A New Simple Method for Maturity of Finite Groups and Application to Fullerenes and Fluxional Molecules

Ali Moghani

Department of Color Physics, Institute for Colorants Paint and Coating (ICPC), Tehran, Iran

Received May 19, 2008; E-mail: moghani@icrc.ac.ir

Matured and unmatured groups were introduced by S. Fujita who used them in the Q-conjugacy character table of a finite group (*Bull. Chem. Soc. Jpn.* **1998**, *71*, 2071). He then applied his results in this area of research to enumerate isomers of molecules. In this paper, we introduce a new simple method to specify how a given finite group is matured or unmatured via some useful examples. The Q-conjugacy character tables of the fullerene C_{80} and tetranitrocubane are then verified.

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.[1] Let G be a finite group and $h_1, h_2 \in G$. We say h_1, h_2 are Q-conjugate if there exists $t \in G$ such that $t^{-1}\langle h_1\rangle t = \langle h_2\rangle$.

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 nonredundant set of cyclic subgroups of G denoted by *SCSG*. In order to develop new methods of combinatorial enumeration of isomers, some relationship between character tables containing characters for irreducible representations and mark tables containing marks for coset representations have been clarified by Fujita who proposed not only markaracter tables, which enable us to discuss characters and marks on a common basis, but Q-conjugacy character tables, which are obtained for finite groups.[1–10]

A molecule is said to be non-rigid if there are several local minima on the potential energy surface easily surmountable by the molecular system via a tunneling rearrangement. A non-rigid molecule typically possesses several potential valleys separated by relatively low energy barriers, and thus exhibits large amplitude tunneling dynamics among various potential minima. Because of this deformability, the non-rigid molecules exhibit some interesting properties of intramolecular dynamics, spectroscopy, dynamic NMR and so, all of which can be interpreted resorting to group theory. Group theory is the best formal method to describe the symmetry concept of molecular structures. Group theory for non-rigid molecules is becoming increasingly relevant and its numerous applications to large amplitude vibrational spectroscopy of small organic molecules are in the literature.[11,12]

The molecular symmetry group of a non-rigid molecule was defined by Longuet-Higgins[13] although there have been earlier works that suggested the need for such a framework by Hougen.[14] Bunker and Papoušek[15] extended the definition of the molecular symmetry group to linear molecules using an extended molecular symmetry. The operations of the molecular symmetry group and the three-dimensional rotation group are used together to treat the symmetry properties of molecules in electric and magnetic fields by Watson.[16] The complete set of the molecular conversion operations that commute with the nuclear motion operator will contain overall rotation operations that describe a molecule rotating as a whole, and intramolecular motion operations that describe molecular moieties moving with respect to the rest of the molecule. These operations form a group which is called the full non-rigid molecule group (f-NRG) by Smeyers.[17] The notation we use is standard and the reader may consult,[18,19] besides, the non-rigid group theory also finds applications in the enumeration of isomers and substituted aromatics.[20]

The present study investigates a new simple method to specify how a given finite group is matured or unmatured via some useful examples in the third section, and finally, the Q-conjugacy character tables of the fullerene C_{80} and tetranitrocubane are verified in the fourth section.

Theoretical

In this section we first describe some notation which will be kept throughout. 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. 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 we are given a mapping P: $X \times G \rightarrow X$ via $(x, g) \rightarrow xg$ such that holds the following: $(xg)g' = x(gg')$ 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. One considers the set of its right cosets H_{g_i} and the corresponding partition of G into these cosets: $G = H_{g_1} + H_{g_2} + \ldots + H_{g_m}$. 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, correspondingly, a permutation representation which is denoted by $G(/H)$, following Fujita's notation.[1]

Published on the web September 9, 2009; doi:10.1246/bcsj.82.1103

If M is a normal subgroup of G and K is another subgroup of G such that $M \cap K = \{e\}$ and $G = MN = \langle M, N\rangle$, then G is called a semi direct product of N by M which is denoted by $N{:}M$. Suppose K and H be groups and let H act on the set Γ. Then the wreath product of K by H, denoted by $K \sim H$ is defined to be the semi direct product $K^{\Gamma}{:}H$, where K^{Γ} is the set of all functions f: $\Gamma \to K$.[18,19]

The Maturity of Finite Groups. The aim of this section is to specify a simple method to verify a given finite group is matured or unmatured. The concept of maturity has been introduced by Fujita.[2] Let C be a $u \times u$ matrix of character table of a given finite group G. Then, C is transformed into a more concise form called the Q-conjugacy character table that we denote its $s \times s$ matrix by C^Q ($s \leq u$) as follows: If $u = s$, then $C = C^Q$ i.e., G is a matured group. Otherwise $s < u$, for each $G_i \in SCSG$ (the corresponding dominant class K_i) set $t_i = m(G_i)/\phi(|G_i|)$ where $m(G_i) = |N_G(G_i)|/|C_G(G_i)|$ (called the maturity discriminant), ϕ is the Euler function and finally $N_G(G_i)$ and $C_G(G_i)$ denote the normalizer and centralizer of G_i in G, respectively for $i = 1, \ldots, s$.

If $t_i = 1$ then, K_i is exactly a conjugacy class so there is no reduction in row and column of C, but if $t_i > 1$ then K_i is a union of t_i-conjugacy classes of G (i.e., reduction in column), therefore the sum of t_i rows of irreducible characters via the same degree in C (reduction in rows) gives us a reducible character which is called the Q-conjugacy character with integer-valued in both cases.[21,22]

Assume G_i to be an arbitrary finite group with the corresponding character table C_i, for $i = 1, 2, \ldots, n$, let G be the direct product of $G_1, G_2, \ldots, G_n$ (i.e., $G = G_1 \times G_2 \times \ldots \times G_n$), with the corresponding character table C. We have two following cases.

Case 1, G_i is matured group for each i: Suppose χ_{G_i} be an arbitrary irreducible character of G_i in C_i (for $i = 1, 2, \ldots, n$), it is well-known that all irreducible characters of G, χ_G in C is defined as a tensor product of its corresponding characters, i.e., $\chi_G = \otimes_{i=1}^{n} \chi_{G_i}$ such that for each $g_i \in G_i$, expressed as follows:

$$\chi_G(g_1, g_2, \ldots, g_n) = \chi_{G_1}(g_1) \times \chi_{G_2}(g_2) \times \ldots \times \chi_{G_n}(g_n) \quad (1)$$

Because all the above irreducible characters in C are the product of real-valued characters so they are real numbers too, thus $C = C^Q$.

Case 2, there is k such that G_k is an unmatured group: In this situation, according to the above discussion and definition of maturity discriminant, there exists at least an irreducible character χ_{G_k} in C_k with a non-real value, therefore G should have at least an irreducible character χ_G in C with non-real value, so $C \neq C^Q$.

Similarly, the above discussion is valid for semi direct products and wreath products of finite groups, therefore, we summarize the results as the following theorem.

Main Theorem: (i) The direct product of the matured groups again is a matured group. But the direct product of at least one unmatured group is an unmatured group.

(ii) The semi direct product of the matured groups again is a matured group. But the semi direct product of at least one unmatured group is an unmatured group.

(iii) The wreath product of the matured groups again is a matured group. But the wreath product of at least one unmatured group is an unmatured group.

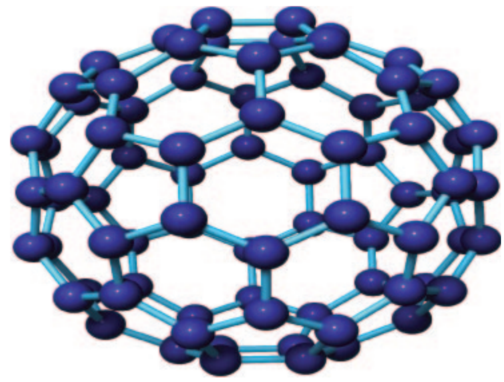

Figure 1. The big fullerene C_{80}.

The *Q*-Conjugacy Character Tables. The author presented an algorithm for computing symmetry of fullerenes.[23] The symmetry of the fullerene C_{80} is the direct product of C_2 and A_5 (i.e., $F = C_2 \times A_5$), where C_2 and A_5 are a cyclic group of order 2 and an alternating group on 5 letters, respectively (Figure 1). Since A_5 is an unmatured group, by our main theorem, F is an unmatured group.

GAP SYSTEM[24] is a group theory software package which is free and extendable. We run the following program at the GAP prompt to compute the character table and the set $SCSG$ of the symmetry of C_{80} as follows:

```
LogTo("Fullerene.txt");
    C2:=CyclicGroup(IsPermGroup,(2));
  A5:=AlternatingGroup(IsPermGroup,(5));
    F:=DirectProduct(c2,A5);
      CharC80:=CharacterTable(F);
      Order(F);IsPermGroup(F);
s:=ConjugacyClassesSubgroups(F);
      Sort("s");
Full:=List(ConjugacyClassesSubgroups(F),x->Elements(x));
  Len:=Length(Full); y:=[];
    for i in [1,2...Len]do
      if IsCyclic(Full[i][1])then Add(y,i);
        fi;
      od;
    Display(CharC80);
  Display(s);
        Print("CharC80", "\n");
    Print("Full", "\n");
Print("Fullerene.txt", "\n");
      LogTo( );
```

To denote the consecutive classes of elements of order n, 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. here x denotes an arbitrary conjugacy class. After running the program, symmetry of C_{80}, F has exactly 8 dominant classes as follow: $D_1 = 1a$, $D_2 = 2a$, $D_3 = 2b$, $D_4 = 2c$, $D_5 = 3a$, $D_6 = 5a \cup 5b$, $D_7 = 6a$, and $D_8 = 10a \cup 10b$, furthermore, D_6 and D_8 are unmatured dominant classes. Besides, a non-redundant set of cyclic subgroups of symmetry C_{80} contains the following elements: $G_1 = \mathrm{id}$, $G_2 = \langle(1,2)\rangle$, $G_3 = \langle(1,2)(4,5)(6,7)\rangle$, $G_4 = \langle(4,5)(6,7)\rangle$, $G_5 = \langle(5,6,7)\rangle$, $G_6 = \langle(3,4,5,6,7)\rangle$, $G_7 = \langle(5,6,7),(1,2)\rangle$, and $G_8 = \langle(3,4,5,6,7),(1,2)\rangle$. Therefore, by using the above calculations, we are able to calculate C^Q. See the Q-conjugacy character table of group $F = C_2 \times A_5$ stored in Table 1.

The f-NRG of tetranitrocubane, showed by Darafsheh et al.[25] which is $C_2 \sim S_4$, where S_4 is the symmetric group on four letters (Figure 2). Let W be the f-NRG of tetranitrocubane, i.e., $W = C_2 \sim S_4$. Remove W with F and add the following statements in the previous GAP program:

```
S4:=SymmetricGroup(IsPermGroup,(4));
    W:=WreathProduct(c2,s4);
```

Now, according to our main theorem W should be a matured group. Hence, we try to verify it. The non-redundant set of cyclic subgroups of symmetry W contains the following elements: $G_1 = \mathrm{id}$, $G_2 = \langle(1,2)\rangle$, $G_3 = \langle(1,2)(3,4)\rangle$, $G_4 = \langle(1,2)(3,4)(5,6)\rangle$, $G_5 = \langle(1,2)(3,4)(5,6)(7,8)\rangle$, $G_6 = \langle(5,7),(6,8)\rangle$, $G_7 = \langle(1,2)(5,7)(6,8)\rangle$, $G_8 = \langle(1,2)(3,4)(5,7)(6,8)\rangle$, $G_9 = \langle(1,5)(2,6)(3,7)(4,8)\rangle$, $G_{10} = \langle(3,7,5)(4,8,6)\rangle$, $G_{11} = \langle(5,6)(7,8),(5,7)(6,8)\rangle$, $G_{12} = \langle(1,2)(5,6),(1,5,2,6)(3,7)(4,8)\rangle$, $G_{13} = \langle(1,2)(3,4)(5,6)(7,8),(1,5,2,6)(3,7,4,8)\rangle$, $G_{14} = \langle(1,5,3,7)(2,6,4,8)\rangle$, $G_{15} = \langle(5,6)(7,8),(5,7,6,8)\rangle$, $G_{16} = \langle(5,6)(7,8),(1,2)(3,4)(5,7,6,8)\rangle$, $G_{17} = \langle(3,4)(5,6)(7,8),(3,7,5)(4,8,6)\rangle$, $G_{18} = \langle(1,2)(3,4)(5,6)(7,8),(3,7,5)(4,8,6)\rangle$, $G_{19} = \langle(1,2),(3,7,5)(4,8,6)\rangle$, and $G_{20} = \langle(1,2)(3,4)(5,6)(7,8),(1,5,3,7,26,4,8)\rangle$. Furthermore, the dominant classes of W are $K_1 = 1\mathrm{a}$, $K_2 = 2\mathrm{a}$, $K_3 = 2\mathrm{b}$, $K_4 = 2\mathrm{c}$, $K_5 = 2\mathrm{d}$, $K_6 = 2\mathrm{e}$, $K_7 = 2\mathrm{f}$, $K_8 = 2\mathrm{g}$, $K_9 = 2\mathrm{h}$, $K_{10} = 3\mathrm{a}$, $K_{11} = 4\mathrm{a}$, $K_{12} = 4\mathrm{b}$, $K_{13} = 4\mathrm{c}$, $K_{14} = 4\mathrm{d}$, $K_{15} = 4\mathrm{e}$, $K_{16} = 4\mathrm{f}$, $K_{17} = 6\mathrm{a}$, $K_{18} = 6\mathrm{b}$, $K_{19} = 6\mathrm{c}$, and $K_{20} = 8\mathrm{a}$ which are all matured dominate classes, thus $C = C^Q$, see Table 2.

Finally, we list some useful examples and verify our main theorem as follows.

Example 1: In terms of its circumference (q) and its length (p), an arbitrary polyhex nanotorus denoted $T\,[p,q]$, (Figures 3). To study maturity for $T\,[p,q]$, at first we need to assume the dihedral group of order $2p$, i.e. $D_{2p} = \langle x, y | x^p = y^2 = 1, xy = x^{-1}\rangle$ (the dihedral group of degree p).[26] It is clear that, the non-redundant set of cyclic subgroups of

Table 1. The Q-Conjugacy Character Table of Symmetry for Fullerene C_{80}

C^Q	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8
ϕ_1	1	1	1	1	1	1	1	1
ϕ_2	1	1	−1	−1	1	1	−1	−1
ϕ_3	6	−2	6	−2	0	−1	0	−1
ϕ_4	6	−2	−6	2	0	−1	0	1
ϕ_5	4	0	4	0	1	−1	1	−1
ϕ_6	4	0	−4	0	1	−1	−1	1
ϕ_7	5	1	5	1	−1	0	−1	0
ϕ_8	5	1	−5	−1	−1	0	1	0

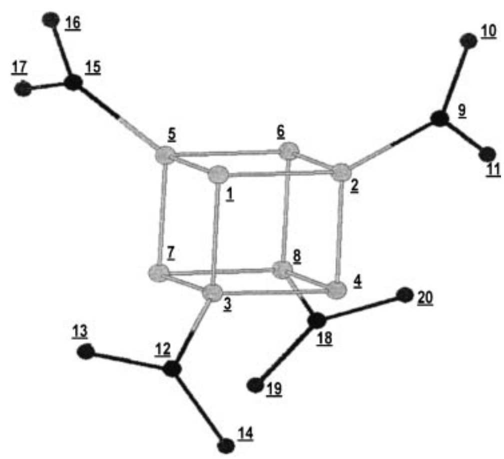

Figure 2. The structure of tetranitrocubane.

Table 2. The Q-Character Table for the Full Non-Rigid Group Tetranitrocubane

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}	K_{16}	K_{17}	K_{18}	K_{19}	K_{20}
X_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
X_2	1	−1	1	−1	1	1	−1	−1	1	1	−1	1	−1	−1	1	1	−1	−1	1	1
X_3	1	−1	1	1	−1	1	−1	1	1	1	−1	−1	1	−1	1	−1	1	1	1	−1
X_4	1	1	1	−1	−1	1	1	−1	1	1	1	−1	−1	1	1	−1	−1	−1	1	−1
X_5	2	0	2	−2	0	2	0	−2	2	−1	0	0	−2	0	2	0	1	1	−1	0
X_6	2	0	2	2	0	2	0	2	2	−1	0	0	2	0	2	0	−1	−1	−1	0
X_7	3	−1	−1	−3	1	3	−1	−3	3	0	1	1	1	−1	−1	1	0	0	0	−1
X_8	3	−1	−1	3	−1	3	−1	3	3	0	1	−1	−1	−1	−1	−1	0	0	0	1
X_9	3	1	−1	−3	−1	3	1	−3	3	0	−1	−1	1	1	−1	−1	0	0	0	1
X_{10}	3	1	−1	3	1	3	1	3	3	0	−1	1	−1	1	−1	1	0	0	0	−1
X_{11}	4	−2	0	−2	0	0	2	2	−4	1	0	2	0	0	0	−2	−1	1	−1	0
X_{12}	4	−2	0	2	0	0	2	−2	−4	1	0	−2	0	0	0	2	1	−1	−1	0
X_{13}	4	2	0	−2	0	0	−2	2	−4	1	0	−2	0	0	0	2	−1	1	−1	0
X_{14}	4	2	0	2	0	0	−2	−2	−4	1	0	2	0	0	0	−2	1	−1	−1	0
X_{15}	6	2	2	0	0	−2	2	0	6	0	0	0	0	−2	−2	0	0	0	0	0
X_{16}	6	−2	2	0	0	−2	−2	0	6	0	0	0	0	2	−2	0	0	0	0	0
X_{17}	6	0	−2	0	2	−2	0	0	6	0	0	−2	0	0	2	−2	0	0	0	0
X_{18}	6	0	−2	0	−2	−2	0	0	6	0	0	2	0	0	2	2	0	0	0	0
X_{19}	8	0	0	−4	0	0	0	4	−8	−1	0	0	0	0	0	0	1	−1	1	0
X_{20}	8	0	0	4	0	0	0	−4	−8	−1	0	0	0	0	0	0	−1	1	1	0

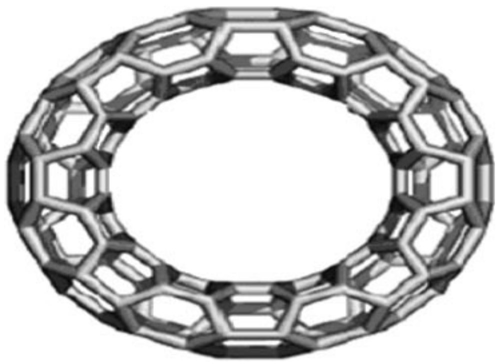

Figure 3. A polyhex nanotorus.

D_{2p} for prime p and $p \geq 3$, contains the following elements: $G_1 = \text{id}$, $G_2 = \langle \prod_{i=0}^{\frac{p-1}{2}} (2+i, p-i) \rangle$, $G_3 = \langle (1,2,3,\ldots,p) \rangle$ and $G_4 = D_{2p}$.

Let K_p be a dominant class of order p. Then, K_p is the union of $(p-1)/2$ conjugacy classes of elements order p in character table of D_{2p}. Therefore the reducible Q-conjugacy character χ of D_{2p} which is the sum of $(p-1)/2$ irreducible characters via degree 2 as follows:

$$\chi = \sum_{i=3}^{(p+3)/2} \chi_i \qquad (2)$$

Therefore, according to the previous section D_{2p} for prim p and $p \geq 3$, is an unmatured group. The symmetry of an arbitrary polyhex nanotorus has been defined as semi direct product of a dihedral group with C_2, see theorem in,[26] thus $C \neq C^Q$.

Example 2: 1,3,5-Triamino-2,4,6-trinitrobenzene with symmetry $L = S_2 \sim S_3$;[27] since for each n, the symmetric group S_n is a matured group, L must be a matured group.

Example 3: 2,3-Dimethylbutane with symmetry $K = (C_3 \times C_3 \times C_3 \times C_3){:}C_2$; hexamethylbenzene with symmetry $P = C_3 \sim D_6$; 1,4-dimethylbenzene with symmetry $X = C_2 \times (C_3 \sim C_2)$ and tetra-*tert*-butyltetrahedrane with symmetry $W = (C_3 \sim C_3) \sim S_4$.[28–31] Since C_3 is an unmatured group, K, P, X, and W are unmatured groups.

Example 4: Octanitrocubane with symmetry $O = C_2 \sim (S_4 \times C_2)$; water pentamer with symmetry $Z = S_2 \sim S_5$ and tetraammineplatinum(II) with symmetry $T = S_3 \sim (C_2 \times C_2)$.[21,32–34] Similarly, both S_n and C_2 are matured groups, thus, O, Z, and T should be matured groups.

Conclusion

We introduced a simple method to specify how a given finite group is matured or unmatured and verified with some examples like polyhex nanotorus: 1,3,5-triamino-2,4,6-trinitrobenzene, 2,3-dimethylbutane, hexamethylbenzene, 1,4-dimethylbenzene, tetra-*tert*-butyltetrahedrane, octanitrocubane, water pentamer, and tetraammineplatinum(II). Then, the Q-conjugacy character tables of the fullerene C_{80} and tetranitrocubane are verified.[35–37]

References

1 S. Fujita, *Symmetry and Combinatorial Enumeration in Chemistry*, Springer-Verlag, Berlin-Heidelberg, **1991**.
2 S. Fujita, *Bull. Chem. Soc. Jpn.* **1998**, *71*, 2071.
3 S. Fujita, *Bull. Chem. Soc. Jpn.* **1998**, *71*, 1587.
4 S. Fujita, *Bull. Chem. Soc. Jpn.* **1998**, *71*, 2309.
5 S. Fujita, *J. Math. Chem.* **1993**, *12*, 173.
6 S. Fujita, *MATCH* **2005**, *54*, 251.
7 S. Fujita, *MATCH* **2006**, *55*, 5.
8 S. Fujita, *MATCH* **2006**, *55*, 237.
9 S. Fujita, *MATCH* **2007**, *57*, 5.
10 S. Fujita, *Diagrammatical Approach to Molecular Symmetry and Enumeration of Stereoisomers*, MCM, Kragujevac, **2007**.
11 P. R. Bunker, P. Jensen, *Molecular Symmetry and Spectroscopy*, 2nd ed., NRC Research Press, Ottawa, **1998**.
12 J. Maruani, J. Serre, *Symmetries and Properties of Non-rigid Molecules*, Elsevier, Amsterdam, **1983**.
13 H. C. Longuet-Higgins, *Mol. Phys.* **1963**, *6*, 445.
14 J. T. Hougen, *J. Chem. Phys.* **1962**, *37*, 1433.
15 P. R. Bunker, D. Papoušek, *J. Mol. Spectrosc.* **1969**, *32*, 419.
16 J. K. G. Watson, *Can. J. Phys.* **1975**, *53*, 2210.
17 Y. G. Smeyers, *Adv. Quantum Chem.* **1992**, *24*, 1.
18 I. M. Isaacs, *Character Theory of Finite Groups*, Academic Press, New York, **1978**.
19 D. E. Littlewood, *The Theory of Group Characters and Matrix Representations of Groups*, 2nd ed., AMS Chelsea Publishing, Rhode Island, **2006**.
20 J. R. Dias, *Handbook of Polycyclic Aromatic Compounds*, *Part A*, Elsevier, New York, **1987**; *Handbook of Polycyclic Aromatic Compounds*, *Part B*, Elsevier, New York, **1988**.
21 A. Moghani, *J. Serb. Chem. Soc.* **2008**, *73*, 189.
22 M. R. Darafsheh, A. Moghani, *Bull. Chem. Soc. Jpn.* **2008**, *81*, 979.
23 A. Moghani, S. Naghdi, A. R. Ashrafi, A. Ahmadi, *London Math. Soc.* **2007**, *340*, 630.
24 *GAP: Groups, Algorithms and Programming*, http://www.gap-system.org, Lehrstuhl De für Mathematik, RWTH, Aachen, **1995**.
25 M. R. Darafsheh, Y. Farjami, A. R. Ashrafi, *MATCH* **2005**, *54*, 331.
26 M. Yavari, A. R. Ashrafi, *Int. J. Mol. Sci.* **2009**, in press.
27 K. Balasubramanian, *Chem. Phys. Lett.* **2004**, *398*, 15.
28 M. R. Darafsheh, A. R. Ashrafi, A. Darafsheh, *MATCH* **2007**, *58*, 47.
29 M. R. Darafsheh, A. R. Ashrafi, A. Darafsheh, *Chem. Phys. Lett.* **2006**, *421*, 566.
30 M. R. Darafsheh, A. Darafsheh, *MATCH* **2006**, *56*, 271.
31 M. R. Darafsheh, A. R. Ashrafi, A. Darafsheh, *Int. J. Quantum Chem.* **2005**, *105*, 485.
32 M. R. Darafsheh, Y. Farjami, A. R. Ashrafi, *MATCH* **2005**, *54*, 53.
33 K. Balasubramanian, *J. Phys. Chem. A* **2004**, *108*, 5527.
34 M. R. Darafsheh, Y. Farjami, A. R. Ashrafi, *Bull. Chem. Soc. Jpn.* **2005**, *78*, 996.
35 M. R. Darafsheh, A. Moghani, *J. Serb. Chem. Soc.* **2009**, *74*, 45.
36 M. R. Darafsheh, A. Moghani, S. Naghdi Sedeh, *Acta Chim. Slov.* **2008**, *55*, 602.
37 M. R. Darafsheh, A. Moghani, M. Karami, A. Zaeembashi, S. Naghdi, *Int. J. Chem. Model.* **2009**, in press.