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Full non-rigid group of Sponge and Pina

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The non-rigid molecule group theory (NRG) in which the dynamical symmetry operations are defined as physical operations is a new field in chemistry. Smeyers and Villa computed the r-NRG of the triple equivalent methyl rotation in pyramidal trimethylamine with inversion and proved that the r-NRG of this molecule is a group of order 648, containing a subgroup of order 324 without inversions (see J. Math. Chem. **28**(4) (2000) 377–388). In this work, a computational method is described, by means of which it is possible to calculate the symmetry group of molecules. We study the full non-rigid group (f-NRG) of Sponge and Pina molecules with C_2 and C_i point groups, respectively. It proved that these are groups of order 162 and 13122 with 54 and 3240 conjugacy classes, respectively. The character tables of these groups are also computed.

KEY WORDS: non-rigid group, character table, Sponge, Pina

1. Introduction

Following Smeyers [1,2], a non-rigid molecule is a molecular system, which presents large amplitude vibration modes. This kind of motion appears whenever the molecule possesses various isoenergetic forms separated by relatively low energy barriers. In such cases, intramolecular transformations occur.

The complete set of the molecular conversion operations which commute with the nuclear motion operator will contain overall rotation operations, describing the molecule rotating as a whole, and intramolecular motion operations,

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describing molecular moieties moving with respect to the rest of the molecule. Such a set forms a group, which we call the full non-rigid group (f-NRG).

Group theory for non-rigid molecules is getting everyday more and more relevance and numerous application to large amplitude vibrations in spectroscopy of small organic molecules are appearing in the literature [3–6].

Longuet-Higgins [7] investigated the symmetry groups of non-rigid molecules, where changes from one conformation to another can occur easily. In many cases, these symmetry groups are not isomorphic with any of the familiar symmetry groups of rigid molecules, and their character tables are not known. It is therefore of some interest and importance to develop simple methods of calculating these character tables, which are needed for classification of wave functions, determination of selection rules, and so on.

The method as it is described here is appropriate for molecules, which consist of a number of XO_2 or XH_3 groups attached to a rigid framework. An example of such a molecule is Pina and Sponge molecules, which is considered here in some detail. It is not appropriate in cases where the framework is linear, as in ethane, but Bunker [8] has shown how to deal with such molecules. We use the standard notation and terminology on character theory [9,10].

Lomont [11], has given two methods for calculating character tables. These are satisfactory for small group, but both of them require knowledge of the class constant and hence of the group multiplication table and they become very unwieldy as soon as the order of the group becomes even moderately large. For non-rigid molecules, whose symmetry groups may have several thousand elements, they are usually quite impracticable.

Smeyers and Villa [12] investigated the r-NRG of planer trimethylamine and proved that this is a group of order 324. Furthermore, they showed that this molecule has a pyramidal inversion and so the order of r-NRG of trimethylamine is 648.

In [13], Stone described a method, which it is appropriate for molecules with a number of XH_3 groups attached to a rigid framework. It is not appropriate in cases where the framework is linear, as in ethane and dimethylacetylene.

We described a method by which it is possible to find the character table of large molecules [14–18]. In this paper, using this and a new method, we investigate the f-NRG of Pina and Sponge molecules. We prove that these are groups of order 162 and 5184 for the point group of types C_2 and C_i, respectively.

Throughout this paper, all groups considered are assumed to be finite. Our notation is standard and taken mainly from refs. [1], [9] and [10].

2. Method

Suppose $G = A \times B$ is a finite group with subgroups A and B. It is a well-known fact that if X is a conjugacy class of A and Y is a conjugacy class of B then $X \times Y$ is a conjugacy class of G and every conjugacy class of G has this form. Suppose $\mathbb{C}$

denotes the set of complex numbers. If $\chi: A \longrightarrow \mathbb{C}$ is an irreducible character of A and $\psi: B \longrightarrow \mathbb{C}$ is an irreducible character of B then the map $\varphi: G \longrightarrow \mathbb{C}$ with $\varphi(g) = \chi(a)\psi(b)$, for every element $g = (a, b) \in G$, is an irreducible character for G, and that, every irreducible character of G has such a form. We use this simple fact to compute the character tables of f-NRG of Pina and Sponge molecules.

Suppose H and G are the full non-rigid group of Pina and Sponge molecules, respectively. The process of enumerating the symmetry operations of these molecules and arranging them in classes can be explained as adopting a numbering convention for the proton carbon nuclei as shown in figures 1 and 2. Let us define the following operations:

$$X_1 = (1,8)(2,9)(3,10)(6,7)(11,16)(12,14)(13,15)(17,20)(18,21)(19,22)(23,29)(24,30)(25,31)(26,32)(27,33)(28,34),$$

$$X_2 = (1,8)(2,9)(3,10)(6,7)(11,16)(12,14)(13,15)(17,20)(18,21)(19,22)(23,29,24,30,25,31)(26,32,27,33,28,34),$$

$$X_3 = (23,24,25),$$

$$X_4 = (26,27,28),$$

$$X_5 = (29,30,31),$$

$$X_6 = (32,33,34),$$

$$X_7 = (1,8)(2,9)(3,10)(6,7)(11,16)(12,14)(13,15)(17,20)(18,21)(19,22)(23,29,24,30,25,31)(26,32)(27,33)(28,34),$$

$$X_8 = (1,8)(2,9)(3,10)(6,7)(11,16)(12,14)(13,15)(17,20)(18,21)(19,22)(23,29)(24,30)(25,31)(26,32,27,33,28,34),$$

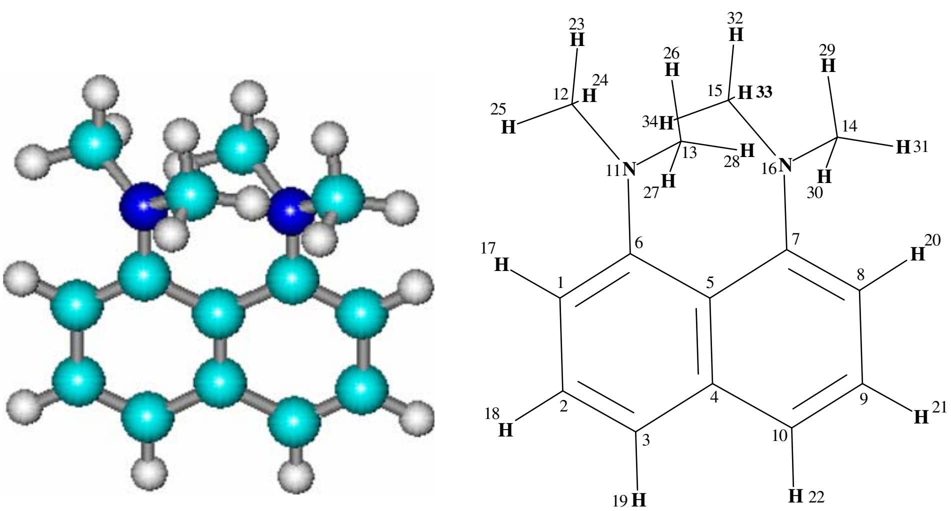

Figure 1. Sponge with C_2 point group.

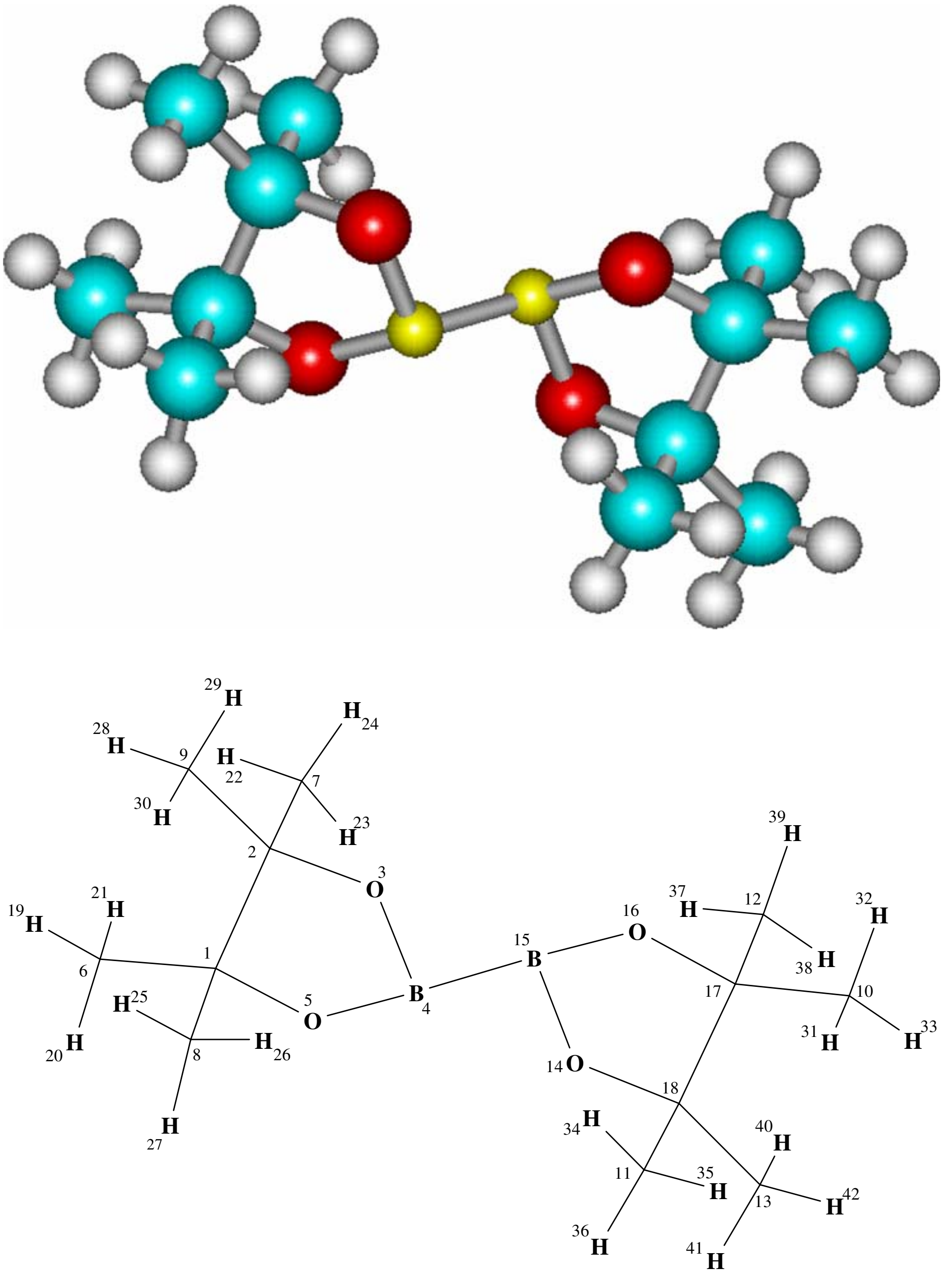

Figure 2. Pina with C_{i} point group.

Using figure 1, we can see that these operations generate the f-NRG of Sponge molecule. We now apply GAP SYSTEM [19] to find the structure of the group G and its character table. At first, we can see that G is also generated by the elements X_1, X_2 and X_3. To find the structure of the group G, we define:

$$
\begin{aligned}
Y_1 &= (1,8)(2,9)(3,10)(6,7)(11,16)(12,14)(13,15)(17,20)(18,21)(19,22)\\
&\quad (23,29)(24,30)(25,31)(26,32)(27,33)(28,34),\\
Y_2 &= (23,25,24)(29,30,31),\\
Y_3 &= (23,24,25)(26,27,28)(29,30,31)(32,33,34).
\end{aligned}
$$

Set $A = \langle X_6, Y_1, Y_2\rangle$ and $B = \langle Y_3\rangle$. Then A and B are normal subgroups of G of orders 54 and 3, respectively. Since $A \cap B = \langle()\rangle$, G is isomorphic to $A \times B$. We now consider the following operations:

$$
\begin{aligned}
Z_1 &= (1,8)(2,9)(3,10)(6,7)(11,16)(12,14)(13,15)(17,20)(18,21)(19,22)\\
&\quad (23,29)(24,30)(25,31)(26,32)(27,33)(28,34),\\
Z_2 &= (26,28,27)(32,33,34),\\
Z_3 &= (26,27,28)(32,33,34).
\end{aligned}
$$

Next we suppose that $B_1 = \langle Z_1, Z_2, Y_2\rangle$ and $B_2 = \langle Z_3\rangle$. Using GAP, it is easy to see that, $|B_1| = 18$, $|B_2| = 3$, $B_1 \cap B_2 = \langle()\rangle$ and so B is isomorphic to $B_1 \times B_2$. Therefore, $G \cong A \times B_1 \times B_2$ and G has order 162. Since A and B_2 are cyclic groups of order 3 and conjugacy classes and character tables of cyclic groups are known, it is enough to find the conjugacy classes and character table of the group B_1. In tables 1 and 2, we find conjugacy classes and character table of the group B_1.

We now consider the Pina molecule to find the f-NRG and its character table. Let us define the following operations:

Table 1
The representatives of conjugacy classes of the group B_1.

No.	Representatives	Size
1	()	1
2	(26,27,28)(32,34,33)	2
3	(23,24,25)(29,31,30)	2
4	(23,24,25)(26,27,28)(29,31,30)(32,34,33)	2
5	(23,24,25)(26,28,27)(29,31,30)(32,33,34)	2
6	(1,8)(2,9)(3,10)(6,7)(11,16)(12,14)(13,15)(17,20)(18,21) (19,22)(23,29)(24,30)(25,31)(26,32)(27,33)(28,34)	9

Table 2
The character table of the group B_1.

	1a	3b	2c	6a	3c	6b
χ_1	1	1	1	1	1	1
χ_2	1	1	1	1	1	−1
χ_3	2	2	−1	−1	−1	0
χ_4	2	−1	2	−1	−1	0
χ_5	2	−1	−1	−1	2	0
χ_6	2	−1	−1	2	−1	0

$$
\begin{aligned}
\alpha_1 &= (1,17)(2,18)(3,14)(4,15)(5,16)(6,10)(7,11)(8,12)(9,13)(19,31)(20,33)\\
&\quad (21,32)(22,35)(23,34)(24,36)(25,38)(26,37)(27,39)(28,40)(29,42)(30,41),\\
\alpha_2 &= (1,17)(2,18)(3,14)(4,15)(5,16)(6,10)(7,11)(8,12)(9,13)(19,31,20,33,21,32)\\
&\quad (22,35)(23,34)(24,36)(25,38)(26,37)(27,39)(28,40)(29,42)(30,41),\\
\alpha_3 &= (1,17)(2,18)(3,14)(4,15)(5,16)(6,10)(7,11)(8,12)(9,13)(22,35,23,34,24,36)\\
&\quad (19,31)(20,33)(21,32)(25,38)(26,37)(27,39)(28,40)(29,42)(30,41),\\
\alpha_4 &= (1,17)(2,18)(3,14)(4,15)(5,16)(6,10)(7,11)(8,12)(9,13)(25,38,26,37,27,39)\\
&\quad (19,31)(20,33)(21,32)(22,35)(23,34)(24,36)(28,40)(29,42)(30,41),\\
\alpha_5 &= (1,17)(2,18)(3,14)(4,15)(5,16)(6,10)(7,11)(8,12)(9,13)(28,40,29,42,30,41)\\
&\quad (19,31)(20,33)(21,32)(22,35)(23,34)(24,36)(25,38)(26,37)(27,39),\\
\alpha_6 &= (1,17)(2,18)(3,14)(4,15)(5,16)(6,10)(7,11)(8,12)(9,13)(19,31,20,33,21,32)\\
&\quad (22,35,23,34,24,36)(25,38,26,37,27,39)(28,40,29,42,30,41),\\
\alpha_7 &= (19,20,21),\\
\alpha_8 &= (22,23,24),\\
\alpha_9 &= (25,26,27),\\
\alpha_{10} &= (28,29,30),\\
\alpha_{11} &= (31,32,33),\\
\alpha_{12} &= (34,35,36),\\
\alpha_{13} &= (37,38,39),\\
\alpha_{14} &= (40,41,42).
\end{aligned}
$$

Using figure 2, we can see that these operations generate the f-NRG of Pina molecule. We apply again GAP to find the structure of the group H and its character table. At first, we can see that H is also generated by the elements $\alpha_1,\ldots,\alpha_5$. To find the structure of the group H, we define:

$$
\begin{aligned}
U_1 &= (40,41,42),\\
U_2 &= (34,35,36),
\end{aligned}
$$

$U_3 = (31, 32, 33),$
$U_4 = (1, 17)(2, 18)(3, 14)(4, 15)(5, 16)(6, 10)(7, 11)(8, 12)(9, 13)(19, 31)(20, 33)$
$(21, 32)(22, 35)(23, 34)(24, 36)(25, 38)(26, 37)(27, 39)(28, 40)(29, 42)(30, 41),$
$U_5 = (25, 26, 27)(37, 38, 39),$
$U_6 = (19, 21, 20)(22, 24, 23)(25, 26, 27)(31, 32, 33)(34, 35, 36)(37, 39, 38).$

Set $C = \langle U_1, U_2, U_3, U_4, U_5\rangle$ and $D = \langle U_6\rangle$. Then C and D are normal subgroups of H of orders 4374 and 3, respectively. Since $C \cap D = \langle()\rangle$ and $|G| = |C| \times |D|$, H is isomorphic to $C \times D$. We now consider the following operations:

$V_1 = (19, 21, 20)(22, 23, 24)(31, 32, 33)(34, 36, 35)$
$V_2 = (40, 41, 42),$
$V_3 = (31, 32, 33),$
$V_4 = (1, 17)(2, 18)(3, 14)(4, 15)(5, 16)(6, 10)(7, 11)(8, 12)(9, 13)(19, 31)(20, 33)$
$(21, 32)(22, 35)(23, 34)(24, 36)(25, 38)(26, 37)(27, 39)(28, 40)(29, 42)(30, 41),$
$V_5 = (22, 23, 24)(34, 35, 36),$
$V_6 = (25, 26, 27)(37, 38, 39).$

Suppose $C_1 = \langle V_1\rangle$ and $C_2 = \langle V_1, V_2, V_3, V_4, V_5\rangle$. Then a similar argument as above, shows that C is isomorphic to $C_1 \times C_2$. We now consider the group C_2 of order 1458. The heart of our method is decomposing the group into a direct product of their subgroups. We find other permutations to decompose C_2. Define

$W_1 = (40, 41, 42),$
$W_2 = (1, 17)(2, 18)(3, 14)(4, 15)(5, 16)(6, 10)(7, 11)(8, 12)(9, 13)(19, 31)(20, 33)$
$(21, 32)(22, 35)(23, 34)(24, 36)(25, 38)(26, 37)(27, 39)(28, 40)(29, 42)(30, 41),$
$W_3 = (19, 20, 21)(31, 32, 33),$
$W_4 = (22, 23, 24)(34, 35, 36),$
$W_5 = (25, 26, 27)(37, 38, 39),$
$W_6 = (19, 20, 21)(31, 33, 32),$

and consider the subgroups $C_{2,1} = \langle W_1, W_2, W_3, W_4, W_5\rangle$ and $C_{2,2} = \langle W_6\rangle$. Then $C_{2,1}$ and $C_{2,2}$ are normal subgroups of C_2 of orders 486 and 3, respectively, which have trivial intersection. Thus, $C_2 \cong C_{2,1} \times C_{2,1}$. Finally, we choose the following permutations:

$R_1 = (1, 17)(2, 18)(3, 14)(4, 15)(5, 16)(6, 10)(7, 11)(8, 12)(9, 13)(19, 31)(20, 33)$
$(21, 32)(22, 35)(23, 34)(24, 36)(25, 38)(26, 37)(27, 39)(28, 40)(29, 42)(30, 41),$
$R_2 = (19, 20, 21)(31, 32, 33),$
$R_3 = (22, 23, 24)(34, 35, 36),$

$R_4 = (25, 26, 27)(37, 38, 39)$,
$R_5 = (28, 29, 30)(40, 41, 42)$
$R_6 = (28, 29, 30)(40, 42, 41)$.

Then we can see that, $C_{2,1} \cong C_{2,1,1} \times C_{2,1,2}$, such that $C_{2,1,1} = \langle R_1, R_2, R_3, R_4, R_5 \rangle$ and $C_{2,1,2} = \langle R_6 \rangle$ are normal subgroups of $C_{2,1}$ of orders 162 and 3, respectively. Therefore, $H \cong D \times C_1 \times C_{2,2} \times C_{2,1,2} \times C_{2,1,1}$ and G has order 13122. Since $D, C_1, C_{2,2}$, and $C_{2,1,2}$ are cyclic groups of order 3, it is enough to find the conjugacy classes and character table of the group $C_{2,1,1}$. In tables 3 and 4, we find conjugacy classes and character table of this group.

Table 3
The representatives of conjugacy classes of the group $C_{2,1,1}$.

No.	Representatives	Size
1	()	1
2	(28,29,30)(40,41,42)	2
3	(25,26,27)(37,38,39)	2
4	(25,26,27)(28,29,30)(37,38,39)(40,41,42)	2
5	(25,26,27)(28,30,29)(37,38,39)(40,42,41)	2
6	(22,23,24)(34,35,36)	2
7	(22,23,24)(28,29,30)(34,35,36)(40,41,42)	2
8	(22,23,24)(28,30,29)(34,35,36)(40,42,41)	2
9	(22,23,24)(25,26,27)(34,35,36)(37,38,39)	2
10	(22,23,24)(25,26,27)(28,29,30)(34,35,36)(37,38,39)(40,41,42)	2
11	(22,23,24)(25,26,27)(28,30,29)(34,35,36)(37,38,39)(40,42,41)	2
12	(22,23,24)(25,27,26)(34,35,36)(37,39,38)	2
13	(22,23,24)(25,27,26)(28,29,30)(34,35,36)(37,39,38)(40,41,42)	2
14	(22,23,24)(25,27,26)(28,30,29)(34,35,36)(37,39,38)(40,42,41)	2
15	(19,20,21)(31,32,33)	2
16	(19,20,21)(28,29,30)(31,32,33)(40,41,42)	2
17	(19,20,21)(28,30,29)(31,32,33)(40,42,41)	2
18	(19,20,21)(25,26,27)(31,32,33)(37,38,39)	2
19	(19,20,21)(25,26,27)(28,29,30)(31,32,33)(37,38,39)(40,41,42)	2
20	(19,20,21)(25,26,27)(28,30,29)(31,32,33)(37,38,39)(40,42,41)	2
21	(19,20,21)(25,27,26)(31,32,33)(37,39,38)	2
22	(19,20,21)(25,27,26)(28,29,30)(31,32,33)(37,39,38)(40,41,42)	2
23	(19,20,21)(25,27,26)(28,30,29)(31,32,33)(37,39,38)(40,42,41)	2
24	(19,20,21)(22,23,24)(31,32,33)(34,35,36)	2
25	(19,20,21)(22,23,24)(28,29,30)(31,32,33)(34,35,36)(40,41,42)	2
26	(19,20,21)(22,23,24)(28,30,29)(31,32,33)(34,35,36)(40,42,41)	2
27	(19,20,21)(22,23,24)(25,26,27)(31,32,33)(34,35,36)(37,38,39)	2
28	(19,20,21)(22,23,24)(25,26,27)(28,29,30)(31,32,33)(34,35,36)(37,38,39)(40,41,42)	2
29	(19,20,21)(22,23,24)(25,26,27)(28,30,29)(31,32,33)(34,35,36)(37,38,39)(40,42,41)	2

Table 3
Continued.

No.	Representatives	Size
30	(19,20,21)(22,23,24)(25,27,26)(31,32,33)(34,35,36)(37,39,38)	2
31	(19,20,21)(22,23,24)(25,27,26)(28,29,30) (31,32,33)(34,35,36)(37,39,38)(40,41,42)	2
32	(19,20,21)(22,23,24)(25,27,26)(28,30,29) (31,32,33)(34,35,36)(37,39,38)(40,42,41)	2
33	(19,20,21)(22,24,23)(31,32,33)(34,36,35)	2
34	(19,20,21)(22,24,23)(28,29,30)(31,32,33)(34,36,35)(40,41,42)	2
35	(19,20,21)(22,24,23)(28,30,29)(31,32,33)(34,36,35)(40,42,41)	2
36	(19,20,21)(22,24,23)(25,26,27)(31,32,33)(34,36,35)(37,38,39)	2
37	(19,20,21)(22,24,23)(25,26,27)(28,29,30) (31,32,33)(34,36,35)(37,38,39)(40,41,42)	2
38	(19,20,21)(22,24,23)(25,26,27)(28,30,29) (31,32,33)(34,36,35)(37,38,39)(40,42,41)	2
39	(19,20,21)(22,24,23)(25,27,26)(31,32,33)(34,36,35)(37,39,38)	2
40	(19,20,21)(22,24,23)(25,27,26)(28,29,30) (31,32,33)(34,36,35)(37,39,38)(40,41,42)	2
41	(19,20,21)(22,24,23)(25,27,26)(28,30,29) (31,32,33)(34,36,35)(37,39,38)(40,42,41)	2
42	(1,17)(2,18)(3,14)(4,15)(5,16)(6,10)(7,11)(8,12)(9,13)(19,31)(20,33) (21,32)(22,34)(23,36)(24,35)(25,37)(26,39)(27,38)(28,40)(29,42)(30,41)	81

Table 4
The character table of the group $C_{2,1,1}$.

	1a	3a	3b	3c	3d	3e	3f	3g	3h	3i	3j	3k	3l	3m	3n	3o	3p	3q	3r	3s	3t
χ_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
χ_3	2	2	2	2	2	2	2	2	2	2	2	2	2	2	−1	−1	−1	−1	−1	−1	−1
χ_4	2	2	2	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	2	2	2	2	2	2	2
χ_5	2	2	−1	−1	−1	2	2	2	−1	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	−1
χ_6	2	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2
χ_7	2	−1	−1	−1	2	2	−1	−1	−1	−1	2	−1	2	−1	2	−1	−1	−1	−1	2	−1
χ_8	2	−1	−1	2	−1	2	−1	−1	−1	2	−1	−1	−1	2	2	−1	−1	−1	2	−1	−1
χ_9	2	−1	2	−1	−1	−1	−1	2	−1	−1	2	−1	−1	2	2	−1	−1	2	−1	−1	2
χ_{10}	2	−1	2	−1	−1	−1	2	−1	−1	2	−1	−1	2	−1	2	−1	−1	2	−1	−1	2
χ_{11}	2	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	−1	−1	2	−1	−1	2	−1
χ_{12}	2	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	−1	2	−1	−1	2	−1	−1
χ_{13}	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	2	2	2	2	2	2	−1	−1	−1	−1
χ_{14}	2	2	−1	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	2	2	2	−1	−1	−1	−1
χ_{15}	2	2	−1	−1	−1	2	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	2
χ_{16}	2	2	−1	−1	−1	2	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	2	2	2	−1
χ_{17}	2	2	2	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1
χ_{18}	2	2	2	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1

Table 4
Continued.

	3u	3v	3w	3x	3y	3z	3a′	3b′	3C′	3d′	3e′	3f′	3g′	3h′	3i′	3j′	3k′	3l′	3m′	3n′	2a
χ_{19}	2	−1	−1	−1	2	−1	−1	2	−1	2	−1	2	−1	−1	2	−1	−1	−1	−1	2	−1
χ_{20}	2	−1	−1	−1	2	−1	−1	2	−1	2	−1	2	−1	−1	−1	−1	2	−1	2	−1	2
χ_{21}	2	−1	−1	−1	2	−1	−1	2	−1	2	−1	2	−1	−1	−1	2	−1	2	−1	−1	−1
χ_{22}	2	−1	−1	−1	2	2	−1	−1	−1	−1	2	−1	2	−1	−1	−1	2	−1	2	−1	2
χ_{23}	2	−1	−1	−1	2	2	−1	−1	−1	−1	2	−1	2	−1	−1	2	−1	2	−1	−1	−1
χ_{24}	2	−1	−1	2	−1	2	−1	−1	−1	2	−1	−1	−1	2	−1	−1	2	2	−1	−1	−1
χ_{25}	2	−1	−1	2	−1	2	−1	−1	−1	2	−1	−1	−1	2	−1	2	−1	−1	−1	2	2
χ_{26}	2	−1	2	−1	−1	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1
χ_{27}	2	−1	2	−1	−1	−1	−1	2	−1	−1	2	−1	−1	2	−1	2	−1	−1	2	−1	−1
χ_{28}	2	−1	2	−1	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	−1	2	−1	−1	2	−1
χ_{29}	2	−1	2	−1	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1
χ_{30}	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	−1	−1	−1	2
χ_{31}	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	2	2	2	−1
χ_{32}	2	2	−1	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	2
χ_{33}	2	2	−1	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	−1	−1	−1	2	2	2	−1
χ_{34}	2	−1	−1	−1	2	−1	2	−1	2	−1	−1	−1	−1	2	2	−1	−1	−1	−1	2	−1
χ_{35}	2	−1	−1	−1	2	−1	2	−1	2	−1	−1	−1	−1	2	−1	−1	2	−1	2	−1	2
χ_{36}	2	−1	−1	−1	2	−1	2	−1	2	−1	−1	−1	−1	2	−1	2	−1	2	−1	−1	−1
χ_{37}	2	−1	−1	2	−1	−1	−1	2	2	−1	−1	−1	2	−1	2	−1	−1	−1	2	−1	−1
χ_{38}	2	−1	−1	2	−1	−1	2	−1	−1	−1	2	2	−1	−1	2	−1	−1	−1	2	−1	−1
χ_{39}	2	−1	−1	2	−1	−1	−1	2	2	−1	−1	−1	2	−1	−1	−1	2	2	−1	−1	−1
χ_{40}	2	−1	−1	2	−1	−1	−1	2	2	−1	−1	−1	2	−1	−1	2	−1	−1	−1	2	2
χ_{41}	2	−1	−1	2	−1	−1	2	−1	−1	−1	2	2	−1	−1	−1	−1	2	2	−1	−1	−1
χ_{42}	2	−1	−1	2	−1	−1	2	−1	−1	−1	2	2	−1	−1	−1	2	−1	−1	−1	2	2
χ_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
χ_3	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	0
χ_4	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	0
χ_5	2	2	2	2	2	−1	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	−1	−1	−1	0
χ_6	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	0
χ_7	2	−1	2	−1	−1	−1	−1	2	−1	2	−1	2	−1	−1	−1	−1	2	−1	2	−1	0
χ_8	−1	2	2	−1	−1	−1	2	−1	−1	−1	2	2	−1	−1	−1	2	−1	−1	−1	2	0
χ_9	−1	−1	−1	−1	2	−1	−1	2	−1	−1	2	−1	2	−1	−1	2	−1	−1	2	−1	0
χ_{10}	−1	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	−1	2	−1	−1	2	−1	−1	2	0
χ_{11}	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	0
χ_{12}	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	−1	0
χ_{13}	−1	−1	−1	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	2	2	2	−1	−1	−1	0
χ_{14}	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	2	2	2	0
χ_{15}	2	2	−1	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	−1	−1	−1	2	2	2	0
χ_{16}	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	0
χ_{17}	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	2	2	2	2	2	2	2	2	2	0
χ_{18}	−1	−1	2	2	2	2	2	2	2	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	0
χ_{19}	−1	−1	−1	−1	2	−1	2	−1	2	−1	−1	−1	2	−1	2	−1	−1	−1	−1	2	0
χ_{20}	2	−1	−1	2	−1	2	−1	−1	−1	−1	2	2	−1	−1	−1	−1	2	−1	2	−1	0

Table 4
Continued.

	3u	3v	3w	3x	3y	3z	3a′	3b′	3C′	3d′	3e′	3f′	3g′	3h′	3i′	3j′	3k′	3l′	3m′	3n′	2a
χ_{21}	−1	−1	2	−1	−1	−1	−1	2	−1	2	−1	−1	−1	2	−1	2	−1	2	−1	−1	0
χ_{22}	−1	2	−1	−1	2	−1	2	−1	2	−1	−1	−1	−1	2	−1	2	−1	2	−1	−1	0
χ_{23}	−1	−1	−1	2	−1	2	−1	−1	−1	−1	2	−1	2	−1	2	−1	−1	−1	−1	2	0
χ_{24}	−1	2	−1	−1	2	2	−1	−1	−1	2	−1	−1	−1	2	2	−1	−1	−1	2	−1	0
χ_{25}	2	−1	−1	2	−1	−1	−1	2	2	−1	−1	−1	2	−1	−1	−1	2	2	−1	−1	0
χ_{26}	−1	−1	−1	2	−1	−1	2	−1	−1	2	−1	2	−1	−1	2	−1	−1	2	−1	−1	0
χ_{27}	−1	2	2	−1	−1	2	−1	−1	2	−1	−1	−1	−1	2	−1	−1	2	−1	−1	2	0
χ_{28}	2	−1	2	−1	−1	2	−1	−1	2	−1	−1	−1	2	−1	−1	2	−1	−1	2	−1	0
χ_{29}	−1	2	−1	−1	2	−1	−1	2	−1	−1	2	2	−1	−1	2	−1	−1	2	−1	−1	0
χ_{30}	2	−1	−1	−1	−1	2	2	2	−1	−1	−1	2	2	2	−1	−1	−1	−1	−1	−1	0
χ_{31}	2	2	2	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	2	2	2	0
χ_{32}	−1	−1	2	2	2	−1	−1	−1	−1	−1	−1	−1	−1	−1	2	2	2	−1	−1	−1	0
χ_{33}	2	2	−1	−1	−1	−1	−1	−1	2	2	2	2	2	2	−1	−1	−1	−1	−1	−1	0
χ_{34}	−1	−1	−1	2	−1	2	−1	−1	−1	−1	2	−1	−1	2	−1	2	−1	2	−1	−1	0
χ_{35}	2	−1	2	−1	−1	−1	−1	2	−1	2	−1	−1	2	−1	2	−1	−1	−1	−1	2	0
χ_{36}	−1	−1	−1	−1	2	−1	2	−1	2	−1	−1	2	−1	−1	−1	−1	2	−1	2	−1	0
χ_{37}	−1	2	−1	−1	2	2	−1	−1	−1	2	−1	−1	2	−1	−1	−1	2	2	−1	−1	0
χ_{38}	−1	2	−1	2	−1	−1	−1	2	2	−1	−1	−1	−1	2	2	−1	−1	−1	2	−1	0
χ_{39}	−1	2	−1	2	−1	−1	−1	2	2	−1	−1	2	−1	−1	−1	2	−1	−1	−1	2	0
χ_{40}	−1	−1	2	−1	−1	−1	2	−1	−1	−1	2	−1	−1	2	2	−1	−1	−1	2	−1	0
χ_{41}	2	−1	2	−1	−1	−1	2	−1	−1	−1	2	−1	2	−1	−1	−1	2	2	−1	−1	0
χ_{42}	−1	−1	−1	−1	2	2	−1	−1	−1	2	−1	2	−1	−1	−1	2	−1	−1	−1	2	0

3. Conclusion

It is far from true that every finite group is a direct product of two of its non-trivial proper normal subgroups. But in some cases it is possible to find two subgroups A and B such that A is a normal subgroup of G and $A \cap B = \langle () \rangle$. In such a case, G is called the semidirect product of A by B. In the case that $|A| = 1/2|G|$, the method of subgroups of index 2 is the best method to find the character table of G[10]. In other cases, we must find some properties of the parent group to calculate the character table of the group. But, for the group of small order, GAP is the most powerful tools for computing character tables.

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