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Journal of the Serbian Chemical Society

JSCS@tmf.bg.ac.yu • www.shd.org.rs/JSCS

J. Serb. Chem. Soc. 74 (1) 45–52 (2009)
JSCS–3807

UDC 519.111:547.216–125
Original scientific paper

Q-Conjugacy character table for the non-rigid group of 2,3-dimethylbutane

MOHAMMAD REZA DARAFSHEH[1] and ALI MOGHANI[2]*

[1]*School of Mathematics, College of Science, University of Tehran, Tehran and* [2]*Department of color physics, Institute for Colorants Paint and Coating (ICPC), Tehran, Iran*

(Received 9 April 2008)

Abstract: Maturated and unmaturated groups were introduced by the Japanese chemist Shinsaku Fujita, who used them in the markaracter table and the Q-conjugacy character table of a finite group. He then applied his results in this area of research to enumerate isomers of molecules. Using the non-rigid group theory, it was shown by the second author that the full non-rigid (f-NRG) group of 2,3--dimethylbutane is isomorphic to the group $(Z_3\times Z_3\times Z_3\times Z_3):Z_2$ of order 162 with 54 conjugacy classes. Here $(Z_3\times Z_3\times Z_3\times Z_3):Z_2$ denotes the semi direct product of four copies of Z_3 by Z_2, where Z_n is a cyclic group of order n. In this paper, it is shown with the GAP program that this group has 30 dominant classes (similarly, Q-conjugacy characters) and that 24 of them are unmatured (similarly, Q-conjugacy characters such that they are the sum of two irreducible characters). Then, the Q-conjugacy character table of the unmatured full non-rigid group 2,3-dimethylbutane is derived.

Keywords: full non-rigid group; Q-conjugacy character; 2,3-dimethylbutane.

INTRODUCTION

In order to develop new methods of combinatorial enumeration of isomers, some relationship between character tables containing characters for irreducible representations[1,2] and mark tables containing marks for coset representations were clarified by Shinsaku Fujita.[3–14]

Fujita proposed not only markaracter tables, which enable characters and marks to be discussed on a common basis,[15,16] but also Q-conjugacy character tables,[7–9] which are obtained for finite groups. The enumeration of chemical compounds has been accomplished by various methods but the Pólya–Redfield theorem has been a standard method for combinatorial enumerations of graphs and chemical compounds. A dominant class[15] is defined as a disjoint union of conjugacy classes that corresponds to the same cyclic subgroup, which is selected

* Corresponding author. E-mail: moghani@icrc.ac.ir
doi: 10.2298/JSC0901045D

as a representative of conjugate cyclic subgroups. Let G be a finite group and h_1, $h_2 \in$ G. It is said that h_1, h_2 are Q-conjugate if there exists $t \in$ G such that $t^{-1} = = \langle h_1 \rangle$ and $t = \langle h_2 \rangle$. It is easy to see that the Q-conjugacy is an equivalence relation on G and generates equivalence classes which are called dominant classes, *i.e.*, the group G is partitioned into dominant classes as follows: $G = K_1 + K_2 + \ldots + K_s$ in which K_i corresponds to the cyclic (dominant) subgroup G_i selected from a non-redundant set of cyclic subgroups of G denoted by SCSG.[15]

Now, let $\mathbf{C} = \mathbf{C}_{u\times u}$ be the matrix of the character table of the finite group G. Thereby, it is transformed to a more concise form called a Q-conjugacy character table, the $s\times s$-matrix of which is denoted by $\mathbf{C}^Q$ where $s \leq u$, as follows: If $u = s$, then $\mathbf{C} = \mathbf{C}^Q$, *i.e.*, G is a maturated group. Assuming $s < u$, then according to literature,[7–9] since the dimension of the Q-conjugacy character table of G and the corresponding markaracter table of G are equal, $t = \varphi(|H|)/m(H)$ is set, where $m(H)$ is maturity discriminate.[10–16]

If $t = 1$ (*i.e.*, K_i is exactly a conjugacy class), then there is no reduction in the rows and columns of **C** but, if $t > 1$ (K_i is a union of t-conjugacy classes of G, *i.e.*, a reduction in the correspondence columns in the character table **C**), the sum of the t-rows of the irreducible characters *via* the same degree in **C** (reduction in rows) gives a reducible character, which are called Q-conjugacy characters in both cases.

A rigid molecule is defined as being such that the barriers between its versions are insuperable and there are no observable tunneling splittings. For non-rigid molecules, there are one or more contortional large amplitude vibrations, such as inversion or internal rotation that give rise to tunneling splittings. Due to this deformability, non-rigid molecules exhibit some interesting properties of intramolecular dynamics, which can be more easily studied by resorting to group theory. The group theory for non-rigid molecules finds numerous applications ranging from rovibronic spectroscopy of molecules exhibiting large amplitude motions, chemical reactions to dynamic stereochemistry to weakly-bound van der Waals complexes. Following the pioneering works of Longuet–Higgins,[19] the symmetry group of a non-rigid molecule group consists of all permutations and permutation–inversion operations, which become feasible as molecules tunnel through a number of potential energy maxima separated by multiple minima. Subsequently, several other workers[19–32,34–36] formulated different ways of characterizing non-rigid groups (NRG).

The complete set of molecular conversion operations which commute with the nuclear motion operator contains overall rotation operations, describing the molecule rotating as a whole, and non-rigid tunneling motion operations, descrybing 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[19] investigated the symmetry groups of non-rigid molecules, where

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.

The present study investigates Q-conjugacy character tables of the f-NRG of 2,3-dimethylbutane. The motivation for this study is also outlined in literature,[26–36] and the reader is encouraged to consult these papers for background material as well as basic computational techniques with the aid of GAP.[33] For instance, an algorithm to work with big chemical graphs, such as the big fullerene C_{80}, was introduced by the second author[29,35] and a Q-conjugacy character table for the f--NRG of petra-amine platinum (II) was presented.[36]

The symmetry groups of 2,3-dimethylbutane was found as a semi-direct product by the first author (see Fig. 1).[30] In the present paper, it is shown that the f--NRG of 2,3-dimethylbutane is an unmatured group of order 162 with 30 dominant classes (similarly, Q-conjugacy characters), such that there are 24 unmatured (*i.e.*, there are 24 row (column) reductions in the character table of the f-NRG of 2,3-dimethylbutane).

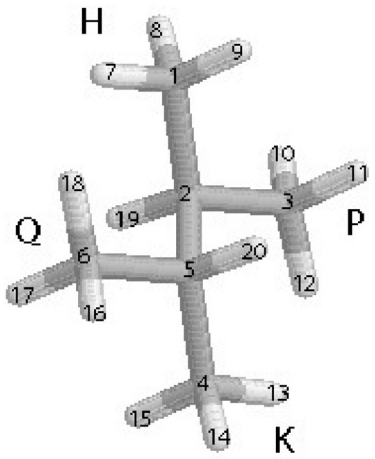

Fig. 1. Structure of 2,3-dimethylbutane.

COMPUTATIONAL METHOD AND DISCUSSION

A permutation representation P of a finite group G is obtained when the group G acts on a finite set $X = \{x_1, x_2, \ldots, x_t\}$ from the right, which means that the following mapping is given:

P: $X \times G \rightarrow X$ *via* $(x,g) \rightarrow xg$ such that the following holds: $(xg)g' = x(gg')$ and $x_1 = x$, for each $g,g' \in G$ and $x \in X$. Now let it be assumed that an action P of G on X and a subgroup H of G are given. Considering the set of its right cosets H_{gi} and the corresponding partition of G into these cosets: $G = H_{g1} + H_{g2} + \ldots + H_{gm}$.

If the cosets from the right are multiplied by a group element g, these cosets are permuted. In fact, one obtains an action of G on the set X of cosets and cor-

respondingly a permutation representation which is denoted by G(/H), following Fujita's notation.

If M is a normal subgroup of G and K is another subgroup of G such that M ∩ K = {e} and G = MK = <M,K>, then G is called a semi-direct product of K by M denoted by K:M.

The first author described[30] that the f-NRG of 2,3-dimethylbutane is isomorphic to the semidirect product of four copies of Z_3 by Z_2, where Z_n is a cyclic group of order *n*, as follows: using numbers {1,2,3,4,5,6} to indicate the carbon atoms, the numbers {7,8,9} to label the three hydrogen atoms on the 1 corner and {10,11,12} to label the hydrogen atoms on the 3 corner and so on, see Fig. 1, then the symmetry of order 2 of the framework in terms of permutations is: σ = = (1,4)(2,5)(3,6)(7,13)(8,14)(9,15)(10,16)(11,17)(12,18)(19,20).

The group of symmetries of each CH_3 group in terms of a generating system is: H = <(7,8,9)>, K = <(13,14,15)>, P = <(10,11,12)> and Q = <(16,17,18)>.

Since the effect of σ on the carbon atoms is not needed, its effect on the hydrogen atoms is considered, *i.e.*, σ' = (7,13)(8,14)(9,15)(10,16)(11,17)(12,18). Therefore, the f-NRG of this molecule in terms of generators is G = <θ_1,θ_2,θ_3,θ_4,σ'>, where θ_1 = (7,8,9), θ_2 = (13,14,15), θ_3 = (10,11,12) and θ_4 = = (16,17,18).

The computations of the symmetry properties of the molecules were carried out using of GAP.[33] GAP stands for Groups, Algorithms and Programming. The name was chosen to reflect the aim of the system, which is group theoretical software for solving computational problems in computational group theory. This software was constructed by the GAP team in Aachen. GAP is a free and extendable software package.

Now, at the prompt of GAP, the following program was run to compute the character table and the set SCSG of the f-NRG of 2,3-dimethylbutane D = $(Z_3 \times Z_3 \times Z_3 \times Z_3):Z_2$ as follow:

```
LogTo("Computations.txt");
a := (7,8,9);
   b:= (10,11,12);
     c := (13,14,15);
        d := (16, 17, 18);
             e := (7,13)(8,14)(9,15)(10,16) (11,17)(12,18);
                  D : = GroupWithGenerators(a,b,c,d,e);
                       Char := CharacterTable(D);
Order(D);IsPermGroup(D);
   s:=ConjugacyClassesSubgroups(D);
      Sort("s");
         SCSG:=List(ConjugacyClassesSubgroups(G),x->Elements(x));
            Len:=Length(a); y:=[];
```

```
for i in [1,2...z]do
   if IsCyclic(a[i])then Add(y,i);
      fi;
         od;
           Display(Char);
             Display(s);
                Print("Char", "\n");
                   Print("SCSG", "\n");
                      LogTo( );
```

In addition, since the dimensions of the Q-conjugacy character table of D = = $(Z_3 \times Z_3 \times Z_3 \times Z_3):Z_2$ and its corresponding markaracter table[7–9] are equal, $|SCSG| = 30$.

Now, on running the program, it can be seen that D has exactly 30 dominant (Q-conjugacy) classes as follow:

K_1 = 1a, K_2 = 2a, K_3 = 3a ∪ 3b, K_4 = 3c ∪ 3f, K_5 = 3d ∪ 3h, K_6 = 3e ∪ 3g, K_7 = 3i ∪ 3q, K_8 = 3j, K_9 = 3k ∪ 3u, K_{10} = 3l ∪ 3w, K_{11} = 3m ∪ 3v, K_{12} = 3n ∪ ∪ 3r, K_{13} = 3o ∪ 3t, K_{14} = 3p ∪ 3s, K_{15} = 3x ∪ 3am, K_{16} = 3y ∪ 3ao, K_{17} = 3z ∪ ∪ 3an, K_{18} = 3aa, K_{19} = 3ab ∪ 3aj, K_{20} = 3ac ∪ 3af, K_{21} = 3ad ∪ 3ar, K_{22} = 3ae ∪ ∪ 3aq, K_{23} = 3ag ∪ 3al, K_{24} = 3ah, K_{25} = 3ai ∪ 3ap, K_{26} = 3ak, K_{27} = 6a ∪ 6b, K_{28} = 6c ∪ 6f, K_{29} = 6d ∪ 6h, K_{30} = 6e ∪ 6g.

Here, just K_1, K_2, K_8, K_{18}, K_{24} and K_{26} are matured dominant classes (similar discussion for Q-conjugacy characters). Therefore, by the above computations, the Q-conjugacy character table (C^Q) of group D = $(Z_3 \times Z_3 \times Z_3 \times Z_3):Z_2$, which are stored in Table I and II, can be introduced. More details are given in the literature.[37]

TABLE I. Q-conjugacy character table from K_1 to K_{15} of the f-NRG of 2,3-dimethylbutane

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}	K_{13}	K_{14}	K_{15}
ϕ_1	1	1	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	1	1	1
ϕ_3	2	2	–1	–1	–1	2	2	–1	–1	–1	–1	–1	–1	–1	–1
ϕ_4	2	2	–1	–1	–1	2	2	–1	–1	–1	–1	–1	–1	–1	–1
ϕ_5	2	–1	2	–1	–1	–1	2	–1	2	–1	–1	–1	2	2	–1
ϕ_6	2	–1	2	–1	–1	–1	2	–1	–1	2	–1	–1	2	2	–1
ϕ_7	2	–1	–1	–1	2	–1	2	–1	2	–1	2	–1	–1	–1	2
ϕ_8	2	–1	–1	–1	2	–1	2	–1	2	–1	2	–1	–1	–1	2
ϕ_9	2	–1	–1	2	–1	–1	2	2	–1	–1	–1	2	–1	–1	–1
ϕ_{10}	2	–1	–1	2	–1	–1	2	2	–1	–1	–1	2	–1	–1	–1
ϕ_{11}	2	–1	2	–1	–1	2	–1	–1	2	–1	–1	2	–1	2	–1
ϕ_{12}	2	2	–1	–1	–1	2	2	–1	–1	–1	–1	–1	–1	2	2
ϕ_{13}	2	–1	–1	–1	2	2	–1	2	–1	–1	–1	–1	2	2	–1
ϕ_{14}	2	–1	–1	2	–1	2	–1	–1	–1	2	2	–1	–1	2	–1
ϕ_{15}	4	–2	–2	1	1	4	–2	1	–2	1	1	–2	1	–2	1

TABLE 1. Continued

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}	K_{13}	K_{14}	K_{15}
ϕ_{16}	4	1	–2	1	–2	–2	–2	1	4	1	–2	–2	1	–2	–2
ϕ_{17}	4	1	–2	–2	1	–2	–2	–2	–2	1	1	4	1	–2	1
ϕ_{18}	4	1	4	1	1	–2	–2	1	–2	–2	1	–2	–2	4	1
ϕ_{19}	4	4	1	1	1	4	4	1	1	1	1	1	1	–2	–2
ϕ_{20}	4	–2	1	1	–2	–2	4	1	–2	1	–2	1	1	–2	4
ϕ_{21}	4	–2	1	–2	1	–2	4	–2	1	1	1	–2	1	–2	–2
ϕ_{22}	4	–2	–2	1	1	–2	4	1	1	–2	–1	–1	–2	4	–2
ϕ_{23}	4	–2	1	1	–2	4	–2	–2	1	1	1	1	–2	–2	1
ϕ_{24}	4	–2	1	–2	1	4	–2	1	1	–2	–2	1	1	–2	1
ϕ_{25}	4	1	–2	1	–2	–2	–2	–2	1	–2	1	1	4	4	1
ϕ_{26}	4	1	–2	–2	1	–2	–2	1	1	4	–2	1	–2	4	1
ϕ_{27}	4	1	1	1	4	–2	–2	–2	–2	1	–2	1	–2	–2	–2
ϕ_{28}	4	1	1	–2	–2	–2	–2	1	–2	–2	4	1	1	–2	–2
ϕ_{29}	4	1	1	–2	–2	–2	–2	4	1	1	1	–2	–2	–2	1
ϕ_{30}	4	1	1	4	1	–2	–2	–2	1	–2	–2	–2	1	–2	1

Table II. Q-conjugacy character table from K_{16} to K_{30} of the f-NRG of 2,3-dimethylbutane

C^Q	K_{16}	K_{17}	K_{18}	K_{19}	K_{20}	K_{21}	K_{22}	K_{23}	K_{24}	K_{25}	K_{26}	K_{27}	K_{28}	K_{29}	K_{30}
ϕ_1	1	1	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	–1	–1	–1
ϕ_3	–1	2	2	2	–1	–1	2	2	–1	2	–2	–2	1	1	1
ϕ_4	–1	2	2	2	–1	–1	2	2	–1	2	2	2	–1	–1	–1
ϕ_5	–1	2	–1	–1	–1	2	–1	2	–1	2	–2	1	–2	1	1
ϕ_6	–1	2	–1	–1	–1	2	–1	2	–1	2	2	–1	2	–1	–1
ϕ_7	–1	2	–1	–1	–1	–1	–1	2	2	2	–2	1	1	1	–2
ϕ_8	–1	2	–1	–1	–1	–1	–1	2	2	2	2	–1	–1	–1	2
ϕ_9	2	2	–1	–1	2	–1	–1	2	–1	2	–2	1	1	–2	1
ϕ_{10}	2	2	–1	–1	2	–1	–1	2	–1	2	2	–1	–1	2	–1
ϕ_{11}	–1	2	–1	–1	2	–1	2	–1	2	–1	0	0	0	0	0
ϕ_{12}	2	–1	–1	–1	2	2	–1	–1	2	–1	0	0	0	0	0
ϕ_{13}	–1	–1	–1	2	2	–1	–1	–1	2	2	0	0	0	0	0
ϕ_{14}	–1	–1	2	–1	2	–1	–1	2	2	–1	0	0	0	0	0
ϕ_{15}	1	4	–2	–2	–2	1	4	–2	–2	–2	0	0	0	0	0
ϕ_{16}	1	4	1	1	–2	1	–2	–2	4	–2	0	0	0	0	0
ϕ_{17}	–2	4	1	1	4	1	–2	–2	–2	–2	0	0	0	0	0
ϕ_{18}	1	4	1	1	–2	–2	–2	–2	–2	–2	0	0	0	0	0
ϕ_{19}	–2	–2	–2	–2	–2	–2	–2	–2	–2	–2	0	0	0	0	0
ϕ_{20}	–2	–2	1	1	–2	–2	1	–2	4	–2	0	0	0	0	0
ϕ_{21}	4	–2	1	1	4	–2	1	–2	–2	–2	0	0	0	0	0
ϕ_{22}	–2	–2	1	1	–2	4	1	–2	–2	–2	0	0	0	0	0
ϕ_{23}	1	–2	4	4	2	1	–2	–2	–2	4	0	0	0	0	0
ϕ_{24}	1	–2	4	–2	–2	1	–2	4	–2	–2	0	0	0	0	0
ϕ_{25}	1	–2	1	–2	–2	–2	1	–2	–2	4	0	0	0	0	0
ϕ_{26}	1	–2	–2	1	–2	–2	1	4	–2	–2	0	0	0	0	0

TABLE 2. Continued

C^Q	K_{16}	K_{17}	K_{18}	K_{19}	K_{20}	K_{21}	K_{22}	K_{23}	K_{24}	K_{25}	K_{26}	K_{27}	K_{28}	K_{29}	K_{30}
ϕ_{27}	1	–2	1	–2	–2	1	1	–2	4	4	0	0	0	0	0
ϕ_{28}	1	–2	–2	1	–2	1	1	4	4	–2	0	0	0	0	0
ϕ_{29}	–2	–2	1	–2	4	1	1	–2	–2	4	0	0	0	0	0
ϕ_{30}	–2	–2	–2	1	4	1	1	4	–2	–2	0	0	0	0	0

The derived Q-conjugacy character tables could also be valuable in other applications, such as in the context of chemical applications of graph theory and aromatic compounds.[10–14]

И З В О Д

ТАБЛИЦА КАРАКТЕРА Q-КОНЈУГАЦИЈЕ ЗА НЕРИГИДНУ ГРУПУ СИМЕТРИЈЕ 2,3-ДИМЕТИЛБУТАНА

MOHAMMAD REZA DARAFSHEH[1] и ALI MOGHANI[2]

[1]School of Mathematics, College of Science, University of Tehran, Tehran, Iran и [2]Department of color physics, Institute for Colorants Paint and Coating (ICPC), Tehran, Iran

Јапански хемичар Shinsaku Fujita увео је матуриране и нематуриране групе, које је користио у теорији таблица марк-карактера и таблица карактера Q-конјугације коначних група. Он је онда применио ове резултате за пребројавање изомера. Користећи теорију неригидних група, један од садашњих аутора показао је да је потпуна неригидна група (f-NRG) 2,3-диметилбутана изоморфна са групом $(Z_3\times Z_3\times Z_3\times Z_3):Z_2$ реда 162 са 54 класа конјугације. Овде $(Z_3\times Z_3\times Z_3\times Z_3):Z_2$ означава семидиректни производ четири копије групе Z_3 са групом Z_2, где је Z_n циклична група реда n. У овом раду је применом програма GAP показано да ова група има 30 доминантних класа (односно карактера Q-конјугације), и да су 24 од њих нематуриране (односно карактери Q-конјугације су збир два иредуцибилна карактера). Након тога, одређена је таблица катактера Q-конјугације за нематурирану потпуну неригидну групу симетрије 2,3-диметилбутана.

(Примљено 9. априла 2008)

REFERENCES

1. F. A. Cotton, *Chemical Application of Group Theory*, Wiley-International, New York, 1971
2. I. Hargittai, H. Hargitta, *Symmetry through the Eyes of a Chemist*, VCH, Weinheim, 1986
3. S. Fujita, *J. Math. Chem*. **12** (1999) 173
4. S. Fujita, *J. Graph Theory* **18** (1994) 349
5. S. Fujita, *J. Org. Chem.* **67** (2002) 6055
6. S. Fujita, *J. Comput. Chem. Jpn.* (2004) 113
7. S. Fujita, *Bull. Chem. Soc. Japan* **71** (1998) 2071
8. S. Fujita, *Bull. Chem. Soc. Japan* **71** (1998) 2309
9. S. Fujita, *Bull. Chem. Soc. Japan* 71(1998) 1587
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*, MCM, Kragujevac, 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. M. R. Darafsheh, Y. Farjami, A. R. Ashrafi, *Acta Chim. Slov.* **52** (2005) 282
19. H. C. Longuet-Higgins, *Mol. Phys.* **6** (1963) 445
20. Y. G. Smeyers, *Adv. Quantum. Chem.* **24** (1992) 1
21. S. L. Altmann, *Induced Representation in Crystal & Molecules*, Academic Press, London, 1977
22. P. R. Bunker, *Molecular Symmetry in Spectroscopy*, Academic Press, New York, 1979
23. J. S. Lomont, *Applications of Finite Groups*, Academic, New York, 1959
24. A. J. Stone, *J. Chem. Phys.* **41** (1964) 1568
25. Y. G. Smeyers, M. Villa, *J. Math. Chem.* **28** (2000) 377
26. K. Balasubramanian, *J. Phys. Chem.* **10** (2004) 5527
27. K. Balasubramanian, *Chem. Phys. Lett.* **391** (2004) 64
28. K. Balasubramanian, *Chem. Phys. Lett.* **398** (2004) 15
29. A. Moghani, S. Naghdi, A. R. Ashrafi, A. Ahmadi, *London Math. Soc.* **340** (2007) 630
30. M. R. Darafsheh, A Darafsheh, A. R. Ashrafi, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 47
31. M. R. Darafsheh, A. Darafsheh, A. R. Ashrafi, *Int. J. Quantum Chem.* **107** (2007) 340
32. M. R. Darafsheh,; A. R. Ashrafi, A. Darafsheh, *Chem. Phys. Lett*. **421** (2006) 566
33. GAP, Groups, Algorithms and Programming, Lehrstuhl De für Mathematik, RWTH, Aachen, http://www.gap-system.org (1995)
34. M. R. Darafsheh, Y. Farjami, A. R. Ashrafi, M. Hamadanian, *J. Math. Chem.* **41** (2007) 315
35. A. Moghani, A. R. Ashrafi, *Croat. Chem. Acta* **79** (2006) 465
36. A. Moghani, *J. Serb. Chem. Soc.* **73** (2008) 189
37. M. R. Darafsheh, A. Moghani, *Bull. Chem. Soc. Japan* (2008), in press.