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FULL NON-RIGID GROUP OF 2,3 ,5, 6-TETRAMETHYLEPYRAZINE AS WREATH PRODUCT AND ITS SYMMETRY

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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 deduce the character table of the full non-rigid molecule group (f-NRG) of 2,3,5,6-Tetramethylpyrazine The f-NRG of this molecule is seen to be isomorphic to the group $\mathbb{Z}_3 \wr (\mathbb{Z}_2 \times \mathbb{Z}_2)$, where $\mathbb{Z}_n$ is the cyclic group of order n, of order 324 which has 45 conjugacy classes. We determine the some properties and relations between characters of the group. Also, we examine the symmetry group of this molecule and show that its symmetry group is $\mathbb{Z}_2 \times \mathbb{Z}_2$.

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1. Introduction

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, intermolecular transformations occur.

Following Y. G. Smeyers [17]-[19] the complete set of the molecular conversion operations that commute with the nuclear motion operator will contain overall rotation operations that describe the molecule rotating as a whole, and intermolecular motion operations that describe molecular moieties moving with respect to the rest of the molecule. Such a set forms a group, which we call the full non-rigid molecule group (f-NRG).

Balasubramanian (see for example [6] and [7]) was the first chemist who calculated the non-rigid group of molecules using wreath product formalism. He

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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.

The method described in the present study is appropriate for molecules that consist of a number of XH_3 groups attached to a rigid framework [20]. An example of this molecule is 2, 3, 5, 6-Tetramethylpyrazine, which is considered in some detail. We first specify the algebraic structure of the full non-rigid group of 2, 3, 5, 6-Tetramethylpyrazine. We will show that the f-NRG of 2, 3, 5, 6-Tetramethylpyrazine can be represented by the wreath product of some known groups. Then based on the structure of the group we apply a useful programming language, namely GAP [22], and compute the character table of f-NRG of this molecule. Note that we can use GAP to find many properties of the groups.

We use reference [13] for the standard notations and terminology of character theory. The motivation for this study is outlined in [1]-[12], [14]-[20], [23] and the references therein, and the reader is encouraged to consult these papers for background material as well as basic computational techniques.

In this paper we also compute the symmetry group of 2, 3, 5, 6 - Tetramethylpyrazine. Symmetry operations on a graph are called graph automorphisms. They affect only the labels of vertices by per-muting them so that the adjacency matrix of the graph remains unchanged. The graph symmetry is completely determined by all the automorphisms it has, i.e. by specifying all the permutations that leave the adjacency matrix intact.

The automorphism group of a graph depends only on the connectivity of the graph but does not depend on how the graph is represented in three dimensions. That is, a graph, in general, can be represented in different ways in three dimensions such that two representations can yield different three-dimensional symmetries and yet their automorphism groups are the same since the latter depend only on which vertices are connected in the graph. For this reason the symmetry of a graph was thought to be quite different from the point group symmetry and it is apparent that the two symmetries need not be related to each other. Randic [14], [15] showed a graph can be depicted in different ways such that its point group symmetry or three dimensional perception may differ, but the underlying connectivity symmetry is still the same as characterized by the automorphism group of the graph which by definition comprises permutations of the vertices of the graph that leave the adjacency matrix invariant. However, the molecular symmetry depends on the coordinates of the various nuclei that are related directly to their three dimensional geometry. Although the symmetry as perceived in graph theory by the automorphism group of the graph and the molecular group are quite different, Balasubramanian has shown that the two symmetries are connected [8].

The topic of perceiving the symmetry of a graph through the automorphism group of the graph has been studied in considerable depth (see for example [11], [8], [12], [14]-[16]) but the connection between the graph automorphism problem and the symmetry of a molecule has not been explored as much. Although the

symmetry as perceived in graph theory by the automorphism group of the graph and the molecular group is quite different, it is shown in this paper that the two symmetries are connected for 2, 3, 5, 6-Tetramethylpyrazine. By symmetry we mean the automorphism group symmetry of a graph. The symmetry of a graph, which is also called a topological symmetry, accounts only for the bond relations between atoms, and does not fully determine molecular geometry. The symmetry of a graph does not need to be the same as (i.e., isomorphic to) the molecular point group symmetry. However, it does represent the maximal symmetry the geometrical realization of a given topological structure may possess. The reader is encouraged to consult references [1], [4], [5], [6], [23], for background material and computational techniques on this topic.

2. Wreath product

In this section we describe briefly some notation which will be used in the next section. Let N be a normal subgroup and H be a subgroup of a group G such that $N \cap H = \{e\}$ and $G = NH = \{xy \mid x \in N, y \in H\}$. Then we say that G is a semidirect product of N by H denoted by $N \rtimes H$. Note that if H is also a normal subgroup of G, then $G = N \times H$ is the direct product of N and H. If $G = N \rtimes H$, then each $x \in G$ can be written uniquely as $x = nh$ for some $n \in N$ and $h \in H$, and there is homomorphism $\varphi : H \to \mathrm{Aut}(N)$, such that $(h)\varphi = \varphi_h$, where $\varphi_h : N \to N$ is defined by $(n)\varphi_h = h^{-1}nh$. We call φ conjugation homomorphism of the semi direct product G and write $G = N \rtimes_\varphi H$.

We can see that if the homomorphism $\varphi : H \to \mathrm{Aut}(N)$ defined above is trivial, then the semidirect product reduces to the direct product $N \times H$. It is a well-known fact that the homomorphism completely determines the semidirect product.

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. Let H be group acting on X. This is equivalent to the existence a homomorphism from H into S_X. Suppose also that G is 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 $GWr(X)H = G^X \rtimes H = \{(f, \pi) \mid f \in G^X, \pi \in H\}$. For $f \in G^X$ and $\pi \in H$, we define an action of H on G^X, by $f^\pi \in G^X$ by $f^\pi = f^\pi(x) = f(x\pi)$, where $x\pi = (x)\pi$ is the image of $x \in G$ under the permutation π. It is easy to check that the following law of composition

$$(f, \pi)(g, \sigma) = (fg^\pi, \pi\sigma),$$

makes G Wr(X) H into a group. This group is called the wreath product of G by H with respect to the action of H on X. If the action of H on X is faithful, that is the homomorphism from H into S_X is one to one, then H is a subgroup of S_X and we call H a permutation group on X. In this case G Wr(X) H is called the standard wreath product of G by H and denoted by $G \wr H$. Note that each function $f \in G^X$ can be identified with its image $(a_1, a_2, \ldots a_n)$, where $a_i = f(i)$.

Therefore G^X can be identified with G, $G \times G \times \cdots \times G = \{(a_1, a_2, \ldots, a_n) \mid a_i \in G\}$, the group of n-tuples of elements of G. Now if $f = (a_1, a_2, \ldots, a_n) \in G^X$ and $\pi \in H$, then $f^\pi = (a_{(1)\pi}, a_{(2)\pi}, \ldots, a_{(n)\pi})$. Hence $G \wr H = G^X \rtimes H = \{(a_1, a_2, \ldots, a_n; \pi) \mid a_i \in G, \pi \in H\}$ and

$$(a_1, a_2, \ldots, a_n; \pi)(b_1, b_2, \ldots, b_n; \sigma) = (a_1 b_{(1)\pi}, a_2 b_{(n)\pi}, \ldots, a_n b_{(n)\pi}; \pi\sigma).$$

3. Full non-rigid group of 2, 3, 5, 6-Tetramethylpyrazine

We know that full non-rigid group a molecule is semidirect product of the point group and the internal isometric group [10]. First of all, we consider the point group of the molecule in the rigid state. The point group of 2, 3, 5, 6-Tetramethylpyrazine is C_{2v}.The process of enumerating the symmetry operations of this molecule and arranging them in classes entails the adoption of a numbering convention for the central atom of the molecule, central atom of every methyl group, and the other atoms, such as proton nuclei, as shown in Figure 1. We define the operations C_{31}, C_{32}, C_{33} and C_{34}, which are rotations, in a positive sense, of four methyl groups. The existence of the four equivalent methyl groups implies the existence of 3^4 isoenergetic conformations, described by four equivalent C_3 non-rigid subgroups. The internal isometric group is a direct product of these four non-rigid subgroups, which generate with C_{3i} for $i = 1, \ldots, 4$ and contains 81 dynamical symmetry operations which describe 81 potential energy wells on the potential energy hyper surface.

Let us first consider operations that leave the framework of the molecule unchanged. These operations are grouped according to their cycle structure; operations which rotate different numbers of methyl groups must belong to different conjugacy classes. For a small group, the classes are conveniently found by conjugating a particular element with all other elements. The resulting set then forms one class, and repetition of this process eventually gives all the classes. This becomes impracticable for large groups. However, it is simpler to find the classes by inspection. Next, consider the operations that permute the nuclei of the framework; these fall into sets corresponding to the classes of C_{2v}. It is clear that the point group C_{2v} has exactly two different types of non-identity elements of the group C_2 and σ_v.

To deduce the classes, the full non-rigid operations were divided into three sets:

$$(< C_{31} > \times < C_{32} > \times < C_{33} > \times < C_{34} >) \rtimes \sigma_v$$

$$(< C_{31} > \times < C_{32} > \times < C_{33} > \times < C_{34} >) \rtimes \sigma_{v'}$$

$$(< C_{31} > \times < C_{32} > \times < C_{33} > \times < C_{34} >) \rtimes C_2,$$

where $\rtimes$ denotes the semidirect product and $\sigma_{v'} = C_2\sigma_v$.

Let us denote the operation $C_{31}^i C_{32}^j C_{33}^k C_{34}^r$ by a_{ijkr}. We use the notation of Smeyers and Villa [19]. The multiplication of the first set by all similarity operations of the group permits to separate its elements into 33 classes:

$$a_1 = E = a_{0000} \qquad a_2 = a_{2000} + a_{0200} + a_{0020} + a_{0002}$$
$$a_3 = a_{1000} + a_{0100} + a_{0010} + a_{0001} \qquad a_4 = a_{1200} + a_{2100} + a_{0012} + a_{0021}$$
$$a_5 = a_{1100} + a_{0011} \qquad a_6 = a_{2200} + a_{0022}$$
$$a_7 = a_{2020} + a_{0202} \qquad a_8 = a_{1020} + a_{2010} + a_{0102} + a_{0201}$$
$$a_9 = a_{1002} + a_{2001} + a_{0120} + a_{0210} \qquad a_{10} = a_{1202} + a_{2021} + a_{2120} + a_{0212}$$
$$a_{11} = a_{1120} + a_{1102} + a_{2011} + a_{0211} \qquad a_{12} = a_{2020} + a_{0220}$$
$$a_{13} = a_{2220} + a_{2202} + a_{2022} + a_{0222} \qquad a_{14} = a_{1220} + a_{2102} + a_{2012} + a_{0221}$$
$$a_{15} = a_{1010} + a_{0101} \qquad a_{16} = a_{1001} + a_{0110}$$
$$a_{17} = a_{1201} + a_{2110} + a_{1021} + a_{0112} \qquad a_{18} = a_{1110} + a_{1101} + a_{1011} + a_{0111}$$
$$a_{19} = a_{2210} + a_{2201} + a_{1022} + a_{0122} \qquad a_{20} = a_{1210} + a_{2101} + a_{2101} + a_{0121}$$
$$a_{21} = a_{1212} + a_{2121} \qquad a_{22} = a_{1211} + a_{1112} + a_{1121} + a_{2111}$$
$$a_{23} = a_{1222} + a_{2212} + a_{2221} + a_{2122} \qquad a_{24} = a_{1221} + a_{2112}$$
$$a_{25} = a_{1111} \qquad a_{26} = a_{1122} + a_{2211}$$
$$a_{27} = a_{2222}$$

$$a_{28} = [a_{2121} + a_{2211} + a_{2001} + a_{1122} + a_{1212} + a_{1002} + a_{0012} + a_{0021} + a_{0000}]\sigma_v$$
$$a_{29} = [a_{1122} + a_{2101} + a_{2221} + a_{2212} + a_{2011} + a_{2002} + a_{1120} + a_{1102} + a_{1222} + a_{1210} + a_{1012} + a_{1121} + a_{0100} + a_{0220} + a_{0211} + a_{0010} + a_{0001}]\sigma_v$$
$$a_{30} = [a_{2120} + a_{2111} + a_{2210} + a_{2201} + a_{2021} + a_{2000} + a_{1121} + a_{1112} + a_{1211} + a_{1202} + a_{1022} + a_{1001} + a_{0122} + a_{0110} + a_{0212} + a_{0200} + a_{0020} + a_{0002}]\sigma_v$$
$$a_{31} = [a_{2112} + a_{2100} + a_{2220} + a_{2202} + a_{2022} + a_{2010} + a_{1110} + a_{1101} + a_{1221} + a_{1200} + a_{1020} + a_{1011} + a_{0111} + a_{0102} + a_{0222} + a_{0201} + a_{0021} + a_{0012}]\sigma_v$$
$$a_{32} = a_{2110} + a_{2200} + a_{2020} + a_{1111} + a_{1201} + a_{1021} + a_{0112} + a_{0202} + a_{0022}]\sigma_v$$
$$a_{33} = a_{2102} + a_{2222} + a_{2012} + a_{1100} + a_{1220} + a_{1010} + a_{0101} + a_{0221} + a_{0011}]\sigma_v,$$

Where by $[x+y+\cdots]z$, we mean that $xz, yz, \ldots$ are belong to the same conjugacy classes. In the same way, the multiplication of the second set by all the similarity operations of the group permits us to select 6 classes:

$$b_1 = [a_{2121} + a_{2112} + a_{2100} + a_{1221} + a_{1212} + a_{1200} + a_{0021} + a_{0012} + a_{0000}]\sigma_{v'}$$
$$b_2 = [a_{2122} + a_{2110} + a_{2101} + a_{2221} + a_{2212} + a_{2200} + a_{1222} + a_{1210} + a_{1201} + a_{1021} + a_{1012} + a_{1000} + a_{0121} + a_{0112} + a_{0100} + a_{0022} + a_{0010} + a_{0001}]\sigma_{v'}$$
$$b_3 = [a_{2120} + a_{2111} + a_{2102} + a_{2021} + a_{2012} + a_{2000} + a_{1121} + a_{1112} + a_{1100} + a_{1220} + a_{1211} + a_{1202} + a_{0221} + a_{0212} + a_{0200} + a_{0020} + a_{0011} + a_{0002}]\sigma_{v'}$$
$$b_4 = [a_{2222} + a_{2210} + a_{2201} + a_{1022} + a_{1010} + a_{1001} + a_{0122} + a_{0110} + a_{0101}]\sigma_{v'}$$
$$b_5 = [a_{2220} + a_{2211} + a_{2202} + a_{2022} + a_{2010} + a_{2001} + a_{1122} + a_{1110} + a_{1101} + a_{1020} + a_{1011} + a_{1002} + a_{0120} + a_{0111} + a_{0102} + a_{0222} + a_{0210} + a_{0201}]\sigma_{v'}$$
$$b_6 = [a_{2020} + a_{2011} + a_{2002} + a_{1120} + a_{1111} + a_{1102} + a_{0220} + a_{0211} + a_{0202}]\sigma_{v'}$$

Finally, the multiplication of the third set furnishes 6 classes:

$$c_1 = [a_{0000} + a_{0201} + a_{0102} + a_{1020} + a_{1221} + a_{1122} + a_{2010} + a_{2211} + a_{2112}]C_2$$

$$c_2 = [a_{0002} + a_{0020} + a_{0200} + a_{0221} + a_{0101} + a_{0122} + a_{1010} + a_{1022} + a_{1211} + a_{1220} + a_{1112} + a_{1121} + a_{2000} + a_{2012} + a_{2201} + a_{2210} + a + a_{2102} + a_{2111}]C_2$$

$$c_3 = [a_{0001} + a_{0010} + a_{0202} + a_{0211} + a_{0100} + a_{0112} + a_{1000} + a_{1021} + a_{1201} + a_{1222} + a_{1102} + a_{1120} + a_{2011} + a_{2020} + a_{2212} + a_{2221} + a_{2110} + a_{2122}]C_2$$

$$c_4 = [a_{0012} + a_{0021} + a_{0210} + a_{0222} + a_{0111} + a_{0120} + a_{1002} + a_{1011} + a_{1200} + a_{1212} + a_{1101} + a_{1110} + a_{2001} + a_{2022} + a_{2202} + a_{2220} + a_{2100} + a_{2121}]C_2$$

$$c_5 = [a_{0011} + a_{0212} + a_{0110} + a_{1001} + a_{1202} + a_{1100} + a_{2021} + a_{2222} + a_{2120}]C_2$$

$$c_6 = [a_{0022} + a_{0220} + a_{0121} + a_{1012} + a_{1210} + a_{1111} + a_{2002} + a_{2200} + a_{2101}]C_2.$$

Therefore 45 conjucacy classes are obtained.

In order to separate the possible irreducible representations, it is convenient to distinguish five types of possible symmetry eigenvectors:

(1) The functions conserve the C_3 symmetry of the four methyl groups,
(2) The functions conserve the C_3 symmetry of only three of them,
(3) The functions conserve the C_3 symmetry of only two of them,
(4) The functions conserve the C_3 symmetry of only one of them,
(5) The functions do not exhibit any C_3 symmetry at all.

From the symmetry eigenvectors the characters of each representation are easily deduced for all the classes by simple application of the symmetry operations. In addition, the orthogonality rules between the different representations may be used. But it takes tremendous computations. In below we use GAP package to compute the character table of the non-rigid group of this molecule.

We construct the non-rigid group of the molecule under consideration, so that one can handle it by GAP. First of all, we consider the point group of the molecule in the case of a rigid framework. We consider the full non-rigid group W (f-NRG) of this molecule, each equilibrium co formation of which has an ordinary point group symmetry C_{2v}.

In order to characterize full non-rigid of this molecule, we first note that each dynamic symmetry operation of the molecule, considering the rotations of methyl groups is composed of two sequential physical symmetry operations. We first have a physical symmetry of framework (as we have to map the methyl groups on methyl groups). Before going into the details of the computations of the molecule, 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.

Now consider symmetry operations of this framework. This operations form an abelian group H of order 4, which is not cyclic so it is isomorphic to Klein's group. This group is isomorphic to $\mathbb{Z}_2 \times \mathbb{Z}_2$, where $\mathbb{Z}_2$ is cyclic group of size 2.

After accomplishing the first framework symmetry operation we have to map each methyl group on itself which forms the group G isomorphic to $\mathbb{Z}_3$, cyclic group of size 3. The number of all such operations is 324. The composition of such dynamic symmetry operations are described as follows. We first note that

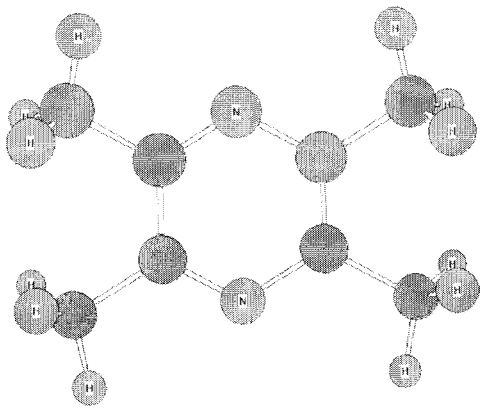

FIGURE 1. The structure of 2, 3, 5, 6-Tetramethylpyrazine.

each dynamic symmetry operation of this molecule, considering the rotations of CH_3 groups, discomposed of two sequential physical operations. First we have a physical symmetry of the molecule, consist of four carbon atoms (that form methyl groups) which are denoted by a, b, c, d; and four carbon atoms which are denoted by A, B, C, D; and two nitrogen atoms which are denoted by E and F, as shown in Figure 1. Such operations are exactly the symmetries of the decagon framework $\{a, b, c, d, A, B, C, D, E, F\}$ which form a group H of order four. Under the reflection with respect to the plane containing two nitrogen atoms carbon atoms are interchanged and hence we should have inserted

$$X_1 = (a, b)(A, B)(d, c)(D, C)$$

in H. The reflection with respect to the plane bisecting AD and BC yields that

$$X_2 = (a, d)(A, D)(b, c)(B, C)(E, F)$$

is an element of H. Clearly the group H generates by these permutation, and so

$$H = \{(), (a, b)(A, B)(d, c)(D, C), (a, d)(A, D)(b, c)(B, C), (a, c)(A, C)(b, d)(B, D)\}.$$

The f-NRG of the molecule is completely characterized the motion of methyl groups, as the other carbon atoms and nitrogen atoms follow the motion of the methyl groups. So A, B, C, and D don't have any effect on our calculations. Therefore we may omitted the permutation $(A, B), (D, C), (B, C)$ and (B, D); and in this case we have

$$H = \{(), (a, b)(d, c), (a, d)(b, c), (a, c)(b, d)\}.$$

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 are possible, therefore the symmetry group of each CH_3 is the set of all even permutations

on 3 letters, namely $\mathbb{Z}_3$. 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:

$$K_1 = \langle (1,2,3) \rangle, K_2 = \langle (4,5,6) \rangle, K_3 = \langle (7,8,9) \rangle, K_4 = \langle (10,11,12) \rangle.$$

Therefore the full non-rigid group of 2, 3, 5, 6 tetramethylpyrazine has the following structure

$$W = (K_1 \times K_2 \times K_3 \times K_4) \rtimes H,$$

where $\rtimes$ denotes the semi-direct product. Hence, we can identify every element of W, as a vector $(a_1, a_2, a_3, a_4; b)$ such that that $a_i \in K_i$ and $b \in H$. It is clear that H permutes K_i and so W can be written in terms of wreath product $W = K \wr H \cong \mathbb{Z}_3 \wr (\mathbb{Z}_2 \times \mathbb{Z}_2)$, where K is the cyclic group of order 3. Note that W has order 324. We now apply GAP to construct a group isomorphic to this group as follows

```
H:=Group((1,2)(3,4),(1,3)(2,4));
G:=Group((1,2,3));
W:=WreathProduct(G,H);
MinimalGeneratingSet(W);
```

$$[(1,4,3,6,2,5)(7,10,8,11,9,12), (1,9)(2,7)(3,8)(4,11,5,12,6,10)]$$

By above description it is clear that wreath product of G by H, denoted by W, is the full non-rigid group of this molecule. W is generated by

$$\{(1,4,3,6,2,5)(7,10,8,11,9,12), (1,9)(2,7)(3,8)(4,11,5,12,6,10)\}.$$

The character table and representative and sizes of the conjugacy classes of full non-rigid group of this molecule can be found by GAP.

4. Character table of f-NRG of 2, 3, 5, 6-Tetramethylpyrazine

In this section we find, using GAP, other information on the full non-rigid group of the molecule under consideration.

After applying GAP program we find that W has 45 conjugacy classes and therefore have 45 irreducible characters. Since the size of factor group of W modulus

$$W = \langle (7,9,8)(10,11,12), (4,6,5)(7,8,9), (1,2,3)(4,5,6)(7,8,9)(10,11,12) \rangle,$$

the derived subgroup of W, is 12. So W has exactly 12 irreducible characters of degree 1. Let us denote these characters by χ_1, χ_2 , χ_3, χ_4 , χ_5, χ_6 , χ_7, χ_8 , χ_9, χ_{10} , χ_{11}, χ_{12}. It can be seen that the group of linear characters of W is generated by two linear characters of order 2 and 6, namely χ_3 and χ_5. We find that W has 18 characters of degrees 2 and 15 characters of degrees 4. Also we can see that W has 28 non-trivial normal subgroups. Now find relations between irreducible characters. Put

$N = \langle (4,5,6)(7,9,8), (1,3,2)(4,5,6)(7,9,8)(10,11,12), (1,11,3,10,2,12)(4,8,6,7,5,9)\rangle$
$M = \langle (1,3,2)(4,5,6)(7,9,8)(10,11,12), (1,3,2)(4,5,6), (1,6,2,4,3,5)(7,12,8,10,9,11)\rangle$
$K = \langle (4,5,6)(10,12,11), (1,3,2)(4,5,6)(7,8,9)(10,12,11), (1,8,3,7,2,9)(4,11,6,10,5,12)\rangle$
$D = \langle (1,2,3)(4,5,6)(7,9,8)(10,12,11), (7,9,8)(10,12,11)\rangle$
$E = \langle (1,2,3)(4,5,6)(7,8,9)(10,11,12), (1,2,3)(10,11,12)\rangle$
$F = \langle (1,2,3)(4,5,6)(7,8,9)(10,11,12), (1,2,3)(7,8,9)\rangle$
$G = \langle (1,2,3)(4,5,6)(7,8,9)(10,11,12)\rangle$.

These subgroups of W are all normal in W. The factor groups of W modulus each of N, M, K are isomorphic to S_3, the symmetric group on three symbols. The factor groups of W modulus each of D, E, F are isomorphic to group $S_3 \times S_3$ isomorphic by the group $J := \langle (1,2,3)(5,6), (2,3)(4,5,6)\rangle$; and finally the factor group of W modulus G, is isomorphic to group $L = \langle x, y \mid x^6 = y^6 = 1, x^{-2}y^{-2} = yx^2\rangle$. Now S_3 has one irreducible character of degree 2, so we obtain three irreducible characters of W by lifting this characters to W. We denote these irreducible characters by χ_{14}, χ_{16}, χ_{18}, respectively. Now J is a group of size 36 and has 9 conjugacy classes, four irreducible characters of degree 1, four irreducible character of degree 2 and one of degree 4. Hence we obtain three irreducible characters of W by lifting the irreducible character of J of degree 4 to W; we denote these irreducible characters by χ_{33}, χ_{32}, χ_{31}, respectively. Also L is a group of size 108 and has 15 conjugacy classes, hence has 15 irreducible characters, four of degree 1, six of degree 2 and five of degree 4. The characters χ_{42}, χ_{43} are obtained by lifting the irreducible characters of L of degree 4.

If φ is a linear character of W, then for any irreducible character χ of degree n, the Kronecker product $\varphi\chi$ is also an irreducible character of degree n. Using this fact, we obtain all irreducible characters of W of degree 2 and 4. These characters are

$\chi_{13} = \chi_3\chi_{14}$, χ_{14}, $\chi_{15} = \chi_2\chi_{16}$, χ_{16}, $\chi_{17} = \chi_2\chi_{18}$, χ_{18}, $\chi_{19} = \chi_8\chi_{14}$, $\chi_{20} = \chi_7\chi_{14}$, $\chi_{21} = \chi_6\chi_{14}$, $\chi_{22} = \chi_5\chi_{14}$, $\chi_{23} = \chi_6\chi_{16}$, $\chi_{24} = \chi_5\chi_{16}$, $\chi_{25} = \chi_{10}\chi_{16}$, $\chi_{26} = \chi_9\chi_{16}$, $\chi_{27} = \chi_6\chi_{18}$, $\chi_{28} = \chi_5\chi_{18}$, $\chi_{29} = \chi_8\chi_{18}$, $\chi_{30} = \chi_7\chi_{18}$, χ_{31}, χ_{32}, χ_{33}, $\chi_{34} = \chi_6\chi_{31}$, $\chi_{35} = \chi_5\chi_{31}$, $\chi_{36} = \chi_5\chi_{32}$, $\chi_{37} = \chi_6\chi_{32}$, $\chi_{38} = \chi_5\chi_{33}$, $\chi_{39} = \chi_6\chi_{33}$, $\chi_{40} = \chi_5\chi_{43}$, $\chi_{41} = \chi_6\chi_{42}$, χ_{42}, χ_{43}, $\chi_{44} = \chi_6\chi_{43}$, $\chi_{45} = \chi_5\chi_{42}$.
The resulting character table is given in Table 1. In this Table, X' denote the complex conjugate of X. Also the values a, b, c, d, e and f are: $a = -e^{i\pi/3}$, $b = -3e^{2i\pi/3} + 2e^{i\pi/3}$, $c = -e^{2i\pi/3} - 2e^{i\pi/3}$, $d = e^{2i\pi/3} - 3e^{i\pi/3}$, $e = -2e^{i\pi/3}$, $f = 4e^{2i\pi/3}$.

Note that the representations corresponding to the characters $\chi_1, \chi_3, \chi_5, \chi_6, \chi_{11}, \chi_{12}$ are A representations and the representations corresponding to the characters $\chi_2, \chi_4, \chi_7, \chi_8, \chi_9, \chi_{10}$ are B representations. E representations are the representations corresponding to the characters χ_i for $i = 13, \ldots, 30$. The remaining representations are G representations. Recall that the letters A and B are used for one-dimensional irreducible representations, which are symmetric and antisymmetric with respect to the rotation around the principal axis of the

point group, respectively. Also E is the symbol for two-dimensional and G for four-dimensional representations.

	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8	a_9	a_{10}	a_{11}	a_{12}	a_{13}	a_{14}	a_{15}
	1	4	4	4	2	2	2	4	4	4	4	2	4	4	2
χ_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
χ_3	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
χ_5	1	a	a'	a'	1	a	a'	1	a'	1	a	1	a	a'	a
χ_6	1	a'	a	a	1	a'	a	1	a	1	a'	1	a'	a	a'
χ_7	1	a	a'	a'	1	a	a'	1	a'	1	a	1	a	a'	a
χ_8	1	a'	a	a	1	a'	a	1	a	1	a'	1	a'	a	a'
χ_9	1	a	a'	a'	1	a	a'	1	a'	1	a	1	a	a'	a
χ_{10}	1	a'	a	a	1	a'	a	1	a	1	a'	1	a'	a	a'
χ_{11}	1	a	a'	a'	1	a	a'	1	a'	1	a	1	a	a'	a
χ_{12}	1	a'	a	a	1	a'	a	1	a	1	a'	1	a'	a	a'
χ_{13}	2	-1	-1	2	-1	2	2	-1	-1	-1	2	2	-1	-1	2
χ_{14}	2	-1	-1	2	-1	2	2	-1	-1	-1	2	2	-1	-1	2
χ_{15}	2	-1	-1	-1	2	-1	2	-1	2	-1	-1	-1	-1	2	2
χ_{16}	2	-1	-1	-1	2	-1	2	-1	2	-1	-1	-1	-1	2	2
χ_{17}	2	-1	-1	2	-1	2	-1	2	2	-1	-1	-1	2	-1	-1
χ_{18}	2	-1	-1	2	-1	2	-1	2	2	-1	-1	-1	2	-1	-1
χ_{19}	2	$-a'$	$-a$	e	-1	e'	e	-1	$-a$	-1	e'	-1	$-a'$	$-a$	e'
χ_{20}	2	$-a$	$-a'$	e'	-1	e	e'	-1	$-a'$	-1	e	2	$-a$	$-a'$	e
χ_{21}	2	$-a'$	$-a$	e	-1	e'	e	-1	$-a$	-1	e'	2	$-a'$	$-a$	e'
χ_{22}	2	$-a$	$-a'$	e'	-1	e	e'	-1	$-a'$	-1	e	2	$-a$	$-a'$	e
χ_{23}	2	$-a'$	$-a$	$-a$	2	$-a'$	e	-1	e	-1	$-a'$	2	$-a'$	e	e'
χ_{24}	2	$-a$	$-a'$	$-a'$	2	$-a$	e'	-1	e'	-1	$-a$	-1	$-a$	e'	e
χ_{25}	2	$-a'$	$-a$	$-a$	2	$-a'$	e	$-a$	e	-1	$-a'$	-1	$-a'$	e	e'
χ_{26}	2	$-a$	$-a'$	$-a'$	2	$-a$	e'	-1	e'	-1	$-a$	-1	$-a$	e'	e
χ_{27}	2	$-a'$	$-a$	e	-1	e'	$-a$	2	e	-1	$-a'$	-1	e'	$-a$	$-a'$
χ_{28}	2	$-a$	$-a'$	e'	-1	e	$-a'$	2	e'	-1	$-a$	-1	e	$-a'$	$-a$
χ_{29}	2	$-a'$	$-a$	e	-1	e'	$-a$	2	e	-1	$-a'$	-1	e'	$-a$	$-a'$
χ_{30}	2	$-a$	$-a'$	e'	-1	e	$-a'$	2	e'	-1	$-a$	-1	e	$-a'$	$-a$
χ_{31}	4	1	1	-2	-2	-2	4	1	-2	1	-2	-1	1	-2	4
χ_{32}	4	1	1	-2	-2	-2	-2	-2	4	1	1	-2	-2	-2	-2
χ_{33}	4	1	1	4	1	4	-2	-2	-2	1	-2	1	-2	1	-2
χ_{34}	4	a'	a	$-e$	-2	$-e'$	f'	1	$-e$	1	$-e'$	-2	a'	$-e$	f
χ_{35}	4	a	a'	$-e'$	-2	$-e$	f	1	$-e'$	1	$-e$	-2	a	$-e'$	f'
χ_{36}	4	a	a'	$-e'$	-2	$-e$	$-e'$	-2	f	1	a	-2	$-e$	$-e'$	$-e$
χ_{37}	4	a'	a	$-e$	-2	$-e'$	$-e$	-2	f'	1	a'	1	$-e'$	$-e$	$-e'$
χ_{38}	4	a	a'	f	1	f'	$-e'$	-2	$-e'$	1	$-e$	1	$-e$	a'	$-e$
χ_{39}	4	a'	a	f'	1	f	$-e$	-2	$-e$	1	$-e'$	-2	$-e'$	a	$-e'$
χ_{40}	4	b	b'	$-e'$	1	$-e$	$-e'$	1	$-e'$	c	a	-2	a	a'	$-e$
χ_{41}	4	b'	b	$-e$	1	$-e'$	$-e$	1	$-e$	c'	a'	1	a'	a	$-e'$
χ_{42}	4	c	c'	-2	1	-2	-2	1	-2	c'	1	1	1	1	-2
χ_{43}	4	c'	c	-2	1	-2	-2	1	-2	c	1	1	1	1	-2
χ_{44}	4	d	d'	$-e$	1	$-e'$	$-e$	1	$-e$	c	a'	1	a'	a	$-e'$
χ_{45}	4	d'	d	$-e'$	1	$-e$	$-e'$	1	$-e'$	c'	a	1	a	a'	$-e$

Table 1. Character table of the full non-rigid group of 2,3,5,6 tetramethylpyrazine.

	a_{16}	a_{17}	a_{18}	a_{19}	a_{20}	a_{21}	a_{22}	a_{23}	a_{24}	a_{25}	a_{26}	a_{27}	a_{28}	a_{29}	a_{30}
	2	4	4	4	4	4	4	4	2	1	2	1	9	18	18
χ_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
χ_3	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
χ_5	a	a'	a	a'	1	a	a'	1	1	1	a	a'	−1	$-a$	$-a'$
χ_6	a'	a	a'	a	1	a'	a	1	1	1	a'	a	−1	$-a'$	$-a$
χ_7	a	a'	a	a'	1	a	a'	1	1	1	a	a'	−1	$-a$	$-a'$
χ_8	a'	a	a'	a	1	a'	a	1	1	1	a'	a	−1	$-a'$	$-a$
χ_9	a	a'	a	a'	1	a	a'	1	1	1	a	a'	1	a	a'
χ_{10}	a'	a	a'	a	1	a'	a	1	1	1	a'	a	1	a'	a
χ_{11}	a	a'	a	a'	1	a	a'	1	1	1	a	a'	1	a	a'
χ_{12}	a'	a	a'	a	1	a'	a	1	1	1	a'	a	1	a'	a
χ_{13}	−1	−1	−1	2	−1	2	−1	2	2	−1	−1	2	0	0	0
χ_{14}	−1	−1	−1	2	−1	2	−1	2	2	−1	−1	2	0	0	0
χ_{15}	2	−1	2	−1	−1	2	−1	−1	2	2	−1	2	−2	1	1
χ_{16}	2	−1	2	−1	−1	2	−1	−1	2	2	−1	2	2	−1	−1
χ_{17}	−1	2	2	−1	−1	2	−1	2	−1	2	−1	2	0	0	0
χ_{18}	−1	2	2	−1	−1	2	−1	2	−1	2	−1	2	0	0	0
χ_{19}	$-a'$	$-a$	$-a'$	e	−1	e'	$-a$	2	2	−1	$-a'$	e	0	0	0
χ_{20}	$-a$	$-a'$	$-a$	e'	−1	e	$-a'$	2	2	−1	$-a$	e'	0	0	0
χ_{21}	$-a'$	$-a$	$-a'$	e	−1	e'	$-a$	2	2	−1	$-a'$	e	0	0	0
χ_{22}	$-a$	$-a'$	$-a$	e'	−1	e	$-a'$	2	2	−1	$-a$	e'	0	0	0
χ_{23}	e'	$-a$	e'	$-a$	−1	e'	$-a$	−1	−1	2	$-a'$	e	−2	a'	a
χ_{24}	e	$-a'$	e	$-a'$	−1	e	$-a'$	−1	−1	2	$-a$	e'	−2	a	a'
χ_{25}	e'	$-a$	e'	$-a$	−1	e'	$-a$	−1	−1	2	$-a'$	e	2	$-a'$	$-a$
χ_{26}	e	$-a'$	e	$-a'$	−1	e	$-a'$	−1	−1	2	$-a$	e'	2	$-a$	$-a'$
χ_{27}	$-a'$	e	e'	$-a$	−1	e'	$-a$	2	2	2	$-a'$	e	0	0	0
χ_{28}	$-a$	e'	e	$-a'$	−1	e	$-a'$	2	2	2	$-a$	e'	0	0	0
χ_{29}	$-a'$	e	e'	$-a$	−1	e'	$-a$	2	2	2	$-a'$	e	0	0	0
χ_{30}	$-a$	e'	e	$-a'$	−1	e	$-a'$	2	2	2	$-a$	e'	0	0	0
χ_{31}	−2	1	−2	−2	1	4	1	−2	−2	−2	1	4	0	0	0
χ_{32}	−2	−2	4	1	1	4	1	−2	−2	4	1	4	0	0	0
χ_{33}	1	−2	−2	−2	1	4	1	4	4	−2	1	4	0	0	0
χ_{34}	$-e'$	a	$-e'$	$-e$	1	f	a	−2	−2	−2	a'	f'	0	0	0
χ_{35}	$-e$	a'	$-e$	$-e'$	1	f'	a'	−2	−2	−2	a	f	0	0	0
χ_{36}	$-e$	$-a'$	f'	a'	1	f'	a'	−2	−2	4	a	f	0	0	0
χ_{37}	$-e'$	$-e$	f	a	1	f	a	−2	−2	4	a'	f'	0	0	0
χ_{38}	a	$-e'$	e	$-e'$	1	f'	a'	4	4	−2	a	f	0	0	0
χ_{39}	a'	$-e$	$-e'$	$-e$	1	f	a	4	4	−2	a'	f'	0	0	0
χ_{40}	a	a'	$-e$	a'	c'	f'	d	−2	−2	−2	d'	f	0	0	0
χ_{41}	a'	a	$-e'$	a	c	f	d'	−2	−2	−2	d	f'	0	0	0
χ_{42}	1	1	−2	1	c	4	c	−2	−2	−2	c'	4	0	0	0
χ_{43}	1	1	−2	1	c'	4	c'	−2	−2	−2	c	4	0	0	0
χ_{44}	a'	a	$-e'$	a	c'	f	b	−2	−2	−2	b'	f'	0	0	0
χ_{45}	a	a'	$-e$	a'	c	f'	b'	−2	−2	−2	b	f	0	0	0

Table 1. Continued.

	a_{31}	a_{32}	a_{33}	b_1	b_2	b_3	b_4	b_5	b_6	c_1	c_2	c_3	c_4	c_5	c_6
	18	9	9	9	18	18	9	18	9	9	18	18	18	9	9
χ_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
χ_3	-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
χ_5	$-a'$	-1	$-a$	-1	$-a$	$-a'$	$-a'$	-1	$-a$	1	a	a'	a'	1	a
χ_6	$-a$	-1	$-a'$	-1	$-a'$	$-a$	$-a$	-1	$-a'$	1	a'	a	a	1	a'
χ_7	$-a'$	-1	$-a$	1	a	a'	a'	1	a	-1	$-a$	$-a'$	$-a'$	-1	$-a$
χ_8	$-a$	-1	$-a'$	1	a'	a	a	1	a'	-1	$-a'$	$-a$	$-a$	-1	$-a'$
χ_9	a'	1	a	-1	$-a$	$-a'$	$-a'$	-1	$-a$	-1	$-a$	$-a'$	$-a'$	-1	$-a$
χ_{10}	a	1	a'	-1	$-a'$	$-a$	$-a$	-1	$-a'$	-1	$-a'$	$-a$	$-a$	-1	$-a'$
χ_{11}	a'	1	a	1	a	a'	a'	1	a	1	a	a'	a'	1	a
χ_{12}	a	1	a'	1	a'	a	a	1	a'	1	a'	a	a	1	a'
χ_{13}	0	0	0	0	0	0	0	0	0	-2	1	1	-2	1	-2
χ_{14}	0	0	0	0	0	0	0	0	0	2	-1	-1	2	-1	2
χ_{15}	-2	1	-2	0	0	0	0	0	0	0	0	0	0	0	0
χ_{16}	2	1	2	0	0	0	0	0	0	0	0	0	0	0	0
χ_{17}	0	0	0	-2	1	1	-2	1	-2	0	0	0	0	0	0
χ_{18}	0	0	0	2	-1	-1	2	-1	2	0	0	0	0	0	0
χ_{19}	0	0	0	0	0	0	0	0	0	-2	a'	a	$-e$	1	$-e'$
χ_{20}	0	0	0	0	0	0	0	0	0	-2	a	a'	$-e'$	1	$-e$
χ_{21}	0	0	0	0	0	0	0	0	0	2	$-a'$	$-a$	e	-1	e'
χ_{22}	0	0	0	0	0	0	0	0	0	2	$-a$	$-a'$	e'	-1	e
χ_{23}	$-e$	1	$-e'$	0	0	0	0	0	0	0	0	0	0	0	0
χ_{24}	$-e'$	1	$-e$	0	0	0	0	0	0	0	0	0	0	0	0
χ_{25}	e	-1	e'	0	0	0	0	0	0	0	0	0	0	0	0
χ_{26}	e'	-1	e	0	0	0	0	0	0	0	0	0	0	0	0
χ_{27}	0	0	0	-2	a'	a	$-e$	1	$-e'$	0	0	0	0	0	0
χ_{28}	0	0	0	-2	a	a'	$-e'$	1	$-e$	0	0	0	0	0	0
χ_{29}	0	0	0	2	$-a'$	$-a$	e	-1	e'	0	0	0	0	0	0
χ_{30}	0	0	0	2	$-a$	$-a'$	e'	1	e	0	0	0	0	0	0
χ_{31}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{32}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{33}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{34}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{35}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{36}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{37}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{38}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{39}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{40}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{41}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{42}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{43}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{44}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
χ_{45}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 1. Continued.

For every element k of group K, centralizer k in K is $\{xK \mid xk = kx\}$ where denoted by $C_K(k)$. Two elements x and y of K is said conjugate if there exist g

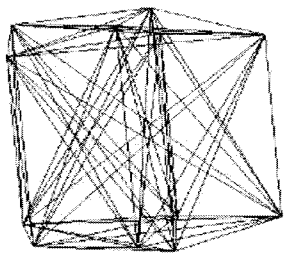

FIGURE 2. The Euclidean graph of the molecule.

K such that $x = g^{-1}yg$, and conjugacy class of every element k of group K is set of all elements of K where are conjugate with k and denoted by $\mathrm{Cl}_K(k)$. If K be finite, then $|C_K(k)| = |K|/|\mathrm{Cl}_K(k)|$ and size of $C_K(k)$ and $\mathrm{Cl}_K(k)$ are called centralizer order and conjugacy length of k in group K respectively. To simplify our argument we denote by na, nb, nc, ... the different conjugacy classes of elements of order n in the group K. If the number of conjugacy classes of K is t then the conjugacy vector of K is a vector with t array such that every array is a conjugacy length for K. Similarly we can define centralizer vector of K.

Now we find these vectors for full non-rigid group of the molecule. Suppose that V is a conjugacy vector and U be centralizer vector of this group. Then we have

$V = (1a, 3a, 3b, 3c, 3d, 3e, 3f, 3g, 3h, 3i, 3j, 3k, 3l, 3m, 3n, 3o, 3p, 3q, 3r, 3s, 3t, 3u,$
$3v, 3w, 3x, 3y, 3z, 2a, 6a, 6b, 6c, 6d, 6e, 2b, 6f, 6g, 6h, 6i, 6j, 2c, 6k, 6l, 6m, 6n, 6o)$

$U = (324, 81, 81, 162, 81, 162, 162, 81, 162, 81, 81, 81, 81, 81, 162, 81, 81, 162, 81, 81,$
$324, 81, 162, 162, 162, 81, 324, 36, 18, 18, 36, 18, 36, 36, 18, 18, 36, 18, 36, 36, 18,$
$18, 36, 18, 36).$

5. Symmetry of 2, 3, 5, 6-Tetramethylpyrazine

In this section we compute the symmetry group of 2, 3, 5, 6 - Tetramethylpyrazine. Let us recall some notations and definitions. Let $V(G)$ and $E(G)$ denote set of vertices and edges of a graph G. Automorphism group of a graph G is set of permutations where permutation g is belong to this group if for two adjacency vertices u and v, $g(u)$ and $g(v)$ be adjacent. This set with operation of composition of permutations is automorphism group on $V(G)$ and denoted by $\mathrm{Aut}(G)$. By symmetry we mean the automorphism group symmetry of a graph. The automorphism group of a graph depends only on the adjacency of vertices of graph and dos not depend on its three dimensional geometry representation. The symmetry of a graph need not be related to point group symmetry, because a graph can be represented in different ways in three dimensions where these two ways can give us two different three dimensional symmetries, however their automorphism groups are the same since this group depends only on which vertices are adjacent in the graph.

A weighted graph is a graph that vertices and edges of graph are weighted by distinct weights. We compute automorphism group of weighted graph of this molecule. Adjacency matrix of a weighted graph is defined as: $A_{ij} = w_{ij}$, if i j and vertices i and j are adjacent by an edge with weight wij, $A_{ij} = v_i$, if $i = j$ and vertex i weighted by v_i; otherwise $A_{ij} = 0$. Note that v_i can be taken as zero if all the nuclei are equivalent. Otherwise one may introduce different weights for nuclei in different equivalence classes and the same weight for nuclei in the same equivalence classes.

Consider 2, 3, 5, 6-Tetramethylpyrazine to illustrate the Euclidean graph and its automorphism group. It suffices to compute the Euclidean distances in terms of the H-H bound lengths and then construct the Euclidean matrix. Since automorphism group of the integer-weighted graph is identical to the automorphism group of the original Euclidean graph, we don't have to work with exact Euclidean distances. Hence we weighted these distances so that distinct Euclidean distances correspond to distinct integers. We compute Cartesian coordinates by HyperChem 6.03 and find the Euclidean distances as shown in Table 2. The Euclidean graph of the molecule is presented as Figure 2.

Note that we have rounded original distances to 2 decimal places. Now let us use a Euclidean edge weighting for 2, 3, 5, 6 tetramethylpyrazine mapped from Euclidean distances as

$(1.78, 3.04, 3.98, 2.47, 6.38, 5.58, 6.13, 6.58, 6.6, 6.82, 5.13, 5.61, 4.59, 6.83, 2.92,$
$3.84, 2.32, 5) \longrightarrow (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18).$

The integer matrix D of this weighted Euclidean graph is computed.

$$D = \begin{bmatrix} 0 & 1 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\ 1 & 0 & 1 & 3 & 11 & 3 & 12 & 13 & 12 & 8 & 14 & 8 \\ 1 & 1 & 0 & 4 & 3 & 2 & 7 & 6 & 5 & 10 & 9 & 8 \\ 2 & 3 & 4 & 0 & 1 & 1 & 8 & 9 & 10 & 5 & 6 & 7 \\ 3 & 11 & 3 & 1 & 0 & 1 & 8 & 14 & 8 & 12 & 13 & 12 \\ 4 & 3 & 2 & 1 & 1 & 0 & 10 & 9 & 8 & 7 & 6 & 5 \\ 5 & 12 & 7 & 8 & 8 & 10 & 0 & 1 & 1 & 15 & 16 & 17 \\ 6 & 13 & 6 & 9 & 14 & 9 & 1 & 0 & 1 & 16 & 18 & 16 \\ 7 & 12 & 5 & 10 & 8 & 8 & 1 & 1 & 0 & 17 & 16 & 15 \\ 8 & 8 & 10 & 5 & 12 & 7 & 15 & 16 & 17 & 0 & 1 & 1 \\ 9 & 14 & 9 & 6 & 13 & 6 & 16 & 18 & 16 & 1 & 0 & 1 \\ 10 & 8 & 8 & 7 & 12 & 5 & 17 & 16 & 15 & 1 & 1 & 0 \end{bmatrix}.$$

Now we apply a MATLAB program to obtain Euclidean graph of the molecule:

```
>> n=size(a,1)
>> A=ones(n,n);
>>for i=1:n
A(i,i)=0;
End
>> gplot ( A,a ) ;
```

A permutation of the vertices of a graph belongs to its automorphism group if it satisfies $P^tAP = A$, where P^t is the transpose of permutation matrix P and A is the adjacency matrix of the graph under consideration. There are $n!$ possible permutation matrices for a graph with n vertices. However, all of them may not satisfy the above relation. Since n is large, to computing automorphism group using GAP, we should split symmetric group (on n symbol) in classes and then find the elements of automorphism group in all cases that need so much time.

0	1.78	1.78	3.04	3.98	2.47	6.38	5.58	6.13	6.58	6.6	6.82
1.78	0	1.78	3.98	5.13	3.98	5.61	4.59	5.61	6.58	6.83	6.58
1.78	1.78	0	2.47	3.98	3.04	6.13	5.58	6.38	6.82	6.6	6.58
3.04	3.98	2.47	0	1.78	1.78	6.58	6.6	6.82	6.38	5.58	6.13
3.98	5.13	3.98	1.78	0	1.78	6.58	6.83	6.58	5.61	4.59	5.61
2.47	3.98	3.04	1.78	1.78	0	6.82	6.6	6.58	6.13	5.58	6.38
6.38	5.61	6.13	6.58	6.58	6.82	0	1.78	1.78	2.92	3.84	2.32
5.58	4.59	5.58	6.6	6.83	6.6	1.78	0	1.78	3.84	5	3.84
6.13	5.61	6.38	6.82	6.58	6.58	1.78	1.78	0	2.32	3.84	2.92
6.58	6.58	6.82	6.38	5.61	6.13	2.92	3.84	2.32	0	1.78	1.78
6.6	6.83	6.6	5.58	4.59	5.58	3.84	5	3.84	1.78	0	1.78
6.82	6.58	6.58	6.13	5.61	6.38	2.32	3.84	2.92	1.78	1.78	0

Table 2. Euclidean distances of 2, 3, 5, 6 tetramethylpyrazine.

Let $\mathrm{Aut}(G) = \{\sigma_1, \sigma_2, \ldots, \sigma_m\}$. The matrix $S = [\sigma_{ij}]$, where $\sigma_{ij} = \sigma_i(j)$ is called a solution matrix for G. It is clear that S have m rows and n columns and every row is a permutation on n symbol, for example if $[2, 1, 3, 6, 5, 4, 7, 8, 9, 10, 11, 12]$ be a row of S then this row correspond $(1, 2)(4, 6)$. So it is clear that it is enough to calculate a solution matrix. For this propose we use the MATLAB program given in [1], and then compute this group. By adding the statement b=round(b*100)/100; before the function "jaigasht" in the MATLAB program [1] we can specify the decimal digits for distances. After apply the MATLAB program in [1], we obtain S:

$$S = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\ 3 & 2 & 1 & 6 & 5 & 4 & 9 & 8 & 7 & 12 & 11 & 8 \\ 4 & 5 & 6 & 1 & 2 & 3 & 10 & 11 & 12 & 7 & 8 & 8 \\ 6 & 5 & 4 & 3 & 2 & 1 & 12 & 11 & 10 & 9 & 8 & 7 \end{bmatrix}.$$

Now apply below simple GAP program to compute automorphism group of the molecule

```
H:=[ ];
n:=Size(S);
for i in [1..n] do
    a:=PermListList(S[1],S[i]);
    AddSet(H,a);
Od;
aut:=AsGroup(H);
```

The automorphism group is
$\mathrm{Aut}(G) = \{(), (1,3)(4,6)(7,9)(10,12), (1,4)(2,5)(3,6)(7,10)(8,11)(9,12),$
$(1,6)(2,5)(3,4)(7,12)(8,11)(9,10)\},$
which is a non cyclic group of order four. So it is isomorphic to $\mathbb{Z}_2 \times \mathbb{Z}_2$. If we change $b = round(b * 100)/100$ to $b = round(b * 10)/10$ we obtain the same result. Thus in these cases automorphism group and point group of this molecule are isomorphic. But if we change to $b = round(b * 1000)/1000$, then we have $\mathrm{Aut}(G) = \{(), (1,3)(4,6)(7,9)(10,12)\}$. In other cases we obtain that $\mathrm{Aut}(G) = \{()\}$.

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