Scientific paper

Group Theory for Tetramethylethylene, II

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Abstract

The maturated and unmaturated groups have been introduced by S. Fujita who used them in the markaracter table and the Q-conjugacy character table of a finite group. Fujita introduced more concise forms called the Q-conjugacy characters with integer-valued of the irreducible characters of finite groups and applied his results in this area of research to enumerate isomers of molecules. In this paper using GAP program all integer-valued characters of the full non-rigid group (f-NRG) of tetramethylethylene (2,3-dimethylbut-2-ene) is calculated by the Q-conjugacy relationships. It is shown that this group has 29 dominant classes (similarly, Q-conjugacy characters) such that 16 of them are unmaturated (similarly, Q-conjugacy characters such that they are the sum of two irreducible characters). Then the markaracter table and Q-conjugacy character table of the f-NRG of tetramethylethylene are derived for the first time.

Keywords: Full non-rigid group, markaracter table, Q-conjugacy character table, tetramethylethylene (2,3-dimethylbut-2-ene).

1. Introduction

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 S. Fujita who proposed not only markaracter tables, which enable us to discuss characters and marks on a common basis, but also Q-conjugacy character tables, 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 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. 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 non-redundant set of cyclic subgroups of G denoted by SCSG.[1–14]

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, dynamical NMR etc., all of which can be interpreted resorting to group theory. Group theory is one of the most powerful mathematical tools in quantum chemistry and spectroscopy. It can predict, interpret, and simplify complex theories and data. 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 described in the literature.[15–19] The molecular symmetry group of a non-rigid molecule was

first defined by Longuet-Higgins[20] although there have been earlier works that suggested the need for such a framework by Hougen.[21] Bunker and Papoušek[22] 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.[23] 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.[24] Calculating the f-NRGs using wreath product formalism was first introduced by Balasubramanian. He also computed the character table of non-rigid groups under consideration.[25–27]

The present study investigates the Q-conjugacy character tables of tetramethylethylene (Figure 1), the f-NRG of which has been previously introduced.[29] In order to derive all of its integer-valued characters, it is shown that its unmaturated group has 16 row- and column-reductions in its character table. The reader is encouraged to consult references[26–32] for background materials. The notation we use is standard and mainly taken from references.[33–34]

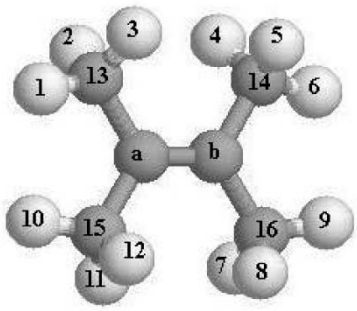

Figure 1. Geometry of Tetramethylethylene (2,3-Dimethylbut-2-ene)

2. Results and Discussion

In this section we first describe some notation. 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 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 the following holds: $(xg)g' = x(gg')$ and $x1 = x$, for each g, $g' \in G$ and $x \in X$. Now let it is 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_1} and the corresponding partition of G into these cosets: $G = H_{g_1} + H_{g_2} + \ldots + H_{g_m}$

For any $g \in G$, the set of all permutations

$$G(/H)_g = \begin{pmatrix} Hg_1 & Hg_2 & \ldots & Hg_m \\ Hg_1g & Hg_2g & \ldots & Hg_mg \end{pmatrix}$$

constructs a permutation representation of G, which is called a coset representation of G by H denoted by G(/H). The degree of G(/H) is $|G| / |H|$, where $|G|$ is the number of elements in G. Obviously, the coset representation G(/H) is transitive, i.e. has just one orbit.[1] 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. 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 $N : M \cong M \times N$.

Let K and H be groups and suppose H acts on the set Γ. Then the wreath product of K by H, denoted by $K \sim H$ is defined to be the semi direct product $K^{\Gamma} : H$ such that $K^{\Gamma} = \{f \mid f: \Gamma \rightarrow K\}$, see references[33–34] for more details.

Let C be a u × u matrix of character table of G. Then, C is transformed into a more concise form called the Q-conjugacy character table that we denote its s × s matrix by C^Q ($s \leq u$) as follows: If u = s, then $C = C^Q$ i.e. G is a maturated 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, …, 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.

It has been shown that the f-NRG of tetramethylethylene is a wreath product of the cyclic group of order three with direct product of two copies of cyclic group of order two,[29] i.e. $C_3 \sim (C_2 \times C_2)$ as follow:

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: $A_1 = \langle (1, 2, 3) \rangle$, $A_2 = \langle (4, 5, 6) \rangle$, $A_3 = \langle (7,8,9) \rangle$, $A_4 = \langle (10,11,12) \rangle$, where A_1, A_2, A_3 and A_4 are the symmetry groups of the CH_3 whose carbon atom is marked as 13, 14, 15 and 16, respectively. Let T be the f-NRG of tetramethylethylene, therefore T has the following structure: $T = (A_1 \times A_2 \times A_3 \times A_4) : V$, where V = {id, (13, 14)(15, 16)(a, b), (13, 16)(14, 15)(a, b), (13, 15)(14, 16)(a, b)} is the Klein's four group, so it is obvious that every element of T is as a vector (a_1, a_2, a_3, a_4, v) such that $a_i \in G_i$ and $v \in V$, i.e. T can be written in terms of wreath product $T = C_3 \sim (C_2 \times C_2)$. Now, the computations of the symmetry properties of molecules were carried out with the aid of GAP SYSTEM,[35] a group theory software package which is free and extendable. We run the following

Table 1: The Markaracter Table for Tetramethylethylene

M^C	G_1	G_2	G_3	G_4	G_5	G_6	G_7	G_8	G_9	G_{10}	G_{11}	G_{12}	G_{13}	G_{14}	G_{15}
$T(/G_1)$	324	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_2)$	162	18	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_3)$	162	0	18	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_4)$	162	0	0	18	0	0	0	0	0	0	0	0	0	0	0
$T(/G_5)$	108	0	0	0	54	0	0	0	0	0	0	0	0	0	0
$T(/G_6)$	108	0	0	0	0	54	0	0	0	0	0	0	0	0	0
$T(/G_7)$	108	0	0	0	0	0	54	0	0	0	0	0	0	0	0
$T(/G_8)$	108	0	0	0	0	0	0	27	0	0	0	0	0	0	0
$T(/G_9)$	108	0	0	0	0	0	0	0	27	0	0	0	0	0	0
$T(/G_{10})$	108	0	0	0	0	0	0	0	0	54	0	0	0	0	0
$T(/G_{11})$	108	0	0	0	0	0	0	0	0	0	54	0	0	0	0
$T(/G_{12})$	108	0	0	0	0	0	0	0	0	0	0	27	0	0	0
$T(/G_{13})$	108	0	0	0	0	0	0	0	0	0	0	0	108	0	0
$T(/G_{14})$	108	0	0	0	0	0	0	0	0	0	0	0	0	54	0
$T(/G_{15})$	108	0	0	0	0	0	0	0	0	0	0	0	0	0	27
$T(/G_{16})$	108	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{17})$	108	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{18})$	108	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{19})$	108	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{20})$	108	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{21})$	54	6	0	0	0	0	0	0	0	0	27	0	0	0	0
$T(/G_{22})$	54	18	0	0	0	0	0	0	0	0	0	0	0	27	0
$T(/G_{23})$	54	0	18	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{24})$	54	0	6	0	0	0	27	0	0	0	0	0	0	0	0
$T(/G_{25})$	54	0	0	6	0	27	0	0	0	0	0	0	0	0	0
$T(/G_{26})$	54	0	0	18	0	0	0	0	0	27	0	0	0	0	0
$T(/G_{27})$	54	6	0	0	0	0	0	0	0	0	0	0	54	0	0
$T(/G_{28})$	54	18	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{29})$	54	0	0	6	0	0	0	0	0	0	0	0	54	0	0

M^C	G_{16}	G_{17}	G_{18}	G_{19}	G_{20}	G_{21}	G_{22}	G_{23}	G_{24}	G_{25}	G_{26}	G_{27}	G_{28}	G_{29}
$T(/G_1)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_2)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_3)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_4)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_5)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_6)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_7)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_8)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_9)$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{10})$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{11})$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{12})$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{13})$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{14})$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{15})$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{16})$	108	0	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{17})$	0	108	0	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{18})$	0	0	108	0	0	0	0	0	0	0	0	0	0	0
$T(/G_{19})$	0	0	0	27	0	0	0	0	0	0	0	0	0	0
$T(/G_{20})$	0	0	0	0	27	0	0	0	0	0	0	0	0	0
$T(/G_{21})$	0	0	0	0	0	3	0	0	0	0	0	0	0	0
$T(/G_{22})$	0	0	0	0	0	0	9	0	0	0	0	0	0	0
$T(/G_{23})$	54	0	0	0	0	0	0	18	0	0	0	0	0	0
$T(/G_{24})$	0	0	0	0	0	0	0	0	3	0	0	0	0	0
$T(/G_{25})$	0	0	0	0	0	0	0	0	0	3	0	0	0	0
$T(/G_{26})$	0	0	0	0	0	0	0	0	0	0	9	0	0	0
$T(/G_{27})$	0	0	0	0	0	0	0	0	0	0	0	6	0	0
$T(/G_{28})$	0	0	54	0	0	0	0	0	0	0	0	0	18	0
$T(/G_{29})$	0	0	0	0	0	0	0	0	0	0	0	0	0	6

Table 2: The Q-Conjugacy Character Table for Tetramethylethylene

C^Q	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	D_{10}	D_{11}	D_{12}	D_{13}	D_{14}	D_{15}
T_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
T_2	1	1	–1	–1	1	1	1	1	1	1	1	1	1	1	1
T_3	1	–1	1	–1	1	1	1	1	1	1	1	1	1	1	1
T_4	1	–1	–1	1	1	1	1	1	1	1	1	1	1	1	1
T_5	2	2	2	2	–1	–1	2	–1	2	–1	2	–1	2	–1	–1
T_6	2	2	–2	–2	–1	–1	2	–1	2	–1	2	–1	2	–1	–1
T_7	2	–2	2	–2	–1	–1	2	–1	2	–1	2	–1	2	–1	–1
T_8	2	–2	–2	2	–1	–1	2	–1	2	–1	2	–1	2	–1	–1
T_9	2	0	–2	0	–1	2	–1	–1	2	2	–1	–1	–1	2	–1
T_{10}	2	0	2	0	–1	2	–1	–1	2	2	–1	–1	–1	2	–1
T_{11}	2	–2	0	0	–1	–1	2	2	–1	2	–1	–1	–1	–1	2
T_{12}	2	2	0	0	–1	–1	2	2	–1	2	–1	–1	–1	–1	2
T_{13}	2	0	0	–2	–1	2	–1	2	–1	–1	–1	2	2	–1	–1
T_{14}	2	0	0	2	–1	2	–1	2	–1	–1	–1	2	2	–1	–1
T_{15}	4	0	–4	0	1	–2	–2	1	4	–2	–2	1	–2	–2	1
T_{16}	4	0	4	0	1	–2	–2	1	4	–2	–2	1	–2	–2	1
T_{17}	4	–4	0	0	1	1	4	–2	–2	–2	–2	1	–2	1	–2
T_{18}	4	4	0	–4	1	1	4	–2	–2	–2	–2	1	–2	1	–2
T_{19}	4	0	0	4	1	–2	–2	–2	–2	1	–2	–2	4	1	1
T_{20}	4	0	0	0	1	–2	–2	–2	–2	1	–2	–2	4	1	1
T_{21}	4	0	0	0	1	–2	–2	–2	–2	4	1	1	1	–2	–2
T_{22}	4	0	0	0	1	–2	–2	4	1	–2	1	–2	–2	1	–2
T_{23}	4	0	0	0	1	4	1	–2	–2	–2	1	–2	–2	–2	1
T_{24}	8	0	0	0	–1	2	–4	2	–4	–4	2	–1	2	2	2
T_{25}	8	0	0	0	–1	2	–4	–4	2	2	2	2	–4	–1	2
T_{26}	8	0	0	0	–1	–4	2	2	–4	2	2	2	–4	2	–1
T_{27}	8	0	0	0	5	2	2	2	2	2	–1	–1	2	–1	–1
T_{28}	8	0	0	0	–1	–4	2	–4	2	–4	–1	2	2	2	2
T_{29}	8	0	0	0	–4	2	2	2	2	2	–1	–1	2	–1	–1

C^Q	D_{16}	D_{17}	D_{18}	D_{19}	D_{20}	D_{21}	D_{22}	D_{23}	D_{24}	D_{25}	D_{26}	D_{27}	D_{28}	D_{29}
T_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
T_2	1	1	1	1	1	1	1	1	–1	–1	–1	–1	–1	–1
T_3	1	1	1	1	1	–1	–1	–1	1	1	1	–1	–1	–1
T_4	1	1	1	1	1	–1	–1	–1	–1	–1	–1	1	1	1
T_5	–1	–1	2	2	2	–1	–1	2	–1	–1	2	–1	–1	2
T_6	–1	–1	2	2	2	–1	–1	2	1	1	–2	1	1	–2
T_7	–1	–1	2	2	2	1	1	–2	–1	–1	2	1	1	–2
T_8	–1	–1	2	2	2	1	1	–2	1	1	–2	–1	–1	2
T_9	2	–1	2	–1	2	0	0	0	1	–2	1	0	0	0
T_{10}	2	–1	2	–1	2	0	0	0	–1	2	–1	0	0	0
T_{11}	2	–1	–1	2	2	1	–2	1	0	0	0	0	0	0
T_{12}	2	–1	–1	2	2	–1	2	–1	0	0	0	0	0	0
T_{13}	2	–1	2	2	–1	0	0	0	0	0	0	1	–2	1
T_{14}	2	–1	2	2	–1	0	0	0	0	0	0	–1	2	–1
T_{15}	–2	1	4	–2	4	0	0	0	–1	2	2	0	0	0
T_{16}	–2	1	4	–2	4	0	0	0	1	–2	–2	0	0	0
T_{17}	–2	1	–2	4	4	–1	2	2	0	0	0	0	0	0
T_{18}	–2	1	–2	4	4	1	–2	–2	0	0	0	0	0	0
T_{19}	–2	1	4	4	–2	0	0	0	0	0	0	–1	2	2
T_{20}	–2	1	4	4	–2	0	0	0	0	0	0	1	–2	–2
T_{21}	4	1	–2	–2	4	0	0	0	0	0	0	0	0	0
T_{22}	4	1	–2	4	–2	0	0	0	0	0	0	0	0	0
T_{23}	4	1	4	–2	–2	0	0	0	0	0	0	0	0	0
T_{24}	–4	–1	–4	–4	8	0	0	0	0	0	0	0	0	0
T_{25}	–4	–1	–4	8	–4	0	0	0	0	0	0	0	0	0
T_{26}	–4	–1	8	–4	–4	0	0	0	0	0	0	0	0	0
T_{27}	–4	–4	–4	–4	–4	0	0	0	0	0	0	0	0	0
T_{28}	8	–1	–4	–4	–4	0	0	0	0	0	0	0	0	0
T_{29}	–4	5	–4	–4	–4	0	0	0	0	0	0	0	0	0

program at the GAP prompt to compute the mark table, the character table and the set SCSG of the f-NRG of tetramethylethylene.

```
        LogTo("Calculations.txt");
C2:=CyclicGroup(2);
        D:=DirectProduct(C2,C2);
                C3=CyclicGroup(3);
                        T:=WreathProduct(C3,D);
                        Char:= CharacterTable(T);
                Order(T);IsPermGroup(T);
        U:=ConjugacyClassesSubgroups(T);
                Sort("U");
        mark:=TableOfMarks(T);
        V:=List(ConjugacyClassesSubgroups(T),x->Elements(x));
                        Len:=Length(V); y:=[];
                for i in [1..Len]do
                if IsCyclic(V[i][1])then Add(y,i);
                                fi;
                od;
                Display(Char);
        Display(s);
                        Display(mark);
                Print("Char", "\n");
Print("V", "\n");
                Print("mark", "\n");
                Print("Calculations.txt", "\n");
LogTo( );
```

After running the program, the following elements belong to the non-redundant set of cyclic subgroups of T: G_1 = id, G_2 = <(1, 7)(2, 8)(3, 9)(4, 10)(5, 11)(6, 12)>, G_3 = <(1, 10)(2, 11)(3, 12)(4, 7)(5, 8)(6, 9)>, G_4 = <(1, 4)(2, 5)(3, 6)(7, 10)(8, 11)(9, 12)>, G_5 = <(1, 2, 3)(4, 6, 5)(7, 9, 8)(10, 11, 12)>, G_6 = <(1, 2, 3)(4, 5, 6)(7, 9, 8)(10, 12, 11)>, G_7 = <(1, 2, 3)(4, 6, 5)(7, 8, 9)(10, 12, 11)>, G_8 = <(1, 2, 3)(4, 5, 6)(7, 8, 9)(10, 11, 12)>, G_9 = <(7, 8, 9)(10, 11, 12)>, G_{10} = <(4, 5, 6)(7, 9, 8)>, G_{11} = <(4, 5, 6)(10,12,11)>, G_{12} = <(4, 5, 6)(7, 8, 9)>, G_{13} = <(7, 8, 9)(10, 12, 11)>, G_{14} = <(4, 5, 6)(10, 11, 12)>, G_{15} = <(4, 5, 6)(7, 9, 8)(10, 11, 12)>, G_{16} = <(4, 5, 6)(7, 8, 9)(10, 11, 12)>, G_{17} = <(4, 5, 6)(7, 8, 9)(10, 12, 11)>, G_{18} = <(1, 2, 3)(4, 5, 6)(7, 8, 9)(10, 12, 11)>, G_{19} = <(10, 11, 12)>, G_{20} = <(4, 5, 6)(7, 9, 8)(10, 12, 11)>, G_{21} = <(1, 2, 3)(4, 5, 6)(7, 9, 8)(10, 12, 11), (1, 4)(2, 5)(3, 6)(7,10)(8,11)(9, 12)>, G_{22} = <(1, 2, 3)(4, 6, 5)(7, 8, 9)(10, 12, 11), (1, 7)(2, 8)(3, 9)(4, 10)(5, 11)(6, 12)>, G_{23} = <(1, 2, 3)(4, 6, 5)(7, 9, 8)(10, 11, 12), (1, 10)(2, 11)(3, 12)(4, 7)(5, 8)(6, 9)>, G_{24} = <(1, 2, 3)(4, 5, 6)(7, 8, 9)(10, 11, 12), (1, 4)(2, 5)(3, 6)(7, 10)(8, 11)(9, 12)>, G_{25} = <(1, 2, 3)(4, 5, 6)(7, 8, 9)(10, 11, 12), (1, 10)(2, 11)(3, 12)(4, 7)(5, 8)(6, 9)>, G_{26} = <(1, 2, 3)(4, 5, 6)(7, 8, 9)(10, 11, 12), (1, 7)(2, 8)(3, 9)(4, 10)(5, 11)(6, 12)>, G_{27} = <(4, 5, 6)(7, 8, 9), (1, 10)(2, 11)(3, 12)(4, 7)(5, 8)(6, 9)>, G_{28} = <(4, 5, 6)(10, 11, 12), (1, 7)(2, 8)(3, 9)(4, 10)(5, 11)(6, 12)> and G_{29} = <(7, 8, 9)(10, 11, 12), (1, 4)(2, 5)(3, 6)(7, 10)(8, 11)(9, 12)>.

See M^C the markaracter table of tetramethylethylene which is derived from $M_{174 \times 174}$, the mark table of T in Table 1. Besides, we can see that T has exactly 29 dominant classes as follow:

D_1 = 1a, D_2 = 2a, D_3 = 2b, D_4 = 2c, D_5 = 3a∪3b, D_6 = 3c∪3e, D_7 = 3d, D_8 = 3f∪3n, D_9 = 3g, D_{10} = 3h∪3q, D_{11} = 3i∪3s, D_{12} = 3j∪3r, D_{13} = 3k, D_{14} = 3l∪3p, D_{15} = 3m∪3o, D_{16} = 3t∪3z, D_{17} = 3u∪3y, D_{18} = 3v, D_{19} = 3w, D_{20} = 3x, D_{21} = 6a∪6b, D_{22} = 6c∪6e, D_{23} = 6d, D_{24} = 6f∪6g, D_{25} = 6h∪6j, D_{26} = 6i, D_{27} = 6k∪6l, D_{28} = 6m∪6o, D_{29} = 6n such that the dominant classes D_i for i ∈ {5, 6, 8, 10, 11, 12, 14, 15, 16, 17, 21, 22, 24, 25, 27, 28} are unmaturated which shows 16 column-reductions (similarly, row-reductions) in $C_{45\times45}$, the character table of T = C_3 ~ (C_2 × C_2) in the reference.[29] There are sixteen unmaturated integer-valued characters in C^Q the Q-conjugacy character table of T with the sum of two irreducible characters via same degrees. All integer-valued characters of tetramethylethylene are presented in Table 2.

3. Conclusions

In this paper using GAP program all integer-valued characters of the f-NRG of tetramethylethylene are calculated by the Q-conjugacy relationships. It is shown that this group has 29 dominant classes (similarly, Q-conjugacy characters) such that 16 of them are unmaturated (similarly, Q-conjugacy characters such that they are the sum of two irreducible characters) and the complete Q-conjugacy character table and the markaracter table of this group is computed successfully. The derived markaracter table and Q-conjugacy character table would also be valuable in other applications such as in the context of chemical applications of graph theory and aromatic compounds.[14–22]

Furthermore, we introduce the following conjecture.

Conjecture. Let G_i be a finite group for i = 1, …, n and W = G_1 ~ G_2 ~ …. ~ G_n. If there exists k ∈ {1, …, n} such that G_k is an unmaturated group, then W is an unmaturated group too.

4. References

1. S. Fujita, *Symmetry and Combinatorial Enumeration in Chemistry*; Springer-Verlag: Berlin-Heidelberg, **1991**.
2. S. Fujita, *Theor. Chim. Acta* **1995**, *91*, 291–314.
3. S. Fujita, *Bull. Chem. Soc. Jpn.* **1998**, *71*, 1587–1596.
4. S. Fujita, *J. Graph Theory* **1994**, *18*, 349–371.
5. S. Fujita, *Bull. Chem. Soc. Jpn.* **1998**, *71*, 2071–2080.
6. S. Fujita, *Bull. Chem. Soc. Jpn.* **1998**, *71*, 2309–2321.
7. S. Fujita, *J. Math. Chem.* **1990**, *5*, 121–156.
8. S. Fujita, *J. Math. Chem.* **2002**, *30*, 249–270.
9. S. Fujita, *J. Math. Chem.* **1999**, *12*, 173–195.
10. S. Fujita, *MATCH Commun. Math. Comput. Chem.* **2005**, *54*, 251–300.

11. S. Fujita, *MATCH Commun. Math. Comput. Chem.* **2006**, *55*, 5–38.
12. S. Fujita, *MATCH Commun. Math. Comput. Chem.* **2006**, *55*, 237–270.
13. S. Fujita, *MATCH Commun. Math. Comput. Chem.* **2007**, *57*, 5–48.
14. S. Fujita, *Diagrammatical Approach to Molecular Symmetry and Enumeration of Stereoisomers*, MCM, Kragujevac, **2007**.
15. P. R. Bunker, P. Jensen, *Molecular Symmetry and Spectroscopy*, NRC Research Press, Ottawa, **1998**.
16. S. L. Altmann, *Induced Representation in Crystal & Molecules*, Academic Press, London, **1977**.
17. J. Maruani, J. Serre, *Symmetries and Properties of Non-rigid Molecules*, Elsevier, Amsterdam, **1983**.
18. Y. G. Smeyers, M. L. Senent, V. Botella, D. C. Moule, *J. Chem. Phys.* **1993**, *98*, 2754–2767.
19. A. van der Avoird, *J. Chem. Phys.* **1993**, *98*, 5327–5336.
20. H. C. Longuet-Higgins, *Mol. Phys.* **1963**, *6*, 445–460.
21. J. T. Hougen, *J. Chem. Phys.* **1962**, *37*, 1433–1441.
22. P. R. Bunker, D. Papoušek, *J. Mol. Spectrosc.* **1969**, *32*, 419–429.
23. J. K. G. Watson, *Cand. J. Phys.* **1975**, *53*, 2210–2220.
24. Y. G. Smeyers, *Adv. Quantum Chem.* **1992**, *24*, 1–77.
25. K. Balasubramanian, *J. Chem. Phys*. **1980**, *72*, 665–677.
26. K. Balasubramanian, *J. Phys. Chem. A*. **2004**, *108*, 5527–5536.
27. K. Balasubramanian, *Chem. Phys. Letters*. **2007**, *441*, 29–38.
28. M. R. Darafsheh, A. Darafsheh, A. R. Ashrafi, *Int. J. Quantum Chem.* **2007**, *107*, 340–344.
29. M. R. Darafsheh, A. R. Ashrafi, A. Darafsheh, *Acta Chim. Slov.* **2005**, *52*, 282–287.
30. M. R. Darafsheh, A. R. Ashrafi, A. Darafsheh, *Chem Phys Letters.* **2006**, *421*, 566–570.
31. M. R. Darafsheh, A. R. Ashrafi, A. Darafsheh, *MATCH Commun. Math. Comput. Chem.* **2007**, *58*, 47–56.
32. M. R. Darafsheh, A. Darafsheh, *MATCH Commun. Math. Comput. Chem.* **2006**, *56*, 271–278.
33. I. M. Isaacs, *Character Theory of Finite Groups*, Academic Press, New York, **1978**.
34. D. E. Littlewood, *The theory of group characters and matrix representations of groups*, AMS Chelsea publishing, Rhode Island, **2006**.
35. M. Schönert, H. U. Besche, Th. Breuer, F. Celler, B. Eick, V. Felsch, A. Hulpke, J. Mnich, W. Nickel, G. Pfeiffer, U. Polis, H. Theißen, A. Niemeyer, *GAP, Groups, Algorithms and Programming*, Lehrstuhl für Mathematik, RWTH: Aachen, **1995**.

Povzetek

Zrele in nezrele grupe je S. Fujita vpeljal v tabele markarakterjev in Q-konjugiranosti končnih grup. Fujita je vpeljal tudi bolj zgoščene oblike, imenovane Q-konjugacijski karakterji s celoštevilčnimi vrednostmi nereducibilnih karakterjev končnih grup ter uporabil svoje rezultate za oštevilčenje izomerov molekul.
V tem prispevku z uporabo programskega paketa GAP in z upoštevanjem odnosov med Q-konjugiranostjo izračunamo vse celoštevilčne karakterje popolne netoge grupe (f-NRG) tetrametiletilena (2,3-dimetilbut-2-en). Pokažemo tudi, da ima ta grupa 29 dominantnih razredov (oz. Q-konjugacijskih karakterjev) in sicer tako, da jih je 16 nezrelih (Q-konjugacijski karakterji so taki, da so vsota dveh nereducibilnih karakterjev). Nato kot prvi izpeljemo tabelo markarakterjev in Q-konjugacijskih karakterjev za f-NRG tetrametiletilena.