Scientific Paper

Group Theory for Tetramethylethylene

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Abstract

The non-rigid molecule group theory in which the dynamical symmetry operations are defined as physical operations is applied to determine the character table for the full non-rigid molecule group (f-NRG) of tetramethylethylene. We show that the f-NRG of this molecule is a group of order 324, the structure of which is formed as the wreath product $Z_3 \wr (Z_2 \times Z_2)$, in which Z_3 is the cyclic group of order 3 and Z_2 denotes the cyclic group of order two. Using the group theory package GAP, we calculate the conjugacy classes and character table of this molecule.

Keywords: non-rigid molecule group, tetramethylethylene, wreath product, character table

Introduction

A molecule is said to be non-rigid if there are several local minima on the potential-energy surface easily attainable by the molecular system via a tunnelling rearrangement. A non-rigid molecule, which possesses various isoenergetic forms separated by relatively low energy barriers, presents large amplitude movements between various possible configurations. Because of this deformability, the non-rigid molecules exhibit some interesting properties of intramolecular dynamics, which can be studied more easily resorting to Group Theory.

Following Y. G. Smeyers,[1–2] 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 internal motion operations describing molecular moieties moving with respect to the rest of the molecule. Such a set forms a group which called the Full Non-Rigid Molecule Group (f-NRG).

Finite group theory is the mathematics of symmetry. It plays an important role in the study of molecules, crystals, and clusters in chemistry although applications have usually been restricted to small or moderately sized systems due to computational limitations. To be practical for large systems, finite group theory requires both computer calculation and the advanced computational methods.

Group theory for non-rigid molecules is more relevant to large amplitude vibrational spectroscopy of small organic molecules and its applications have appeared in the literature.[3–10]

The various vibrational modes of a molecule can be categorized in terms of their behaviour with respect to the symmetry elements of the molecule. In fact, any motion of the molecule including translations, rotations, and vibrations, can be categorized on this basis. The categories to which these motions are assigned are called irreducible representations. Thus it is important to calculate the irreducible representations and so character table of the symmetry group of a molecule.

The symmetry groups of non-rigid molecules, where changes from one conformation to another can occur easily, were investigated by Longuet-Higgins.[11] In many cases, these symmetry groups are not isomorphic to 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 described here is appropriate for molecules which consist of a number of XH_3 or XO_2 groups attached to a rigid framework. An example of these kinds of molecules is tetramethylethylene, which is considered here in some detail. It is not appropriate in cases where the framework is linear, as in ethane, but Bunker[12] has shown how to deal with such molecules.

Our approach here is first to specify the algebraic structure of the f-NRG of tetramethylethylene. With a geometric consideration of dynamic symmetries of the molecule we will show that the f-NRG of tetramethylethylene can be specified by wreath product of some known groups. Then based on the structure of the group we apply GAP,[13] a useful package for

computing the character tables and even the group structure, to compute the character table of the f-NRG of tetramethylethylene.

Balasubramanian[14–19] was the first chemist who calculated the non-rigid group of molecules using wreath product formalism. He also computed the character table of non-rigid groups under consideration, using a well-known method for computing the character table of groups which is representable as a wreath product of two groups.

We use reference[20] for the standard notation and terminology of character theory. The motivation for this study is outlined in references[21–25] and the reader is encouraged to consult these papers for background material as well as basic computational techniques.

In this paper, the f-NRG of tetramethylethylene, Figure 1, is investigated. We prove that this group has order 324 with 45 conjugacy classes and 45 irreducible characters. Computations were carried out with the aid of GAP and this was done by characterizing the algebraic structure of f-NRG as the wreath product of known groups.

Results and discussion

In this section we first describe some notation which will be kept throughout. Let G be a group and N be a subgroup of G. N is called a normal subgroup of G, if for any $g \in G$ and $x \in N$, $g^{-1}xg \in N$. Moreover, if H is another subgroup of G such that $H \cap N = \{e\}$ and $G = HN = \{xy \mid x \in H, y \in N\}$, then we say that G is a semidirect product of H by N denoted by $H \wedge N$. Suppose X is a set. The set of all permutations on X, denoted by S_X, is a group which is called the symmetric group on X. In the case that, $X = \{1, 2, \ldots, n\}$, we denote S_X by S_n or Sym(n).

Let H be a permutation group on X, a subgroup of S_X, and let G be a group. The set of all mappings $X \to G$ is denoted by G^X, i.e. $G^X = \{f \mid f: X \to G\}$. It is clear that $|G^X| = |G|^{|X|}$. We put $G \wr H = G^X \times H = \{(f; \pi) \mid f \in G^X, \pi \in H\}$. For $f \in G^X$ and $\pi \in H$, we define $f_\pi \in G^X$ by $f_\pi = f o \pi^{-1}$, where "o" denotes the composition of functions. It is easy to check that the following law of composition: $(f ; \pi)\ (f'; \pi') = (f f'_\pi ; \pi \pi')$, makes $G \wr H$ into a group. This group is called the wreath product of G by H.

Before going into the details of the computations of tetramethylethylene we should mention that we consider the speed of rotations of methyl groups sufficiently high so that the mean time dynamical symmetry of the molecules makes sense. In order to characterize the f-NRG of tetramethylethylene we first note that each dynamic symmetry operation of this molecule, considering the rotations of CH_3 groups, is composed of two sequential physical operations. First

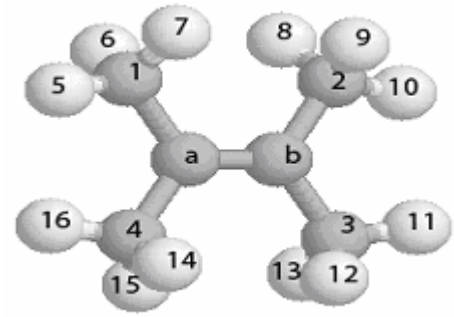

Figure 1. The Structure of Tetramethylethylene.

we have a physical symmetry of the tetramethylethylene consist of six carbon atoms which are denoted by a,b,1,2,3 and 4 in Figure 1. Such operations are exactly the symmetries of the rectangular framework {1,2,3,4} which form the Klein's four group V={Id, (1,2)(4,3), (1,4)(2,3), (1,3)(2,4)}. In fact under the vertical reflection of the frame work the two middle carbons are interchanged and hence we should have inserted (1,2) (4,3) (a,b) in V, and in this case we have V = {Id, (1,2)(4,3)(a,b), (1,4)(2,3), (1,3)(2,4)(a,b)}. Since a and b do not have any effect on our calculations, therefore we omitted the permutation (a,b).

After accomplishing the first framework symmetry operations we must map each CH_3 group on itself. Since one half of the rotations on each CH_3 group is possible, therefore the feasible symmetry group of each CH_3 is the cyclic group of order 3, namely Z_3. Referring to Figure 1, the group of each CH_3 at the four corners of the framework is given in terms of permutations as follows:

$$G_1 = < (5,6,7) >,$$
$$G_2 = < (8,9,10) >,$$
$$G_3 = < (11,12,13) >,$$
$$G_4 = < (14,15,16) >.$$

where G_i is the symmetry group of the CH_3 whose carbon atom is marked as i, $1 \leq i \leq 4$.

Therefore the full symmetry group of tetramethylethylene has the following structure:

$$G = (G_1 \times G_2 \times G_3 \times G_4) : V$$

where ":" denotes the semi-direct product. Therefore we can identify every element of G as a vector (a_1,a_2,a_3,a_4,v) such that $a_i \in G_i$ and $v \in V$. Evidently G can be written in terms of wreath product $G = Z_3 \wr (Z_2 \times Z_2)$. We now apply GAP to obtain the conjugacy classes and character table of the group G, as in Tables 1 and 2. In Table 2, for every entry X, /X denotes the complex conjugate of X and $A = e^{i\pi/3}$, $B = -3A - 2A^2$, $C = -A + 2A^2$, $D = A + 3A^2$, $E = 2A^2$ and $F = 4A$, where $i = \sqrt{-1}$.

Conclusions

The method described in this paper appears to be more efficient in dealing with the construction of the character table of the symmetry group of the molecule. The structure of the group of full symmetries of a non-rigid molecule, which is denoted by f-NRG, is determined by examining various concepts and constructions in group theory. First, all the permutations and inversions which don't change the whole framework of the molecule should be examined. Then using the GAP package the character table of the f-NRG group is computed. The symmetry group of the non-rigid tetramethylethylene molecule which exhibits internal rotations of the CH_3 groups is shown to be the wreath product $Z_3 \wr (Z_2 \times Z_2)$ which contains 324 permutations. This groups falls into 45 conjugacy classes of elements, hence by a famous result in representation theory, the group contains exactly 45 irreducible characters. In Table 1, a representative from each conjugacy class is given and in the column facing it the centralizer size of a representative g is given. Therefore the totality of all elements in a conjugacy class containing g is $|G| / |C_G(g)|$ where $C_G(g)$ denotes the centralizer of g in the group G, i.e. the set of all elements of G which commute with g. In Table 2, where the complete character table is presented, the first row consists of representatives of each conjugacy class, but this time in the GAP notation a representative g is shown by the order of the element g. For example if an element g has order n, then its class is denoted by nx, where x runs over the letters a, b, etc. to denote the consecutive classes of elements of order n. If g belongs to the class nx and if m is 2,3 or 5, then g^m belongs to a class of elements of order n/(n,m), where (n,m) denotes the greatest common divisor of n and m, which are given in a column above nx. The values of the irreducible characters χ_i, $1 \leq i \leq 45$, at each class occupies the rest of Table 2.

Table 1. Representatives and the sizes of the conjugacy classes of G.

No.	Representatives	Size	No.	Representatives	Size
1)	()	1	24)	(1,2,3)(4,6,5)(7,8,9)(10,12,11)	2
2)	(10,11,12)	4	25)	(1,2,3)(4,6,5)(7,9,8)(10,11,12)	2
3)	(10,12,11)	4	26)	(1,2,3)(4,6,5)(7,9,8)(10,12,11)	4
4)	(7,8,9)(10,11,12)	2	27)	(1,3,2)(4,6,5)(7,9,8)(10,12,11)	1
5)	(7,8,9)(10,12,11)	4	28)	(1,4)(2,5)(3,6)(7,10)(8,11)(9,12)	9
6)	(7,9,8)(10,12,11)	2	29)	(1,4)(2,5)(3,6)(7,10,8,11,9,12)	18
7)	(4,5,6)(10,11,12)	2	30)	(1,4)(2,5)(3,6)(7,10,9,12,8,11)	18
8)	(4,5,6)(10,12,11)	4	31)	(1,4,2,5,3,6)(7,10,8,11,9,12)	9
9)	(4,5,6)(7,8,9)	2	32)	(1,4,2,5,3,6)(7,10,9,12,8,11)	18
10)	(4,5,6)(7,8,9)(10,11,12)	4	33)	(1,4,3,6,2,5)(7,10,9,12,8,11)	9
11)	(4,5,6)(7,8,9)(10,12,11)	4	34)	(1,7)(2,8)(3,9)(4,10)(5,11)(6,12)	9
12)	(4,5,6)(7,9,8)	4	35)	(1,7)(2,8)(3,9)(4,10,5,11,6,12)	18
13)	(4,5,6)(7,9,8)(10,11,12)	4	36)	(1,7)(2,8)(3,9)(4,10,6,12,5,11)	18
14)	(4,5,6)(7,9,8)(10,12,11)	4	37)	(1,7,2,8,3,9)(4,10,5,11,6,12)	9
15)	(4,6,5)(10,12,11)	2	38)	(1,7,2,8,3,9)(4,10,6,12,5,11)	18
16)	(4,6,5)(7,8,9)(10,11,12)	4	39)	(1,7,3,9,2,8)(4,10,6,12,5,11)	9
17)	(4,6,5)(7,8,9)(10,12,11)	4	40)	(1,10)(2,11)(3,12)(4,7)(5,8)(6,9)	9
18)	(4,6,5)(7,9,8)	2	41)	(1,10,2,11,3,12)(4,7)(5,8)(6,9)	18
19)	(4,6,5)(7,9,8)(10,11,12)	4	42)	(1,10,3,12,2,11)(4,7)(5,8)(6,9)	18
20)	(4,6,5)(7,9,8)(10,12,11)	4	43)	(1,10,2,11,3,12)(4,7,5,8,6,9)	9
21)	(1,2,3)(4,5,6)(7,8,9)(10,11,12)	1	44)	(1,10,3,12,2,11)(4,7,5,8,6,9)	18
22)	(1,2,3)(4,5,6)(7,8,9)(10,12,11)	4	45)	(1,10,3,12,2,11)(4,7,6,9,5,8)	9
23)	(1,2,3)(4,5,6)(7,9,8)(10,12,11)	2			

Table 2. Character table of the group G and its power map.

		1a	3a	3b	3c	3d	3e	3f	3g	3h	3i	3j	3k	3l	3m	3n	3o	3p	3q	3r
	2p	1a	3b	3a	3e	3d	3c	3n	3g	3q	3s	3r	3k	3p	3o	3f	3m	3l	3h	3j
	3p	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a	1a
	5p	1a	3b	3a	3e	3d	3c	3n	3g	3q	3s	3r	3k	3p	3o	3f	3m	3l	3h	3j
χ_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
χ_3		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
χ_5		1	A	/A	/A	1	A	/A	1	/A	1	A	1	A	/A	A	A	/A	A	/A
χ_6		1	A	/A	/A	1	A	/A	1	/A	1	A	1	A	/A	A	A	/A	A	/A
χ_7		1	A	/A	/A	1	A	/A	1	/A	1	A	1	A	/A	A	A	/A	A	/A
χ_8		1	A	/A	/A	1	A	/A	1	/A	1	A	1	A	/A	A	A	/A	A	/A
χ_9		1	/A	A	A	1	/A	A	1	A	1	/A	1	/A	A	/A	/A	A	/A	A
χ_{10}		1	/A	A	A	1	/A	A	1	A	1	/A	1	/A	A	/A	/A	A	/A	A
χ_{11}		1	/A	A	A	1	/A	A	1	A	1	/A	1	/A	A	/A	/A	A	/A	A
χ_{12}		1	/A	A	A	1	/A	A	1	A	1	/A	1	/A	A	/A	/A	A	/A	A
χ_{13}		2	-1	-1	2	-1	2	2	-1	-1	-1	2	2	-1	-1	2	-1	-1	-1	2
χ_{14}		2	-1	-1	2	-1	2	2	-1	-1	-1	2	2	-1	-1	2	-1	-1	-1	2
χ_{15}		2	-1	-1	-1	2	-1	2	-1	2	-1	-1	-1	-1	2	2	2	-1	2	-1
χ_{16}		2	-1	-1	-1	2	-1	2	-1	2	-1	-1	-1	-1	2	2	2	-1	2	-1
χ_{17}		2	-1	-1	2	-1	2	-1	2	2	-1	-1	-1	2	-1	-1	-1	2	2	-1
χ_{18}		2	-1	-1	2	-1	2	-1	2	2	-1	-1	-1	2	-1	-1	-1	2	2	-1
χ_{19}		2	-A	-/A	E	-1	/E	E	-1	-/A	-1	/E	2	-A	-/A	/E	-A	-/A	-A	E
χ_{20}		2	-A	-/A	E	-1	/E	E	-1	-/A	-1	/E	2	-A	-/A	/E	-A	-/A	-A	E
χ_{21}		2	-/A	-A	/E	-1	E	/E	-1	-A	-1	E	2	-/A	-A	E	-/A	-A	-/A	/E
χ_{22}		2	-/A	-A	/E	-1	E	/E	-1	-A	-1	E	2	-/A	-A	E	-/A	-A	-/A	/E
χ_{23}		2	-A	-/A	-/A	2	-A	E	-1	E	-1	-A	-1	-A	E	/E	/E	-/A	/E	-/A
χ_{24}		2	-A	-/A	-/A	2	-A	E	-1	E	-1	-A	-1	-A	E	/E	/E	-/A	/E	-/A
χ_{25}		2	-A	-/A	E	-1	/E	-/A	2	E	-1	-A	-1	/E	-/A	-A	-A	E	/E	-/A
χ_{26}		2	-A	-/A	E	-1	/E	-/A	2	E	-1	-A	-1	/E	-/A	-A	-A	E	/E	-/A
χ_{27}		2	-/A	-A	-A	2	-/A	/E	-1	/E	-1	-/A	-1	-/A	/E	E	E	-A	E	-A
χ_{28}		2	-/A	-A	-A	2	-/A	/E	-1	/E	-1	-/A	-1	-/A	/E	E	E	-A	E	-A
χ_{29}		2	-/A	-A	/E	-1	E	-A	2	/E	-1	-/A	-1	E	-A	-/A	-/A	/E	E	-A
χ_{30}		2	-/A	-A	/E	-1	E	-A	2	/E	-1	-/A	-1	E	-A	-/A	-/A	/E	E	-A
χ_{31}		4	1	1	-2	-2	-2	4	1	-2	1	-2	-2	1	-2	4	-2	1	-2	-2
χ_{32}		4	1	1	-2	-2	-2	-2	-2	4	1	1	1	-2	-2	-2	-2	-2	4	1
χ_{33}		4	1	1	4	1	4	-2	-2	-2	1	-2	-2	-2	1	-2	1	-2	-2	-2
χ_{34}		4	A	/A	-E	-2	-/E	/F	1	-E	1	-/E	-2	A	-E	F	-/E	/A	-/E	-E
χ_{35}		4	/A	A	-/E	-2	-E	F	1	-/E	1	-E	-2	/A	-/E	/F	E	A	-E	-/E
χ_{36}		4	/A	A	-/E	-2	-E	-/E	-2	F	1	/A	1	-E	-/E	-E	E	-/E	/F	A
χ_{37}		4	A	/A	-E	-2	-/E	-E	-2	/F	1	A	1	-/E	-E	-/E	-/E	-E	F	/A
χ_{38}		4	/A	A	F	1	/F	-/E	-2	-/E	1	-E	-2	-E	A	-E	/A	-/E	-E	-/E
χ_{39}		4	A	/A	/F	1	F	-E	-2	-E	1	-/E	-2	-/E	/A	-/E	A	-E	-/E	-E
χ_{40}		4	B	/B	-/E	1	-E	-/E	1	-/E	C	/A	1	/A	A	-E	/A	A	-E	A
χ_{41}		4	/B	B	-E	1	-/E	-E	1	-E	/C	A	1	A	/A	-/E	A	/A	-/E	/A
χ_{42}		4	C	/C	-2	1	-2	-2	1	-2	/C	1	1	1	1	-2	1	1	-2	1
χ_{43}		4	D	/D	-E	1	-/E	-E	1	-E	C	A	1	A	/A	-/E	A	/A	-/E	/A
χ_{44}		4	/C	C	-2	1	-2	-2	1	-2	C	1	1	1	1	-2	1	1	-2	1
χ_{45}		4	/D	D	-/E	1	-E	-/E	1	-/E	/C	/A	1	/A	A	-E	/A	A	-E	A

Table 2(Continued).

	3s	3t	3u	3v	3w	3x	3y	3z	2a	6a	6b	6c	6d	6e	2b	6f	6g	6h	6i	6j
2p	3i	3z	3y	3v	3w	3x	3u	3t	1a	3c	3e	3t	3v	3z	1a	3f	3n	3t	3w	3z
3p	1a	1a	1a	1a	1a	1a	1a	1a	2a	2a	2a	2a	2a	2a	2b	2b	2b	2b	2b	2b
5p	3i	3z	3y	3v	3w	3x	3u	3t	2a	6b	6a	6e	6d	6c	2b	6g	6f	6j	6i	6h
χ_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
χ_3	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
χ_5	1	A	/A	1	1	1	A	/A	1	A	/A	/A	1	A	1	A	/A	/A	1	A
χ_6	1	A	/A	1	1	1	A	/A	-1	-A	-/A	-/A	-1	-A	-1	-A	-/A	-/A	-1	-A
χ_7	1	A	/A	1	1	1	A	/A	1	A	/A	/A	1	A	-1	-A	-/A	-/A	-1	-A
χ_8	1	A	/A	1	1	1	A	/A	-1	-A	-/A	-/A	-1	-A	1	A	/A	/A	1	A
χ_9	1	/A	A	1	1	1	/A	A	1	/A	A	A	1	/A	1	/A	A	A	1	/A
χ_{10}	1	/A	A	1	1	1	/A	A	-1	-/A	-A	-A	-1	-/A	-1	-/A	-A	-A	-1	-/A
χ_{11}	1	/A	A	1	1	1	/A	A	1	/A	A	A	1	/A	-1	-/A	-A	-A	-1	-/A
χ_{12}	1	/A	A	1	1	1	/A	A	-1	-/A	-A	-A	-1	-/A	1	A	A	A	1	/A
χ_{13}	-1	2	-1	2	2	-1	-1	2	0	0	0	0	0	0	0	0	0	0	0	0
χ_{14}	-1	2	-1	2	2	-1	-1	2	0	0	0	0	0	0	0	0	0	0	0	0
χ_{15}	-1	2	-1	-1	2	2	-1	2	-2	1	1	-2	1	-2	0	0	0	0	0	0
χ_{16}	-1	2	-1	-1	2	2	-1	2	2	-1	-1	2	-1	2	0	0	0	0	0	0
χ_{17}	-1	2	-1	2	-1	2	-1	2	0	0	0	0	0	0	-2	1	1	-2	1	-2
χ_{18}	-1	2	-1	2	-1	2	-1	2	0	0	0	0	0	0	2	-1	-1	2	-1	2
χ_{19}	-1	/E	-/A	2	2	-1	-A	E	0	0	0	0	0	0	0	0	0	0	0	0
χ_{20}	-1	/E	-/A	2	2	-1	-A	E	0	0	0	0	0	0	0	0	0	0	0	0
χ_{21}	-1	E	-A	2	2	-1	-/A	/E	0	0	0	0	0	0	0	0	0	0	0	0
χ_{22}	-1	E	-A	2	2	-1	-/A	/E	0	0	0	0	0	0	0	0	0	0	0	0
χ_{23}	-1	/E	-/A	-1	2	2	-A	E	-2	A	/A	-E	1	-/E	0	0	0	0	0	0
χ_{24}	-1	/E	-/A	-1	2	2	-A	E	2	-A	-/A	E	-1	/E	0	0	0	0	0	0
χ_{25}	-1	/E	-/A	2	-1	2	-A	E	0	0	0	0	0	0	-2	A	/A	-E	1	-/E
χ_{26}	-1	/E	-/A	2	-1	2	-A	E	0	0	0	0	0	0	2	-A	-/A	E	-1	/E
χ_{27}	-1	E	-A	-1	2	2	-/A	/E	-2	/A	A	-/E	1	-E	0	0	0	0	0	0
χ_{28}	-1	E	-A	-1	2	2	-/A	/E	2	-/A	-A	/E	-1	E	0	0	0	0	0	0
χ_{29}	-1	E	-A	2	-1	2	-/A	/E	0	0	0	0	0	0	-2	/A	A	-/E	1	-E
χ_{30}	-1	E	-A	2	-1	2	-/A	/E	0	0	0	0	0	0	2	-/A	-A	/E	-1	E
χ_{31}	1	4	1	-2	4	-2	1	4	0	0	0	0	0	0	0	0	0	0	0	0
χ_{32}	1	4	1	-2	-2	4	1	4	0	0	0	0	0	0	0	0	0	0	0	0
χ_{33}	1	4	1	4	-2	-2	1	4	0	0	0	0	0	0	0	0	0	0	0	0
χ_{34}	1	F	/A	-2	4	-2	A	/F	0	0	0	0	0	0	0	0	0	0	0	0
χ_{35}	1	/F	A	-2	4	-2	/A	F	0	0	0	0	0	0	0	0	0	0	0	0
χ_{36}	1	/F	A	-2	-2	4	/A	F	0	0	0	0	0	0	0	0	0	0	0	0
χ_{37}	1	F	/A	-2	-2	4	A	/F	0	0	0	0	0	0	0	0	0	0	0	0
χ_{38}	1	/F	A	4	-2	-2	/A	F	0	0	0	0	0	0	0	0	0	0	0	0
χ_{39}	1	F	/A	4	-2	-2	A	/F	0	0	0	0	0	0	0	0	0	0	0	0
χ_{40}	/C	/F	D	-2	-2	-2	/D	F	0	0	0	0	0	0	0	0	0	0	0	0
χ_{41}	C	F	/D	-2	-2	-2	D	/F	0	0	0	0	0	0	0	0	0	0	0	0
χ_{42}	C	4	C	-2	-2	-2	/C	4	0	0	0	0	0	0	0	0	0	0	0	0
χ_{43}	/C	F	B	-2	-2	-2	/B	/F	0	0	0	0	0	0	0	0	0	0	0	0
χ_{44}	/C	4	/C	-2	-2	-2	C	4	0	0	0	0	0	0	0	0	0	0	0	0
χ_{45}	C	/F	/B	-2	-2	-2	B	F	0	0	0	0	0	0	0	0	0	0	0	0

Table 2(Continued).

		2c	6k	6l	6m	6n	6o
	2p	1a	3h	3q	3t	3x	3z
	3p	2c	2c	2c	2c	2c	2c
	5p	2c	6l	6k	6o	6n	6m
χ_1		1	1	1	1	1	1
χ_2		1	1	1	1	1	1
χ_3		-1	-1	-1	-1	-1	-1
χ_4		-1	-1	-1	-1	-1	-1
χ_5		1	A	/A	/A	1	A
χ_6		1	A	/A	/A	1	A
χ_7		-1	-A	-/A	-/A	-1	-A
χ_8		-1	-A	-/A	-/A	-1	-A
χ_9		1	/A	A	A	1	/A
χ_{10}		1	/A	A	A	1	/A
χ_{11}		-1	-/A	-A	-A	-1	-/A
χ_{12}		-1	-/A	-A	-A	-1	-/A
χ_{13}		-2	1	1	-2	1	-2
χ_{14}		2	-1	-1	2	-1	2
χ_{15}		0	0	0	0	0	0
χ_{16}		0	0	0	0	0	0
χ_{17}		0	0	0	0	0	0
χ_{18}		0	0	0	0	0	0
χ_{19}		-2	A	/A	-E	1	-/E
χ_{20}		2	-A	-/A	E	-1	/E
χ_{21}		-2	/A	A	-/E	1	-E
χ_{22}		2	-/A	-A	/E	-1	E
χ_{23}		0	0	0	0	0	0
χ_{24}		0	0	0	0	0	0
χ_{25}		0	0	0	0	0	0
χ_{26}		0	0	0	0	0	0
χ_{27}		0	0	0	0	0	0
χ_{28}		0	0	0	0	0	0
χ_{29}		0	0	0	0	0	0
χ_{30}		0	0	0	0	0	0
χ_{31}		0	0	0	0	0	0
χ_{32}		0	0	0	0	0	0
χ_{33}		0	0	0	0	0	0
χ_{34}		0	0	0	0	0	0
χ_{35}		0	0	0	0	0	0
χ_{36}		0	0	0	0	0	0
χ_{37}		0	0	0	0	0	0
χ_{38}		0	0	0	0	0	0
χ_{39}		0	0	0	0	0	0
χ_{40}		0	0	0	0	0	0
χ_{41}		0	0	0	0	0	0
χ_{42}		0	0	0	0	0	0
χ_{43}		0	0	0	0	0	0
χ_{44}		0	0	0	0	0	0
χ_{45}		0	0	0	0	0	0

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Povzetek

Teorijo grup za netoge molekule v kateri so operacije dinamične simetrije definirane kot fizikalne operacije, smo uporabili za določitev tabele karakterjev tertametilena kot popolnoma netoge molekule. Pokazali smo, da to molekulo opiše grupa reda 324, katere strukturo določa ciklični product $Z_3 \wr (Z_2 \times Z_2)$, kjer je Z_3 ciklična grupa 3. reda in Z_2 označuje ciklično grupo 2. reda. Z uporabo paketa programskega paketa za teorijo grup GAP smo izračunali konjugirane vrste in tabelo karakterjev te molecule.