group of non-rigid diethyl ether is identified as a wreath product consisting of 36 permutations. This group decomposes into 18 conjugacy classes and, consequently, admits 18 irreducible characters. In Table 1, each conjugacy class is represented by a selected element g, together with the size of its class.

The number of elements in the conjugacy class containing g is given by

$$\frac{|G|}{|C_G(g)|},$$

where $C_G(g)$ denotes the centralizer of g in the group G.

Table 1: Representatives of conjugacy classes of diethyl ether

S/N	**Representative**	**Size**	**Name**
1	()	1	$1a$
2	$(8,9,10)$	2	$3a$
3	$(8,10,9)$	2	$3b$
4	$(4,5)(6,7)$	1	$2a$
5	$(4,5)(6,7)(8,9,10)$	2	$6a$
6	$(4,5)(6,7)(8,10,9)$	2	$6b$
7	$(1,2,3)(8,9,10)$	1	$3c$
8	$(1,2,3)(8,10,9)$	1	$3d$
9	$(1,2,3)(4,5)(6,7)(8,9,10)$	1	$6c$
10	$(1,2,3)(4,5)(6,7)(8,10,9)$	1	$6d$
11	$(1,3,2)(8,10,9)$	1	$3e$
12	$(1,3,2)(4,5)(6,7)(8,10,9)$	1	$6e$
13	$(1,8)(2,9)(3,10)(4,6)(5,7)$	3	$2b$
14	$(1,8,2,9,3,10)(4,6)(5,7)$	3	$6f$
15	$(1,8,3,10,2,9)(4,6)(5,7)$	3	$6g$
16	$(1,8)(2,9)(3,10)(4,7)(5,6)$	3	$2c$
17	$(1,8,2,9,3,10)(4,7)(5,6)$	3	$6h$
18	$(1,8,3,10,2,9)(4,7)(5,6)$	3	$6i$

Table 2: Character table for diethyl ether

	$1a$	$3a$	$3b$	$2a$	$6a$	$6b$	$3c$	$3d$	$6c$	$6d$	$3e$	$6e$	$2b$	$6f$	$6g$	$2c$	$6h$	$6i$
$2P$	$1a$	$3b$	$3a$	$1a$	$3b$	$3a$	$3e$	$3d$	$3e$	$3d$	$3c$	$3c$	$1a$	$3c$	$3e$	$1a$	$3c$	$3e$
$3P$	$1a$	$1a$	$1a$	$2a$	$2a$	$2a$	$1a$	$1a$	$2a$	$2a$	$1a$	$2a$	$2b$	$2b$	$2b$	$2c$	$2c$	$2c$
$5P$	$1a$	$3b$	$3a$	$2a$	$6b$	$6a$	$3e$	$3d$	$6e$	$6d$	$3c$	$6c$	$2b$	$6g$	$6f$	$2c$	$6i$	$6h$
χ_1	1	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	1	1
χ_3	1	1	1	-1	-1	-1	1	1	-1	-1	1	-1	1	1	1	-1	-1	-1
χ_4	1	1	1	1	1	1	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
χ_5	1	A	$\overline{A}$	-1	$-A$	$-\overline{A}$	$\overline{A}$	1	$-\overline{A}$	-1	A	$-A$	-1	$-A$	$-\overline{A}$	1	A	$\overline{A}$
χ_6	1	$\overline{A}$	A	-1	$-\overline{A}$	$-A$	A	1	$-A$	-1	$\overline{A}$	$-\overline{A}$	-1	$-\overline{A}$	$-A$	1	$\overline{A}$	A
χ_7	1	A	$\overline{A}$	-1	$-A$	$-\overline{A}$	$\overline{A}$	1	$-\overline{A}$	-1	A	$-A$	1	A	$\overline{A}$	-1	$-A$	$-\overline{A}$
χ_8	1	$\overline{A}$	A	-1	$-\overline{A}$	$-A$	A	1	$-A$	-1	$\overline{A}$	$-\overline{A}$	1	$\overline{A}$	A	-1	$-\overline{A}$	$-A$
χ_9	1	A	$\overline{A}$	1	A	$\overline{A}$	$\overline{A}$	1	$\overline{A}$	1	A	A	-1	$-A$	$-\overline{A}$	-1	$-A$	$-\overline{A}$
χ_{10}	1	$\overline{A}$	A	1	$\overline{A}$	A	A	1	A	1	$\overline{A}$	$\overline{A}$	-1	$-\overline{A}$	$-A$	-1	$-\overline{A}$	$-A$
χ_{11}	1	A	$\overline{A}$	1	A	$\overline{A}$	$\overline{A}$	1	$\overline{A}$	1	A	A	1	A	$\overline{A}$	1	A	$\overline{A}$
χ_{12}	1	$\overline{A}$	A	1	$\overline{A}$	A	A	1	A	1	$\overline{A}$	$\overline{A}$	1	$\overline{A}$	A	1	$\overline{A}$	A
χ_{13}	2	-1	-1	-2	1	1	2	-1	-2	1	2	-2	0	0	0	0	0	0
χ_{14}	2	-1	-1	2	-1	-1	2	-1	2	-1	2	2	0	0	0	0	0	0

Table 2 presents the complete character table of the group. The first row lists representatives of each conjugacy class, denoted using GAP notation by the order of the element. Specifically, if an element g has order n, its conjugacy class is labeled by nx, where $x \in \{a, b, c, \ldots\}$ distinguishes different classes of elements having the same order.

If g belongs to the class nx and $m \in \{2, 3, 5\}$, then g^m lies in a conjugacy class of elements of order $n/\gcd(n, m)$, as indicated in the rows labeled $2P$, $3P$, and $5P$. The values of the irreducible characters χ_i, $1 \leq i \leq 18$, are listed for each conjugacy class, completing the character table.

Together, Tables 1 and 2 provide the necessary framework for the classification of molecular wavefunctions, determination of selection rules, and further symmetry-based analysis of the non-rigid diethyl ether molecule.

3. Conclusion

In this paper, we have investigated the non-rigid symmetry of the diethyl ether molecule by computing its associated group, conjugacy classes, and character table. The results, summarized in Tables 1 and 2, reveal that the symmetry group is of order 36 and decomposes into 18 conjugacy classes, thereby admitting 18 irreducible characters. These findings provide a detailed description of the underlying structural symmetries governing the dynamical behavior of diethyl ether.

All computations were carried out using the GAP software package, ensuring both precision and computational reliability. The characterization presented in this work contributes to a deeper understanding of the symmetry properties of non-rigid molecules and establishes a foundation for future investigations into molecular symmetry, spectroscopic selection rules, and related applications.

Declarations

Conflicts of interest: The authors declare that they have no conflicts of interest and all agree to publish this paper under academic ethics.

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