Journal of the Serbian Chemical Society
JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS

J. Serb. Chem. Soc. 75 (1) 91–99 (2010)
JSCS–3944

UDC 547.534.2+519.11:544.01:541
Original scientific paper

The Fujita combinatorial enumeration for the non-rigid group of 2,4-dimethylbenzene

ALI MOGHANI[1]*, SOROOR NAGHDI SEDEH[1] and MOHAMMAD REZA SOROUHESH[2]

[1]*Department of Color Physics, Institute for Colorants, Paints and Coatings (ICPC), Tehran and* [2]*Department of Mathematics, Islamic Azad University, South Branch Tehran, Tehran, Iran*

(Received 1 June, revised 21 July 2009)

Abstract: Using non-rigid group theory, it was previously shown that the full non-rigid group of 2,4-dimethylbenzene is an ummatured and isomorphic to the group $\mathbf{C}_2\times(\mathbf{C}_3\mathrm{wr}\mathbf{C}_2)$ of order 36, where $\mathbf{C}_n$ is the cyclic group of order n, the symbols × and wr stand for the direct and wreath products, respectively. Herein, it is first shown that this group has 12 dominant classes. Then, the Markaracter Table, the Table of all integer-valued characters and the unit subduced cycle index (*USCI*) Table of the full non-rigid group of 2,4-dimethylbenzene are successfully derived for the first time.

Keywords: Full non-rigid group; character; unit subduced cycle index; 2,4-dimethylbenzene.

INTRODUCTION

Shinsaku Fujita proposed the Markaracter Tables, which enabled characters and marks to be discussed on a common basis, then introduced Tables of integer-valued characters[1–3], which are obtained for finite groups.[1–17] Eventually, the Fujita theory was further developed and applied to a variety of problems concerning the enumeration of chemical species.[18–22]

A dominant class is defined as a disjoint union of conjugacy classes that corresponds to the same cyclic subgroup, which is selected as a representative of conjugate cyclic subgroups. Furthermore, the cyclic (dominant) subgroup $\mathbf{G}_i$ selected from a non-redundant set of cyclic subgroups of **G** is denoted by $\mathbf{SCS}_\mathbf{G}$.[15–18,23,24] A rigid molecule is defined as one in which the barriers between its conformers are insuperable and there are no observable tunneling splittings. For non-rigid molecules, there are one or more contortional large amplitude vibration(s), such as inversion or internal rotation that give(s) rise to tunneling splittings. Due to this deformability, non-rigid molecules exhibit some interesting properties of in-

* Corresponding author. E-mail: moghani@icrc.ac.ir
doi: 10.2298/JSC1001091M

tramolecular dynamics which can be studied more easily by resorting to group theory. Following the pioneering works of Longuet–Higgins,[25] the symmetry group of a non-rigid molecule group consists of all permutations and permutation–inversion operations which become feasible as the molecule tunnels through a number of potential energy maxima separated by multiple minima. The complete set of molecular conversion operations which commute with the nuclear motion operator contains overall rotation operations, which describe the rotation of the molecule as a whole, and the non-rigid tunneling motion operations, which describe molecular moieties moving with respect to the rest of the molecule. Such a set forms a group, which is called the full non-rigid group (f-NRG). Longuet–Higgins investigated the symmetry groups of non-rigid molecules in which changes from one conformation to another can occur easily. The method as described here is appropriate for molecules which consist of a number of CH_3 groups attached to a rigid framework.[26–35]

In the present study, the Fujita combinatorial enumeration tables of the f-NRG of 2,4-dimethybenzene (see Fig. 1) are investigated. The motivation for this study with the aid of GAP[36] is outlined and the reader is encouraged to consult these papers for background material as well as the basic computational techniques.[37–40]

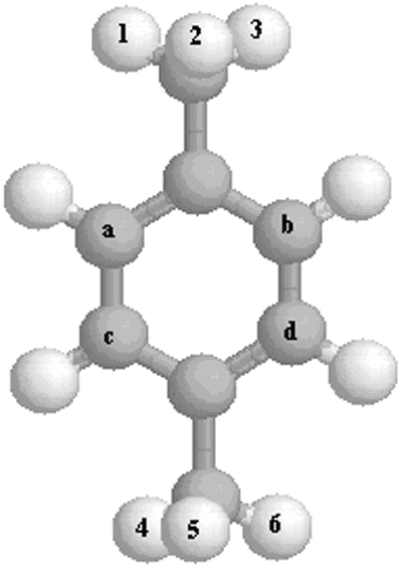

Fig. 1. The structure of 2,4-dimethylbenzene.

COMPUTATIONAL METHOD AND DISCUSSION

In this section, first some notations which will be kept throughout are described. Suppose **X** be a set, a permutation representation **P** of a finite group **G** is obtained when the group **G** acts on a finite set $\mathbf{X} = \{x_1,x_2,\ldots,x_t\}$ from the right,

which means a mapping **P**: **X** × **G** → **X** is given *via* $(x,g) \rightarrow xg$ such that the following holds: $(xg)g' = x(gg')$ and $x1 = x$, for each g, $g' \in$ **G** and $x \in$ **X**. Now let it be assumed that one is given an action **P** of **G** on **X** and a subgroup **H** of **G**. Let $\mathbf{G}_i$ and $\mathbf{G}_j$ be any subgroups of **G**. A subduced representation is denoted by $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$ as a subgroup of the coset representation $\mathbf{G}(/\mathbf{G}_i)$ that contains only elements associated with the elements of $\mathbf{G}_j$. A unit subduced cycle index (*USCI*)[3–6] is defined by:

$$Z(\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j, s_d) = \prod_{g \in \Omega} s_{d_g^{(ij)}}$$

where $s_{d_g^{(ij)}} = |\mathbf{G}_i|/|g^{-1}\mathbf{G}_i g \cap \mathbf{G}_j|$ and Ω is a transversal for the double coset decompositions concerning $\mathbf{G}_i$ and $\mathbf{G}_j$ for $i,j = 1,2,\ldots s$.

If **M** is a normal subgroup of **G** and **K** is another subgroup of **G** such that M ∩ **K** = {*e*} and **G** = **MN** = <**M**, **N**>, then **G** is called the semi direct product of **N** by **M**, which is denoted by **N** : **M**. Let **K** and **H** be groups and suppose **H** acts on the set **Γ**. Then the wreath product of **K** by **H**, denoted by **K** wr **H** is defined to be the semi direct product $\mathbf{K}^{\mathbf{\Gamma}} : \mathbf{H}$ such that $\mathbf{K}^{\mathbf{\Gamma}} = \{f \mid f: \mathbf{\Gamma} \rightarrow \mathbf{K}\}$.[22–24]

The f-NRG of 2,4-dimethylbenzene is described by the direct product of the cyclic group of order two with **G**, where **G** is the wreath product of the cyclic groups three and two, respectively, as follows[18]: if one sets $\alpha = (1,2,3)$, $\beta = (4,5,6)$ and $\gamma = (1,4)(2,5)(3,6)$, then G = $(<\alpha>\times<\beta>) : <\gamma>$, as a matter of fact, one has **G** ≅ $\mathbf{C}_3\text{wr}\mathbf{C}_2$, see Fig. 1. Now the effect of the vertical operation is to interchange the carbon atoms {a,c} with {b,d}. In this event, the methyl frameworks remain fixed and, hence, the f-NRG of the molecule is the direct product of **G** with a cyclic group of order two, namely X = $\mathbf{C}_2\times\mathbf{G}$. Now set **X** = $\mathbf{C}_2\times(\mathbf{C}_3\text{wr}\mathbf{C}2)$ and run the following program at the GAP prompt to compute: the mark table, $M_{22\times22}$; the character table, $C_{18\times18}$ and the set, $SCS_{\mathbf{X}}$ of the f-NRG of 2,4-dimethylbenzene with symmetry **X** = $\mathbf{C}_2\times(\mathbf{C}_3\text{wr}\mathbf{C}_2)$, as follows:

```
LogTo("2,4-Dimethylbenzene.txt");
c2:=CyclicGroup(IsPermGroup,(2));c3:=CyclicGroup(IsPermGroup,(3));
G:=WreathProduct(c3,c2);X:=DirectProduct(c2,G);
Order(X);IsPermGroup(X);
Char:=CharacterTable(X);s:=ConjugacyClassesSubgroups(X);
Sort("s");
V:=List(ConjugacyClassesSubgroups(X),x->Elements(x));
M:=TableOfMarks(X);Len:=Length(V);y:=[];
for i in [1,2..Len]do
if IsCyclic(V[i][1])then Add(y,i);
fi;od;Display(Char);Display(s);
Print("Char", "\n");Print("V", "\n");LogTo( );
Print("2,4-Dimethylbenzene.txt", "\n");
```

After running the program, it can be seen that the non-redundant set of subgroups of X, consists the following elements: G_1 = Id, G_2 = <(1,2)>, G_3 = = <(3,6)(4,7)(5,8)>, G_4 = <(1,2)(3,6)(4,7)(5,8)>, G_5 = <(3,4,5)(6,7,8)>, G_6 = <(3,4,5)>, G_7 = <(3,5,4)(6,7,8)>, G_8 = <(1,2),(3,6)(4,7)(5,8)>, G_9 = <(1,2)(3,4,5)(6,7,8)>, G_{10} = <(1,2)(3,4,5)>, G_{11} = <(3,6)(4,7)(5,8)(3,5,4)(6,7,8)>, G_{12} = <(1,2)(3,5,4)(6,7,8)>, G_{13} = <(3,6)(4,7)(5,8)(3,4,5)(6,7,8)>, G_{14} = <(1,2)(3,6)(4,7)(5,8)(3,4,5)(6,7,8) >, G_{15} = <(1,2)(3,6)(4,7)(5,8)(3,5,4)(6,7,8)>, G_{16} = <(3,4,5)(6,7,8)>, G_{17} = = <(1,2)(3,6)(4,7)(5,8)(3,4,5)(6,7,8)>, G_{18} = <(1,2)(3,6)(4,7)(5,8)(3,4,5)(6,7,8)>, G_{19} = <(1,2)(3,4,5)(6,7,8)>, G_{20} = <(3,6)(4,7)(5,8)(6,7,8)>, G_{21} = <(1,2)(3,6)(4,7)(5,8)(6,7,8)> and G_{22} = **X**.

In addition, **X** has exactly 12 dominant classes as stored in Table I such that $\mathbf{K}_5$, $\mathbf{K}_6$, $\mathbf{K}_8$, $\mathbf{K}_9$, $\mathbf{K}_{10}$ and $\mathbf{K}_{12}$ are unmaturated (*i.e.*, the union of some conjugacy classes), see Table 1.

TABLE I. The dominant classes ($\mathbf{K}_i$) and their corresponding cyclic subgroups ($\mathbf{H}_i$) of f-NRG of 2,4-dimethylbenzene

i	$H_i \in SCG_X$	$\mathbf{K}_i$
1	$\mathbf{G_1}$	1a
2	$\mathbf{G_2}$	2a
3	$\mathbf{G_3}$	2b
4	$\mathbf{G_4}$	2c
5	$\mathbf{G_5}$	3a ∪ 3b
6	$\mathbf{G_6}$	3c ∪ 3e
7	$\mathbf{G_7}$	3d
8	$\mathbf{G_9}$	6a ∪ 6b
9	$\mathbf{G_{10}}$	6c ∪ 6d
10	$\mathbf{G_{12}}$	6e ∪ 6g
11	$\mathbf{G_{13}}$	6f
12	$\mathbf{G_{14}}$	6h ∪ 6i

To compute the Markaracter Table of **X**, *i.e.*, M^C, first, the non-redundant set of cyclic subgroups of **X** (*i.e.*, H_j, j = 1,2,…12) stored in Table 1 is calculated using the above GAP program. Furthermore, the nomenclature for consecutive classes of elements of order n must be defined, thus, 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 calculate the indices of all the unit subduced cycles of X, for instance $Z(G\ (/G_i)\downarrow G_{17}, s_d)$, in addition to the above program, the following GAP program must be applied:

```
G17= GroupWithGenerators (1,2),(3,6)(4,7)(5,8),(3,4,5)(6,7,8));
M17:=TableOfMarks(G17);
Inv:=(M17)^-1;
s17:=ConjugacyClassesSubgroups(G17);Sort(s17);
```

```
A:=[[36,0,0,0,0,0,0,0,0,0],[18,18,0,0,0,0,0,0,0,0],[18,0,6,0,0,0,0,0,0,0],[18,0,0,6
,0,0,0,0,0,0],[12,0,0,0,12,0,0,0,0,0],[12,0,0,0,0,0,0,0,0,0],[12,0,0,0,0,0,0,0,0,0],
[9,9,3,3,0,3,0,0,0,0],[6,6,0,0,6,0,6,0,0,0],[6,6,0,0,0,0,0,0,0,0],[6,0,6,0,0,0,0,0,0,0
],[6,6,0,0,0,0,0,0,0,0],[6,0,2,0,6,0,0,2,0,0],[6,0,0,2,6,0,0,0,2,0],[6,0,0,6,0,0,0,0,0,
0],[4,0,0,0,4,0,0,0,0,0],[3,3,1,1,3,1,3,1,1,1],[3,3,3,3,0,3,0,0,0,0],[2,2,0,0,2,0,2,0,
0,0],[2,0,2,0,2,0,0,2,0,0],[2,0,0,2,2,0,0,0,2,0],[1,1,1,1,1,1,1,1,1,1]];
    Column17:=A*(Inv);
Print("Column17","\n");
```

By using the above calculations, we are able to calculate the Fujita combinatorial enumeration tables (*i.e.*, the Markaracter Table, the Table of integer-valued characters and the USCI Table) of the f-NRG of 2,4-dimethylbenzene stored in Tables II–IV can be calculated, which would also be valuable in other applications, such as in the context of chemical applications of the graph theory and aromatic compounds.[1,27–29]

TABLE II. The Markaracter Table for the f-NRG of 2,4-dimethylbenzene

M^C	H_1	H_2	H_3	H_4	H_5	H_6	H_7	H_8	H_9	H_{10}	H_{11}	H_{12}
$X(/H_1)$	36	0	0	0	0	0	0	0	0	0	0	0
$X(/H_2)$	18	18	0	0	0	0	0	0	0	0	0	0
$X(/H_3)$	18	0	6	0	0	0	0	0	0	0	0	0
$X(/H_4)$	18	0	0	6	0	0	0	0	0	0	0	0
$X(/H_5)$	12	0	0	0	12	0	0	0	0	0	0	0
$X(/H_6)$	12	0	0	0	0	6	0	0	0	0	0	0
$X(/H_7)$	12	0	0	0	0	0	12	0	0	0	0	0
$X(/H_8)$	6	6	0	0	6	0	0	6	0	0	0	0
$X(/H_9)$	6	6	0	0	0	3	0	0	3	0	0	0
$X(/H_{10})$	6	6	0	0	0	0	6	0	0	6	0	0
$X(/H_{11})$	6	0	2	0	6	0	0	0	0	0	2	0
$X(/H_{12})$	6	0	0	2	6	0	0	0	0	0	0	2

TABLE III. The Table of integer-valued characters for the f-NRG of 2,4-dimethylbenzene (here, K_i and ϕ_i are the dominant class and Q-conjugacy character, respectively for i = 1,2,…12)

C^Q	K_1	K_2	K_3	K_4	K_5	K_6	K_7	K_8	K_9	K_{10}	K_{11}	K_{12}
ϕ_1	1	1	1	1	1	1	1	1	1	1	1	1
ϕ_2	1	1	–1	–1	1	1	1	1	–1	–1	–1	–1
ϕ_3	1	–1	1	–1	1	1	1	–1	1	1	1	–1
ϕ_4	1	–1	–1	1	1	1	1	–1	–1	–1	–1	1
ϕ_5	2	2	2	2	–1	–1	2	–1	–1	–1	2	–1
ϕ_6	2	2	–2	–2	–1	–1	2	–1	1	1	–2	1
ϕ_7	2	–2	2	–2	–1	–1	2	1	–1	–1	2	1
ϕ_8	2	–2	–2	2	–1	–1	2	1	1	1	–2	–1
ϕ_9	2	0	–2	0	–1	2	–1	0	1	–2	1	0
ϕ_{10}	2	0	2	0	–1	2	–1	0	–1	2	–1	0
ϕ_{11}	4	0	–4	0	1	–2	–2	0	–1	2	2	0
ϕ_{12}	4	0	4	0	1	–2	–2	0	1	–2	–2	0

TABLE IV. The unit subduced cycle indices for the f-NRG of 2,4-dimethylbenzene (*i.e.*, $Z(G(/G_i) \downarrow G_j, s_d)$ for $i,j = 1,2,\ldots22$)

USCI	$\downarrow G_1$	$\downarrow G_2$	$\downarrow G_3$	$\downarrow G_4$	$\downarrow G_5$	$\downarrow G_6$	$\downarrow G_7$	$\downarrow G_8$	$\downarrow G_9$	$\downarrow G_{10}$	$\downarrow G_{11}$
$G(/G_1)$	s_1^{36}	s_2^{18}	s_2^{18}	s_2^{18}	s_3^{12}	s_3^{12}	s_3^{12}	s_4^{9}	s_6^{6}	s_6^{6}	s_6^{6}
$G(/G_2)$	s_1^{18}	s_1^{18}	s_2^{9}	s_2^{9}	s_3^{6}	s_3^{6}	s_3^{6}	s_2^{9}	s_3^{6}	s_3^{6}	s_6^{3}
$G(/G_3)$	s_1^{18}	s_2^{9}	$s_2^{6}s_1^{6}$	s_2^{9}	s_3^{6}	s_3^{6}	s_3^{6}	$s_2^{3}s_4^{3}$	s_6^{3}	s_6^{3}	s_3^{6}
$G(/G_4)$	s_1^{18}	s_2^{9}	s_2^{9}	$s_2^{6}s_1^{6}$	s_3^{6}	s_3^{6}	s_3^{6}	$s_2^{3}s_4^{3}$	s_6^{3}	s_6^{3}	s_6^{3}
$G(/G_5)$	s_1^{12}	s_2^{6}	s_2^{6}	s_2^{6}	s_1^{12}	s_3^{4}	s_3^{4}	s_4^{3}	s_2^{6}	s_6^{2}	s_6^{2}
$G(/G_6)$	s_1^{12}	s_2^{6}	s_2^{6}	s_2^{6}	s_4^{3}	$s_3^{2}s_1^{6}$	s_4^{3}	s_4^{3}	s_6^{2}	$s_2^{3}s_6$	s_6^{2}
$G(/G_7)$	s_1^{12}	s_2^{6}	s_2^{6}	s_2^{6}	s_4^{3}	s_4^{3}	s_1^{12}	s_4^{3}	s_6^{2}	s_6^{2}	s_6^{2}
$G(/G_8)$	s_1^{9}	s_1^{9}	$s_2^{3}s_1^{3}$	$s_2^{3}s_1^{3}$	s_3^{3}	s_3^{3}	s_3^{3}	$s_2^{3}s_1^{3}$	s_3^{3}	s_3^{3}	s_3^{3}
$G(/G_9)$	s_1^{6}	s_1^{6}	s_2^{3}	s_2^{3}	s_1^{6}	s_3^{2}	s_3^{2}	s_3^{2}	s_1^{6}	s_3^{2}	s_6
$G(/G_{10})$	s_1^{6}	s_1^{6}	s_2^{3}	s_2^{3}	s_3^{2}	$s_1^{3}s_3$	s_3^{2}	s_2^{3}	s_3^{2}	$s_1^{3}s_3$	s_1^{6}
$G(/G_{11})$	s_1^{6}	s_2^{3}	s_1^{6}	s_2^{3}	s_3^{2}	s_3^{2}	s_6	s_2^{3}	s_6	s_6	s_1^{6}
$G(/G_{12})$	s_1^{6}	s_1^{6}	s_2^{3}	s_2^{3}	s_3^{2}	s_3^{2}	s_1^{6}	s_2^{3}	s_3^{2}	s_3^{2}	s_2^{3}
$G(/G_{13})$	s_1^{6}	s_2^{3}	$s_2^{2}s_1^{2}$	s_2^{3}	s_1^{6}	s_3^{2}	s_3^{2}	s_4s_2	s_2^{3}	s_6	s_3^{2}
$G(/G_{14})$	s_1^{6}	s_2^{3}	s_2^{3}	$s_2^{2}s_1^{2}$	s_1^{6}	s_3^{2}	s_3^{2}	s_4s_2	s_2^{3}	s_6	s_6
$G(/G_{15})$	s_1^{6}	s_2^{3}	s_2^{3}	s_1^{6}	s_3^{2}	s_3^{2}	s_1^{6}	s_2^{3}	s_6	s_6	s_2^{3}
$G(/G_{16})$	s_1^{4}	s_2^{2}	s_2^{2}	s_2^{2}	s_1^{4}	s_1^{4}	s_1^{4}	s_4	s_2^{2}	s_2^{2}	s_2^{2}
$G(/G_{17})$	s_1^{3}	s_1^{3}	s_1s_2	s_1s_2	s_1^{3}	s_3	s_3	s_1s_2	s_1^{3}	s_3	s_3
$G(/G_{18})$	s_1^{3}	s_1^{3}	s_1^{3}	s_1^{3}	s_3	s_3	s_1^{3}	s_1^{3}	s_3	s_3	s_1^{3}
$G(/G_{19})$	s_1^{2}	s_1^{2}	s_2	s_2	s_1^{2}	s_1^{2}	s_1^{2}	s_2	s_1^{2}	s_1^{2}	s_2
$G(/G_{20})$	s_1^{2}	s_1^{2}	s_1^{2}	s_2	s_1^{2}	s_1^{2}	s_1^{2}	s_2	s_2	s_2	s_1^{2}
$G(/G_{21})$	s_1^{2}	s_2	s_2	s_1^{2}	s_1^{2}	s_1^{2}	s_1^{2}	s_2	s_2	s_2	s_2
$G(/G_{22})$	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1
$G(/G_1)$	s_6^{6}	s_6^{6}	s_6^{6}	s_6^{6}	s_9^{4}	s_{12}^{3}	s_{12}^{3}	s_{18}^{2}	s_{18}^{2}	s_{18}^{2}	s_{36}
$G(/G_2)$	s_6^{3}	s_6^{3}	s_6^{3}	s_6^{3}	s_9^{2}	s_6^{3}	s_6^{3}	s_9^{2}	s_{18}	s_{18}	s_{18}
$G(/G_3)$	s_6^{3}	$s_6^{2}s_3^{2}$	s_6^{3}	s_6^{3}	s_9^{2}	$s_{12}s_6$	s_6^{3}	s_{18}	s_9^{2}	s_{18}	s_{18}
$G(/G_4)$	s_6^{3}	s_6^{3}	$s_6^{2}s_3^{2}$	s_6^{3}	s_9^{2}	$s_{12}s_6$	s_6^{3}	s_{18}	s_{18}	s_9^{2}	s_{18}

TABLE IV. Continued

USCI	$\downarrow G_{12}$	$\downarrow G_{13}$	$\downarrow G_{14}$	$\downarrow G_{15}$	$\downarrow G_{16}$	$\downarrow G_{17}$	$\downarrow G_{18}$	$\downarrow G_{19}$	$\downarrow G_{20}$	$\downarrow G_{21}$	$\downarrow G_{22}$
$G(/G_5)$	s_6^2	s_2^6	s_2^6	s_6^2	s_3^4	s_4^3	s_{12}	s_6^2	s_6^2	s_6^2	s_{12}
$G(/G_6)$	s_6^2	s_6^2	s_6^2	s_6^2	s_3^4	s_{12}	s_{12}	s_6^2	s_6^2	s_6^2	s_{12}
$G(/G_7)$	s_2^6	s_6^2	s_6^2	s_2^6	s_3^4	s_{12}	s_4^3	s_6^2	s_6^2	s_6^2	s_{12}
$G(/G_8)$	s_3^3	s_6s_3	s_6s_3	s_3^3	s_9	s_6s_3	s_3^3	s_9	s_9	s_9	s_9
$G(/G_9)$	s_3^2	s_3^2	s_3^2	s_6	s_3^2	s_3^2	s_6	s_3^2	s_6	s_6	s_6
$G(/G_{10})$	s_3^2	s_6	s_6	s_6	s_3^2	s_6	s_6	s_3^2	s_6	s_6	s_6
$G(/G_{11})$	s_3^2	s_3^2	s_6	s_2^3	s_3^2	s_6	s_2^3	s_6	s_3^2	s_6	s_6
$G(/G_{12})$	s_1^6	s_6	s_6	s_2^3	s_3^2	s_6	s_2^3	s_3^2	s_6	s_6	s_6
$G(/G_{13})$	s_6	$s_2^2s_1^2$	s_2^3	s_6	s_3^2	s_4s_2	s_6	s_6	s_3^2	s_6	s_6
$G(/G_{14})$	s_6	s_2^3	$s_2^2s_1^2$	s_3^2	s_3^2	s_4s_2	s_6	s_6	s_6	s_3^2	s_6
$G(/G_{15})$	s_2^3	s_6	s_3^2	s_1^6	s_3^2	s_6	s_2^3	s_6	s_6	s_3^2	s_6
$G(/G_{16})$	s_2^2	s_2^2	s_2^2	s_2^2	s_1^4	s_4	s_4	s_2^2	s_2^2	s_2^2	s_4
$G(/G_{17})$	s_3	s_1s_2	s_1s_2	s_3	s_3	s_1s_2	s_3	s_3	s_3	s_3	s_3
$G(/G_{18})$	s_1^3	s_3	s_3	s_1^3	s_3	s_3	s_1^3	s_3	s_3	s_3	s_3
$G(/G_{19})$	s_1^2	s_2	s_2	s_2	s_1^2	s_2	s_2	s_1^2	s_2	s_2	s_2
$G(/G_{20})$	s_2	s_1^2	s_2	s_2	s_1^2	s_2	s_2	s_2	s_1^2	s_2	s_2
$G(/G_{21})$	s_2	s_2	s_1^2	s_1^2	s_1^2	s_2	s_2	s_2	s_2	s_1^2	s_2
$G(/G_{22})$	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1

Acknowledgment. The authors are indebted to the dear referee for useful discussions and suggestions.

И З В О Д

ФУЏИТИНО (FUJITA) КОМБИНАТОРНО ПРЕБРОЈАВАЊЕ ЗА НЕРИГИДНУ ГРУПУ 2,4-ДИМЕТИЛБЕНЗЕНА

ALI MOGHANI[1], SOROOR NAGHDI SEDEH[1] и MOHAMMD REZA SOROUHESH[2]

[1]*Department of color physics, Institute for Colorants Paint and Coating (ICPC), Tehran и* [2]*Department of Mathematics, Islamic Azad University, South branch Tehran, Tehran, Iran*

Применом теорије неригидних група показано је да је потпуна неригидна група 2,4-диметилбензена нематурирана група и да је изоморфна групи $\mathbf{C}_2\times(\mathbf{C}_3\mathrm{wr}\mathbf{C}_2)$ реда 36, где је $\mathbf{C}_n$ циклична група реда n, и где симболи × и wr означавају директни одн. венчасти производ. Показано је да испитивана група има 12 доминантних класа. По први пут су одређене та-

блица марккарактера, таблица свих целобројних карактера, као и таблица јединичних цикличних индекса субдукције (USCI) за све потпуне неригидне групе 2,4-диметилбензена.

(Примљено 1. јуна, ревидирано 21 јула 2009)

REFERENCES

1. S. Fujita, *Bull. Chem. Soc. Jpn*. **71** (1998) 2071
2. S. Fujita, *Bull. Chem. Soc. Jpn*. **71** (1998) 2309
3. S. Fujita, *Bull. Chem. Soc. Jpn*. **71**(1998) 1587
4. F. A. Cotton, *Chemical Application of Group Theory*, Wiley-International, New York, USA, 1971
5. I. Hargittai, H. Hargitta, *Symmetry through the Eyes of a Chemist*, VCH, Weinheim, Germany, 1986
6. S. Fujita, *J. Math. Chem.* **12** (1999) 173
7. S. Fujita, *J. Graph Theory* **18** (1994) 349
8. S. Fujita, *J. Org. Chem*. **67** (2002) 6055
9. S. Fujita, *J. Comput. Chem. Jpn*. (2004) 113
10. S. Fujita, *MATCH Commun. Math. Comput. Chem*. **54** (2005) 251
11. S. Fujita, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 5
12. S. Fujita, *MATCH Commun. Math. Comput. Chem*. **55** (2006) 237
13. S. Fujita, *MATCH Commun. Math. Comput. Chem*. **57** (2007) 5
14. S. Fujita, *Diagrammatical Approach to Molecular Symmetry and Enumeration of Stereoisomers*, University of Kragujevac, Kragujevac, Serbia, 2007
15. S. Fujita, *Theor. Chim. Acta* **91** (1995) 291
16. S. Fujita, *Theor. Chim. Acta* **91** (1995) 315
17. A. Kerber, *MATCH Commun. Math. Comput. Chem*. **46** (2002) 151
18. S. Fujita, *MATCH Commun. Math. Comput. Chem*. **58** (2007) 611
19. S. Fujita, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 509
20. S. Fujita, *MATCH Commun. Math. Comput. Chem*. **61** (2009) 11
21. S. Fujita, *MATCH Commun. Math. Comput. Chem*. **61** (2009) 39
22. S. Fujita, *MATCH Commun. Math. Comput. Chem*. **61** (2009) 71
23. M. R. Darafsheh, A. Darafsheh, *MATCH Commun. Math. Comput. Chem*. **56** (2006) 271
24. A. Moghani, *Bull. Chem. Soc. Jpn*. **82** (2009) 602.
25. H. C. Longuet-Higgins, *Mol. Phys.* **6** (1963) 445
26. Y. G. Smeyers, *Adv. Quantum. Chem.* **24** (1992) 1
27. S. L. Altmann, *Induced Representation in Crystal and Molecules*, Academic Press, London, 1977
28. P. R. Bunker, *Molecular Symmetry in Spectroscopy*, Academic Press, New York, USA, 1979
29. J. S. Lomont, *Applications of Finite Groups*, Academic Press, New York, USA, 1959
30. A. J. Stone, *J. Chem. Phys.* **41** (1964) 1568
31. Y. G. Smeyers, M. Villa, *J. Math. Chem.* **28** (2000) 377
32. K. Balasubramanian, *J. Phys. Chem.* **10** (2004) 5527
33. K. Balasubramanian, *Chem. Phys. Lett*. **391** (2004) 64
34. K. Balasubramanian, *Chem. Phys. Lett*. **398** (2004) 15
35. A. Moghani, S. Naghdi, A. R. Ashrafi, A. Ahmadi, *J. London Math. Soc.* **340** (2007) 630

36. GAP, *Groups, Algorithms and Programming*, Lehrstuhl De für Mathematik, RWTH, Aachen, Germany, http://www.gap-system.org
37. A. Moghani, *J. Serb. Chem. Soc.* **73** (2008) 189
38. M. R Darafsheh, A. Moghani, *Bull. Chem. Soc. Jpn.* **81** (2008) 279
39. M. R. Darafsheh, A. Moghani, S. Naghdi Sedeh, *Acta Chim. Slov.* **55** (2008) 602
40. M. R. Darafsheh, A. Moghani, M. Karami, A. Zaeembashi, S. Naghdi, *Int. J. Chem. Model.* **1** (2009) 435.