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

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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 (N_2H_2). 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 $B(CH_3)_3$ 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 $(\mathbb{Z}_3)wr(\mathbb{Z}_2\times\mathbb{Z}_2)$. 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 $\mathbb{Z}_2 wrS_4$ while that of octanitrocubane was shown to be isomorphic to $(\mathbb{Z}_2)wr(S_4\times\mathbb{Z}_2)$. 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 $\mathbb{Z}_3$ by the cyclic group $\mathbb{Z}_2$, that is, $(\mathbb{Z}_3\times\mathbb{Z}_3\times\mathbb{Z}_3\times\mathbb{Z}_3)\rtimes\mathbb{Z}_2$, 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 $\mathbb{Z}_3\times(\mathbb{Z}_3 wr\mathbb{Z}_2)$ 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_s 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 Cyclohaxanethe groups are found to be isomorphic to the wreath products $C_3 wrC_2$ and $C_2 wrC_6$ 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 Ω be an arbitrary set; we shall often refer to its elements as *points*. A bijective

(a one-to-one, onto mapping) of Ω onto itself is called a *permutation* of Ω. The set of all permutations of Ω forms a group under composition of mappings, called the *Symmetric group* of Ω. We shall denote this group by $Sym(\Omega)$ (or S_Ω), and write S_n to denote the special group $Sym(\Omega)$ when n is a positive integer and $\Omega = \{1,2,\cdots,n\}$. A *permutation group* is just a subgroup of Symmetric group. If Γ and Δ are nonempty sets, then we call Γ^Δ to denote the set of all functions from Δ to Γ. In the case that C is a group, we turn C^Δ into a group by defining product "pointwise"

$$fg(\gamma) := f(\gamma)g(\gamma)$$

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 Δ. 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^Δ via

$$f^d(\gamma) := f\left(\gamma^{d^{-1}}\right)$$

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

$$(f_1, d_1)(f_2, d_2) = \left(f_1 f_2^{d_1^{-1}}, d_1 d_2\right)$$

(See [9])

2.1. f-NRG of Trimethylborane

Consider the trimethylborane compound $B(CH_3)_3$ 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 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 $i, 1 \le i \le 3$. 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 $G := \mathbb{Z}_3 wr \mathbb{Z}_3$. 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):
gap> Order(G);
81
gap>SizesConjugacyClasses(G);
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	9a
14.	(1,4,7,3,6,9,2,5,8)	9	9b
15.	(1,7,4) (2,8,5) (3,9,6)	9	3l
16.	(1,7,5,2,8,6,3,9,4)	9	9c
17.	(1,7,6,3,9,5,2,8,4)	9	9d

Table 2. Character Table for Trimethylborane.

	1a	3a	3b	3c	3d	3e	3f	3g	3h	3i	3j	3k	9a	9b	3l	9c	9d
2P	1a	3b	3a	3f	3e	3d	3c	3j	3i	3h	3g	3l	9d	9c	3k	9b	9a
3P	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a	3g	3j	1a	3g	3j
5P	1a	3b	3a	3f	3e	3d	3c	3j	3i	3h	3g	3l	9d	9c	3k	9b	9a
7P	1a	3a	3b	3c	3d	3e	3f	3g	3h	3i	3j	3k	9a	9b	3l	9c	9d
χ_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	A	A	A	$\overline{A}$	$\overline{A}$	$\overline{A}$
χ_3	1	1	1	1	1	1	1	1	1	1	1	$\overline{A}$	$\overline{A}$	$\overline{A}$	A	A	A
χ_4	1	A	$\overline{A}$	$\overline{A}$	1	1	A	1	A	$\overline{A}$	1	1	A	$\overline{A}$	1	A	$\overline{A}$
χ_5	1	$\overline{A}$	A	A	1	1	$\overline{A}$	1	$\overline{A}$	A	1	1	$\overline{A}$	A	1	$\overline{A}$	A
χ_6	1	A	$\overline{A}$	$\overline{A}$	1	1	A	1	A	$\overline{A}$	1	A	$\overline{A}$	1	$\overline{A}$	1	A
χ_7	1	$\overline{A}$	A	A	1	1	$\overline{A}$	1	$\overline{A}$	A	1	$\overline{A}$	A	1	A	1	$\overline{A}$
χ_8	1	A	$\overline{A}$	$\overline{A}$	1	1	A	1	A	$\overline{A}$	1	$\overline{A}$	1	A	A	$\overline{A}$	1
χ_9	1	$\overline{A}$	A	A	1	1	$\overline{A}$	1	$\overline{A}$	A	1	A	1	$\overline{A}$	$\overline{A}$	A	1
χ_{10}	3	B	$\overline{B}$	$-C$	0	0	C	$\overline{D}$	$\overline{B}$	$-B$	D	0	0	0	0	0	0
χ_{11}	3	$\overline{B}$	B	C	0	0	$-C$	D	$-B$	$\overline{B}$	$\overline{D}$	0	0	0	0	0	0

Continued

χ_{12}	3	C	$-C$	$-B$	0	0	$-\bar{B}$	D	B	$\bar{B}$	D	0	0	0	0	0	0
χ_{13}	3	$-C$	C	$-\bar{B}$	0	0	-B	D	$\bar{B}$	B	$\bar{D}$	0	0	0	0	0	0
χ_{14}	3	$-B$	$-\bar{B}$	B	0	0	$\bar{B}$	D	$-C$	C	$\bar{D}$	0	0	0	0	0	0
χ_{15}	3	$-\bar{B}$	$-B$	$\bar{B}$	0	0	B	$\bar{D}$	C	$-C$	D	0	0	0	0	0	0
χ_{16}	3	0	0	0	D	$\bar{D}$	0	3	0	0	3	0	0	0	0	0	0
χ_{17}	3	0	0	0	$\bar{D}$	D	0	3	0	0	3	0	0	0	0	0	0

where: $A = E(3)^2 = \frac{-1 - Sqrt(-3)}{2}$; $B = -E(3) - 2 * E(3)^2 = \frac{3 + Sqrt(-3)}{2}$;

$C = -E(3) + E(3)^2 = -Sqrt(-3)$; $D = 3 * E(3)^2 = \left(-3 - 3 * Sqrt(-3)\right)/2$.

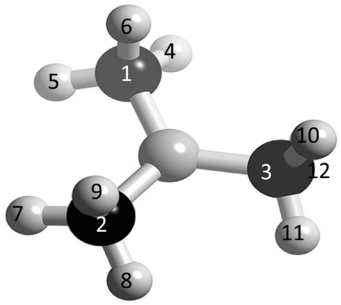

Figure 1. The structure of trimethylborane.

2.2. f-NRG of Cyclohexane

Consider the cyclohexane compound C_6H_{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 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 **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 H_2 whose carbon atom is marked as $i, 1 \le i \le 6$. Therefore, the full symmetry of cyclohexane is:

$G = (B_1 \times B_2 \times B_3 \times B_4 \times B_5 \times B_6) \rtimes A$. 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:

```
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),
(1,3,5,7,9,11)(2,4,6,8,10,12) ])
gap> Elements(G):
gap> Order(G);
384
gap>SizesConjugacyClasses(G);
gap> Display(CharacterTable(G));
```

(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.

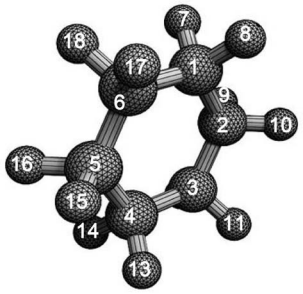

Figure 2. The structure of cyclohexane.

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	12b
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	3a	6c	3b	3b	3b	1a	2e	2k	2m	3a	3a	3a	3b	6e
3P	1a	2a	2b	2c	2d	2e	2f	2g	2h	2i	2j	2k	2l	2m	2n	4c	1a	2i	2m	2n	4a	4b	4c	1a	2i	2m	2n	4c
5P	1a	2a	2b	2c	2d	2e	2f	2g	2h	2i	2j	2k	2l	2m	6f	12b	3b	6d	6e	2n	4a	4b	4c	3a	6b	6c	6a	12a
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	6f	12b	3b	6d	6e	2n	4a	4b	4c	3a	6b	6c	6a	12a
χ_1	1	1	1	1	1	1	1	1	1	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	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	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	1	−1	−1	−1	−1	1	1	1	−1	−1
χ_5	1	−1	1	1	−1	1	−1	−1	1	−1	1	1	−1	1	A	$-A$	$-\overline{A}$	$\overline{A}$	$-\overline{A}$	−1	1	−1	1	$-A$	A	$-A$	$\overline{A}$	$-\overline{A}$
χ_6	1	−1	1	1	−1	1	−1	−1	11	−1	1	1	−1	1	$\overline{A}$	$-\overline{A}$	$-A$	A	$-A$	−1	1	−1	1	$-\overline{A}$	$\overline{A}$	$-\overline{A}$	A	$-A$
χ_7	1	−1	1	1	−1	1	−1	−1	1	−1	1	1	−1	1	$-\overline{A}$	$\overline{A}$	$-A$	A	$-A$	1	−1	1	−1	$-\overline{A}$	$\overline{A}$	$-\overline{A}$	$-A$	A
χ_8	1	−1	1	1	−1	1	−1	−1	1	−1	1	1	−1	1	$-A$	A	$-\overline{A}$	$\overline{A}$	$-\overline{A}$	1	−1	1	−1	$-A$	A	$-A$	$-\overline{A}$	$\overline{A}$
χ_9	1	1	1	1	1	1	1	1	1	1	1	1	1	1	A	A	$-\overline{A}$	$-\overline{A}$	$-\overline{A}$	−1	−1	−1	−1	$-A$	$-A$	$-A$	$\overline{A}$	$\overline{A}$
χ_{10}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	$\overline{A}$	$\overline{A}$	$-A$	$-A$	$-A$	−1	−1	−1	−1	$-\overline{A}$	$-\overline{A}$	$-\overline{A}$	A	A
χ_{11}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	$-\overline{A}$	$-\overline{A}$	$-A$	$-A$	$-A$	1	1	1	1	$-\overline{A}$	$-\overline{A}$	$-\overline{A}$	$-A$	$-A$
χ_{12}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	$-A$	$-A$	$-\overline{A}$	$-\overline{A}$	$-\overline{A}$	1	1	1	1	$-A$	$-A$	$-A$	$-\overline{A}$	$-\overline{A}$
χ_{13}	2	0	−2	2	0	−2	0	0	2	0	−2	2	0	−2	0	0	2	0	−2	0	0	0	0	2	0	−2	0	0
χ_{14}	2	0	−2	2	0	−2	0	0	2	0	−2	2	0	−2	0	0	B	0	$-B$	0	0	0	0	$\overline{B}$	0	$-\overline{B}$	0	0
χ_{15}	2	0	−2	2	0	−2	0	0	2	0	−2	2	0	−2	0	0	$\overline{B}$	0	$-\overline{B}$	0	0	0	0	B	0	$-B$	0	0
χ_{16}	3	−1	−1	−1	3	3	−1	−1	−1	3	−1	3	−1	3	0	0	0	0	0	−3	1	1	−3	0	0	0	0	0
χ_{17}	3	−1	−1	−1	3	3	−1	−1	−1	3	−1	3	−1	3	0	0	0	0	0	3	−1	−1	3	0	0	0	0	0
χ_{18}	3	1	−1	−1	−3	3	1	1	−1	−3	−1	3	1	3	0	0	0	0	0	−3	−1	1	3	0	0	0	0	0
χ_{19}	3	1	−1	−1	−3	3	1	1	−1	−3	−1	3	1	3	0	0	0	0	0	3	1	−1	−3	0	0	0	0	0
χ_{20}	6	−2	−2	2	2	−2	2	2	−2	−6	2	−2	−2	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{21}	6	−2	2	−2	−2	−2	2	2	2	6	−2	−2	−2	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{22}	6	2	−2	2	−2	−2	−2	−2	−2	6	2	−2	2	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{23}	6	2	2	−2	2	−2	−2	−2	2	−6	−2	−2	2	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{24}	6	0	2	−2	0	−6	0	0	−2	0	2	6	0	−6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{25}	6	−4	2	2	0	2	0	0	−2	0	−2	−2	4	−6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{26}	6	0	−2	−2	0	2	−4	4	2	0	2	−2	0	−6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{27}	6	0	−2	−2	0	2	4	−4	2	0	2	−2	0	−6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{28}	6	4	2	2	0	2	0	0	−2	0	−2	−2	−4	−6	0	0	0	0	0	0	0	0	0	0	0	0	0	0

where: $A = -E(3) = \frac{1 - Sqrt(-3)}{2}$; $B = 2 * E(3) = -1 + Sqrt(-3)$.

3. Conclusion

In this paper, we computed the group, the conjugacy classes and character tables of Trimethylborane and Cyclohaxane as seen in Tables 1-4. We found 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 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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