



www.shd.org.yu

J. Serb. Chem. Soc. 73 (2) 189–195 (2008)

JSCS–3701

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

UDC 519.17:547.233'237+546.922:547.97

Original scientific paper

Q-Conjugacy character and Markaracter tables of tetraammineplatinum(II)

ALI MOGHANI*

Department of Color Physics, Institute for Colorants, Paints and Coatings (ICPC), Tehran, Iran

(Received 7 May, revised 8 June 2007)

Abstract: The Q-conjugacy character and Markaracter tables of finite groups were introduced by Fujita, who applied his results in this area of research to enumerate isomers of molecules. In this paper, these tables are computed for tetraammineplatinum(II).

Keywords: Q-conjugacy character table; tetraammineplatinum(II); pigments.

INTRODUCTION

The enumeration of chemical compounds has been accomplished by various methods.^{1–3}

The Pólya–Redfield theorem is a standard method for combinatorial enumerations of graphs, polyhedra and chemical compounds. Only finite groups are treated throughout this paper. The notation is standard and mainly taken from Ref. 4 and the papers by Fujita.^{5–17}

For the sake of completeness, some necessary definitions are mentioned below.

Definition 1. Let G be a finite group and $h_1, h_2 \in G$. If there exists $t \in G$ such that $t^{-1} < h_1 > t = \langle h_2 \rangle$, then h_1, h_2 are said to be Q-conjugate and are denoted by $h_1 \sim_Q h_2$.

It is easy to see that the Q-conjugacy is an equivalence relation and generates equivalence classes which are called dominant classes, *i.e.*, the group G is partitioned into dominant classes as follows: $G = K_1 + K_2 + \dots + K_s$.

Definition 2. A permutation representation P of a finite group G is obtained when the group G acts on a finite set $X = \{x_1, x_2, \dots, x_t\}$ from the right, which means that one is given a mapping $P: X \times G \rightarrow X$ 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 one is given an action P of G on X and a subgroup H of G . One considers the set of its right cosets Hg_i and the corresponding partition of G into these cosets: $G = Hg_1 + Hg_2 + \dots + Hg_m$. If the cosets from the right are multiplied by a group element g , these cosets are permuted, in fact one

* E-mail: moghani@icrc.ac.ir

doi: 10.2298/JSC0802189M

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. When H and H' are conjugate subgroups of G then the induced or coset-representations $G/(H)$ and $G/(H')$ are equivalent.

Recalling from the theory of group actions that the sets $xG = \{xg \mid g \in G\}$, the orbits, form a set partition of X and that the action is called transitive if there is exactly one such orbit. Fujita⁶⁻¹¹ introduced the notations SSG_G and $SCSG_G$. A group contained in $SCSG_G$ is called a dominant subgroup. Any action of G on X induces the set partition of X into its orbits, *i.e.*, into transitive permutation representations. Moreover it can easily be seen that a complete set of pairwise inequivalent transitive permutation representations is formed by the set $\{G/(G_1), \dots, G/(G_r)\}$. Thus each permutation is a unique linear combination $P = \sum \alpha_i G/(G_i)$ (*). The multiplicities α_i can be obtained by using the table of marks introduced by Burnside.¹²⁻¹⁷

Definition 3. The table of marks of G is the matrix $M(G) = (m_{ik}), \{1 \leq i, k \leq r\}$, where m_{ik} is the number of right cosets of G_k in G which remain fixed under right multiplication by the elements of G_i , $m_{ik} = |\{G_k \mid \text{for all } s \in G_i : G_k s = G_k\}|$.¹⁸ If $M(G)$ is restricted to rows and columns that belong to cyclic groups, the Markaracter table of G^9 is obtained and denote it by M^C .

Definition 4. Let H be a cyclic subgroup of G , the maturity of a finite group G is defined by examining how a dominant class (Q-conjugacy class) corresponding to H contains conjugacy classes. If the integer $m(H) = |N_G(H)|/|C_G(H)|$ (called the maturity discriminant) is less than $\varphi(|H|)$ where φ is the Euler function, the group G is concluded to be unmatured concerning H , where $N_G(H)$ and $C_G(H)$ denote the normalizer and centralizer of H within G , respectively.

Corollary 5. Let H be a cyclic group of G , the dominant class $K \cap H$ in the normalizer $N_G(H)$ is the union of $t = \varphi(|H|)/m(H)$ conjugacy classes of G , see Refs. 12-17.

Definition 6. Let $C_{u \times u}$ be the matrix of the character table of G . $C_{u \times u}$ is transformed to a more concise form called the Q-conjugacy character table, the $s \times s$ -matrix of which is denoted by $C^Q(s \leq u)$ as follows: if $u = s$ then $C = C^Q$, *i.e.*, G is a maturated group. Otherwise $s < u$, according to Corollary 5 and Definition 2, since the dimension of the Q-conjugacy character table is equal to that of the corresponding Markaracter table¹² for each $G_i \in SCSG_G$ and the corresponding dominant class K_i , where $i = 1, \dots, s$.

If $t = 1$ (K_i is exactly a conjugacy class), then there is no reduction in row and column of C but if $t > 1$ (K_i is a union of t conjugacy classes of G , *i.e.*, reduction in column), then the sum of the t -rows of irreducible characters, *via* the same degree in C (reduction in rows), give one a reducible character, which are called Q-conjugacy characters in both cases. See Section 2.2 of Ref. 12 and in the special case (Q-conjugacy characters of cyclic groups) Ref. 5 for more details.

COMPUTATIONAL METHOD AND DISCUSSION

Here, a free software package for group theory, named GAP (Groups, Algorithms and Programming), which greatly facilitates these calculations (see <http://www.gap-system.org>), should be brought to the attention of the spectroscopy community. For example, the table of marks of any finite group G is afforded by the following command: "TableOfMarks(G)".

The full, non-rigid group and symmetry properties of tetraammineplatinum(II) of order 5184 with C_{2v} and C_{4v} point groups were computed.^{19,20}

Let G be the symmetry group of tetraammineplatinum(II) (see Fig. 1), then by the following program in GAP:

```
gap>G:=Group((2,3,4,5)(6,9,12,15,7,10,13,16,8,11,14,17),(2,3,4,5)(6,9,12,15,7,10,13,17,8,11,14,16),(2,5)(3,4)(6,15)(7,17)(8,16)(9,12)(10,14)(11,13));
gap> t:=TableOfMarks(G); Sort("t");
gap> c:=CharacterTable(G);
gap>Display(t); Display(c);
```

one obtains the mark and the character tables of tetraammineplatinum(II), hence its $SCSG_G$ can be calculated as follows:

$$SCSG_G = \{G_1 = \text{id}, G_2 = \langle (6,7,8)(9,11,10)(12,14,13)(15,16,17) \rangle,$$

$$G_3 = \langle (9,11,10)(15,16,17) \rangle, G_4 = \langle (12,14,13)(15,17,16) \rangle,$$

$$G_5 = \langle (6,7,8)(9,11,10)(12,13,14) \rangle, G_6 = \langle (15,16,17) \rangle, G_7 = \langle (6,7,8)(9,11,10)(12,14,13)(15,17,16) \rangle,$$

$$G_8 = \langle (9,11,10)(15,16,17), (6,7,8)(9,11,10)(12,14,13)(15,16,17) \rangle,$$

$$G_9 = \langle (12,14,13)(15,17,16), (6,7,8)(9,11,10)(12,14,13)(15,16,17) \rangle,$$

$$G_{10} = \langle (12,14,13)(15,17,16), (9,11,10)(15,16,17) \rangle,$$

$$G_{11} = \langle (12,14,13)(15,17,16), (6,7,8)(9,10,11)(12,14,13)(15,17,16) \rangle,$$

$$G_{12} = \langle (6,7,8)(9,11,10)(12,13,14), (9,11,10)(15,16,17) \rangle,$$

$$G_{13} = \langle (15,16,17), (6,7,8)(9,11,10)(12,14,13)(15,16,17) \rangle,$$

$$G_{14} = \langle (15,16,17), (9,11,10)(15,16,17) \rangle, G_{15} = \langle (15,16,17), (6,8,7)(12,13,14) \rangle,$$

$$G_{16} = \langle (15,16,17), (12,14,13)(15,17,16) \rangle,$$

$$G_{17} = \langle (15,16,17), (9,11,10)(15,16,17), (6,7,8)(9,11,10)(12,14,13)(15,16,17) \rangle,$$

$$G_{18} = \langle (15,16,17), (12,14,13)(15,17,16), (6,7,8)(9,11,10)(12,14,13)(15,16,17) \rangle,$$

$$G_{19} = \langle (12,13,14), (9,11,10)(12,14,13), (6,7,8)(9,10,11)(12,14,13)(15,16,17), (12,14,13)(15,17,16), (2,4)(3,5)(6,12,7,13,8,14)(9,15,10,16,11,17) \rangle,$$

$$G_{20} = \langle (12,14,13)(15,17,16), (6,7,8)(9,10,11)(12,14,13)(15,17,16), (2,4)(3,5)(6,12,7,13,8,14)(9,15,10,16,11,17) \rangle,$$

$$G_{21} = \langle (15,16,17), (9,11,10)(15,16,17), (2,4)(3,5)(6,14)(7,12)(8,13)(9,17)(10,15)(11,16) \rangle,$$

$$G_{22} = \langle (6,7,8)(9,11,10)(12,14,13)(15,17,16), (6,8,7)(12,13,14), (2,4)(3,5)(6,14)(7,12)(8,13)(9,17)(10,15)(11,16) \rangle,$$

$$G_{23} = \langle (7,8)(10,11)(13,14)(16,17) \rangle,$$

$$G_{24} = \langle (6,7,8)(9,11,10)(12,14,13)(15,16,17), (7,8)(10,11)(13,14)(16,17) \rangle,$$

$$\begin{aligned}
G_{25} &= \langle (15,16,17),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{26} &= \langle (12,14,13)(15,17,16),(6,7,8)(9,11,10)(12,14,13)(15,16,17),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{27} &= \langle (12,14,13)(15,17,16),(9,11,10)(15,16,17),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{28} &= \langle (15,16,17),(6,8,7)(12,13,14),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{29} &= \langle (15,16,17),(6,8,7)(9,10,11)(15,16,17),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{30} &= \langle (6,7,8)(9,11,10)(12,14,13)(15,17,16),(9,11,10)(15,16,17),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{31} &= \langle (6,7,8)(9,11,10)(12,14,13)(15,17,16),(12,14,13)(15,17,16),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{32} &= \langle (6,8,7)(9,10,11)(12,13,14),(9,10,11)(12,14,13)(15,16,17),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{33} &= \langle (6,7,8)(15,16,17),(9,11,10)(15,16,17),(12,14,13)(15,17,16),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{34} &= \langle (6,7,8)(12,14,13),(9,11,10),(15,16,17),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{35} &= \langle (15,16,17),(12,14,13)(15,17,16),(6,7,8)(9,11,10)(12,14,13)(15,16,17),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{36} &= \langle (15,16,17),(12,14,13)(15,17,16),(9,11,10)(15,16,17),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{37} &= \langle (6,7,8)(9,11,10)(12,14,13)(15,17,16),(12,14,13)(15,17,16),(9,11,10)(15,16,17),(7,8)(10,11)(13,14)(16,17) \rangle, \\
G_{38} &= \langle (9,11)(15,16) \rangle, G_{39} = \langle (6,8,7)(12,13,14),(6,7,8)(9,10)(12,14,13)(15,17) \rangle, \\
G_{40} &= \langle (15,16,17),(9,11)(15,16) \rangle, G_{41} = \langle (12,14,13),(9,11)(12,14,13)(16,17) \rangle, \\
G_{42} &= \langle (6,8,7)(12,13,14),(15,16,17),(6,7,8)(9,10)(12,14,13)(15,17) \rangle, \\
G_{43} &= \langle (6,7,8)(12,14,13),(9,11,10)(15,16,17),(3,5)(6,7)(9,15)(10,17)(11,16)(13,14) \rangle, \\
G_{44} &= \langle (6,8,7),(12,14,13),(3,5)(6,7)(9,15)(10,17)(11,16)(13,14) \rangle, \\
G_{45} &= \langle (6,7,8)(12,14,13),(9,11,10),(15,16,17),(3,5)(6,7)(9,15)(10,17)(11,16)(13,14) \rangle.
\end{aligned}$$

Now by Definitions 4 and 6, the 45×45 matrices M^C and C^Q of G can be found, which are given in Tables I and II, respectively. Therefore the symmetry of tetraammineplatinum(II) is an unmatred group of order 5184. The reader is encouraged to consult Refs. 20–23 for other monster molecules and pigments.

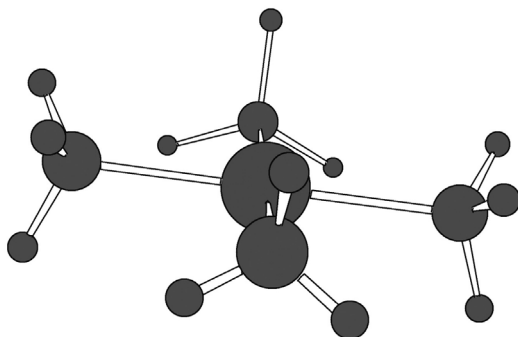


Fig 1. The structure of tetraammineplatinum(II).

ИЗВОД
ТАБЛИЦЕ КАРАКТЕРА Q-КОНЈУГАЦИЈЕ И МАРК-КАРАКТЕРА ЗА
ТЕТРААМИН-ПЛАТИНУ(II)

ALI MOGHANI

Department of Color Physics, Institute for Colorants, Paints and Coatings (ICPC), Tehran, Iran

Fujita је увео таблицу карактера Q-конјугације и таблицу марк-карактера, применивши их за пребројавање изомера. У овом раду ове две таблице су израчунате за тетраамин-платину(II).

(Примљено 7. маја, ревидирано 8. јуна 2007)

REFERENCES

1. N. S. Barta, J. R. Stille, *J. Chem. Educ.* **71** (1994) 20
2. P. S. Beauchamp, *J. Chem. Educ.* **61** (1984) 666
3. A. Kerbe, K. Thurlings, *Combinatorial Theory*, Springer, Berlin, 1982, p. 191
4. J. H. Conway, R. T. Curtis, S. P. Norton, R. A. Parker, R. A. Wilson, *Atlas of Finite Groups*, Oxford University Press, Oxford, 1985
5. S. Fujita, *Bull. Chem. Soc. Jpn.* **71** (1998) 2071
6. S. Fujita, *J. Graph Theory* **18** (1994) 349
7. S. Fujita, *J. Org. Chem.* **67** (2002) 6055
8. S. Fujita, *J. Comput. Chem. Jpn.* (2004) 113
9. S. Fujita, *Theor. Chim. Acta* **91** (1995) 291
10. S. Fujita, *J. Math. Chem.* **5** (1989) 99
11. S. Fujita, *J. Math. Chem.* **12** (1999) 173
12. S. Fujita, *Bull. Chem. Soc. Jpn.* **71** (1998) 2309
13. S. Fujita, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 251
14. S. Fujita, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 5
15. S. Fujita, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 237
16. S. Fujita, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 5
17. S. Fujita, *Diagrammatical Approach to Molecular Symmetry and Enumeration of Stereoisomers*, MCM, Kragujevac, 2007
18. A. Kerber, *MATCH Commun. Math. Comput. Chem.* **46** (2002) 151
19. A. R. Ashrafi, M. Hamadani, *Croat. Chem. Acta* **76** (2003) 299
20. A. Moghani, A. R. Ashrafi, M. Hamadani, *J. Zhejiang Univ. Sci.* **6B** (2005) 222
21. M. R. Darafsheh, Y. Farjami, A. R. Ashrafi, *Bull. Chem. Soc. Jpn.* **78** (2005) 996
22. A. Moghani, A. R. Ashrafi, *Croat. Chem. Acta* **79** (2006) 465
23. A. Moghani, S. Naghdi, A. R. Ashrafi, A. Ahmadi, *London Math. Soc.* **340** (2007) 630.