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On the Mark and Markaracter Tables of Finite Groups

MODJTABA GHORBANI

Department of Mathematics, Faculty of Science, Shahid RajaeeTeacher Training University, Tehran, 16785–136, I. R. Iran

Correspondence should be addressed to M. GHORBANI (Email: *mghorbani@srttu.edu*)

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ABSTRACT. Let G be a finite group and $C(G)$ be the family of representative conjugacy classes ofsubgroups of G. The matrix whose H,K-entry is the number offixed points of the set G/K under the action of H is called thetable of marks of G where H,K run through all elements in$C(G)$. Shinsaku Fujita for the first time introduced the term "markaracter" to discuss marks for permutation representations and characters for linear representations in a common basis. In this paper, we compute these tables for some classes of finite groups.

KEYWORDS group action • automorphism group • mark table • markaracter table

1. INTRODUCTION

A ***graph*** is a collection of points and lines connecting them. Let us to call these points and lines by vertices and edges, respectively. Two vertices x and y are adjacent, if $e = uv$ be an edge of graph. A graph whose all pairs of vertices are connected by a path is called a connected graph. A simple graph is a graph without loop and parallel edges. The vertex and edge-sets of graph G are represented by $V(G)$ and $E(G)$, respectively.

A ***molecular graph*** or a chemical graph is a labeled simple graph whose vertices and edges correspond to the atoms and chemical bonds, respectively. Its vertices are labeled with the kinds of the corresponding atoms and edges are labeled with the types of bonds. In a molecular graph, it is convenient to omit hydrogen atoms. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, see Figure 1. For given graph Γ, it is called a molecular graph if the maximum degree of every vertex reaches to four. Molecular graphs are significantly important in showing the mathematical applications in chemistry.

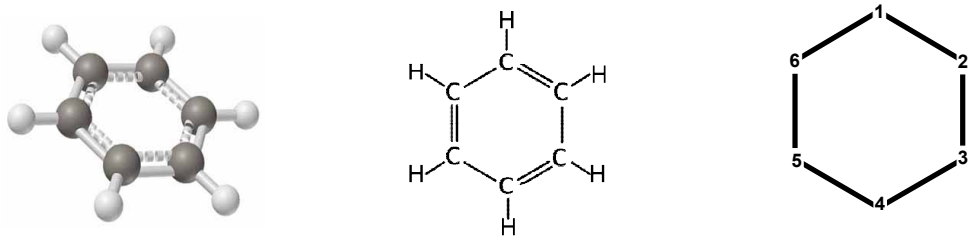

Figure 1. The molecular graph of benzene.

The ***symmetry*** of a molecule has a significant role in the analysis of the molecular structures and spectroscopy of molecules. This means that most often chemists like to classify the molecules according to their symmetry. The elements of symmetry are points, lines, planes and the collection of symmetry elements always form a group called ***point group***. A geometrical figure is said to be symmetrical if there exists permutations which permute its parts while leaving the object as a whole unchanged. An isometry of this kind is called a symmetry.

Groups are often used to describe symmetries of objects. One goal of **Group Theory** is how the symmetry of a molecule is related to its physical properties and provides a method to determine the relevant physical information of the molecule. In other words, the symmetry of a molecule provides many important physical aspects and this is what makes group theory so powerful.

In general, a ***group*** $<G, *>$ is a set of elements with a binary operation "*" which satisfy in three following properties:

1. Associative law, that is for every three elements $a,b,c \in G$, we have $a*(b*c) = (a*b)*c$.
2. There is an identity element, e, so that $a*e = e*a = a$ for any a belonging to the group.
3. Every element has its inverse as the member of the group *i.e.*, if $a \in G$, then $a^{-1} \in G$.

If $a*b = e$ it means that a is the inverse of b and vise versa. For the sake of simplicity, we usually omit the operation "*" and we use ab instead of $a*b$. The order of a group is defined as the number of members of elements present in the group. The symmetries of a given object form a group called the symmetry group of the object. Obviously, every symmetry group is a subgroup of the group of all isometries.

The group G is cyclic if it can be generated by a single element. In this case we say that G has one generator. In other words, if G be a cyclic group, then there is an element g in G, where $G = \{g, g^2, ..., g^n = e\}$. The order of this group is n. A group can be divided in several classes also called ***conjugacy classes***. The importance of classes will be clear in our later studies. Choose any element, perform the so called similarity transformation *i.e.* compute xax^{-1}, where x and a belong to the group. For each a, perform this computation

with x being all members of the group. Hence, for every element $x \in G$, the conjugacy class x^G is as follows:

$$x^G = \{gxg^{-1} : g \in G\}.$$

Example 1. Consider the molecular graph of benzene in Figure 1. Here, we compute its symmetry group. This molecule has the structure of a hexagon with a carbon atom at each corner. Evidently, the simplest symmetry of this molecule is a clock-wise rotation ρ through the angle $\pi/3 = 60^o$. A six-fold repetition of this rotation brings each vertex back to its original position so ρ satisfies the operator equation $\rho^6 = e$. This relation implies that the set $\{\rho, \ldots, \rho^6 = e\}$ compose a group called the rotational symmetry group of a hexagon, or a cyclic group of order 6 and commonly denoted by Z_6. The order of a finite group is the number of elements it contains. The element ρ is said to be a generator of Z_6, because the entire group can be generated from ρ by the group operation. The group Z_6 is completely determined by the condition $\rho^6 = e$ and any such condition on the generators of a group is called a relation of the group. A set of relations which completely determine a group is called a presentation of the group. For Z_6 the presentation consists of the single relation $\rho^6 = e$. The symmetry group of benzene has also another generator δ that is a rotation by π radians about an axis passing through the center of a regular hexagon and vertices 1, 4. Hence, one can easily see that all elements of symmetry group of benzene are as follows:

$$\{\rho, \rho^2, \rho^3, \rho^4, \rho^5, \rho^6 = 1, \delta\rho, \delta\rho^2, \delta\rho^3, \delta\rho^4, \delta\rho^5, \delta\}.$$

Let $X = \{1,2,\ldots,n\}$, a permutation group on X is a group G whose elements are permutations of X, *e.g.* bijective functions from X to X and whose group operation is the composition of permutations in G. The group of all permutations of X is the symmetric group of X denoted by S_X or S_n, where X is finite. By this notation, a finite permutation group is a subgroup of the symmetric group S_n.

Consider the molecular graph H_2O of water molecule as depicted in Figure 2, the function

$$f = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix} = (1,2)$$

is a symmetry element of this graph.

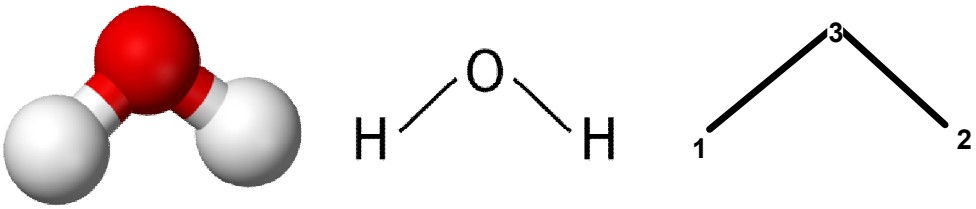

Figure 2. 2-D and 3-D graph of water molecule.

Let G be a group and X a non-empty set. An action of G on X is denoted by (G|X) and X is called a G-set. It induces a group homomorphism φ from G into the symmetric group SX on X, where $\varphi(g)x = gx$ for all $x \in X$. The orbit of x will be denoted by Gx and defines as the set of all $\varphi(g)x$, $g \in G$. The set of all G-orbits will be denoted by $G\backslash\backslash X=\{Gx|x \in X\}$. In the current study, we compute some properties of mark and markaracter tables. In the second and the third sections of the article, we present some elementary properties of these tables and we compute the markaracter tables of product groups in terms of Kronecker product. In the fourth section, we propose a formula for computing the full automorphism group of a graph via the mark table of its symmetry group. In section four, we also compute the symmetry group of some well-known molecular graphs.

2. MAIN RESULTS AND DISCUSSION

The concept of the table of marks of a finite group was introduced by one of the pioneers of finite groups, William Burnside in the second edition of his classical book [1]. This table describes a characterization of the permutation representations of a group G by certain numbers of fixed points and in some detail the partially ordered set of all conjugacy classes of subgroups of G. Hence it provides a very compact description of the subgroup lattice of G, see [2] for details. Suppose the set of fixed points of the subgroup U in the action of G on X is

$$Fix_X(U) = \{x \in X : x.u = x; \forall u \in U\}.$$

Then the ij^{th} entry of mark table of G is as follows:

$$M_{ij}(G) = |Fix_{G/G_j}(G_i)|.$$

Let also U and V be subgroups of G and $v_G(V,U) = |\{U^g : g \in G, U^g \leq V\}|$, thus we have:

Lemma 1. [2] $|Fix_{G/V}(U)| = [G:V]v_G(V,U)/v_G(G,U)$.

Theorem 2. Let G be a finite group and $G_1, G_2, \ldots, G_s$ be all non-conjugated subgroups of G in which $|G_1| \leq |G_2| \leq \ldots \leq |G_s|$. Then the matrix $M(G)$ is a lower triangular matrix and for all $1 \leq i,j \leq s$, $M_{ij}|M_{1j}$.

Proof. By using definition of the markaracter table the first claim can be proved and for the second claim, use Lemma 1.

Lemma 3. Let G be a finite group and $G_i \leq G$ be a subgroup. Then

$$M_{ii} = [N_G(G_i) : G_i].$$

In particular, if G_j be a normal subgroup of G $(1 \le j \le s)$,then

$$M_{ij} = \begin{cases} |G|/|G_j| & G_i \subseteq G_j \\ 0 & otherwise \end{cases}.$$

Proof. By using definition of the mark table, we have:

$$\begin{aligned} M_{ii} &= |\{gG_i : \forall x \in G_i, x.gG_i = gG_i\}| \\ &= |\{gG_i : \forall x \in G_i, g^{-1}xgG_i = G_i\}| \\ &= |\{gG_i : \forall x \in G_i, x \in gG_i g^{-1}\}| \\ &= |\{gG_i : G_i = gG_i g^{-1}\}|. \end{aligned}$$

On the other hand, similar to the proof of Lemma 1, one can see that

$$M_{ij} = \left|\left\{gG_j : G_i \subseteq g^{-1}G_j g\right\}\right|.$$

Since G_j is normal then, $g^{-1}G_j g = G_j$. This completes the proof.

Let the finite group G act on a finite set $X = \{x_1, x_2, \ldots, x_k\}$. The permutation representation $\Re(G)$ is a set of permutations η_g on X, each of which is associated with an element $g \in G$ so that $\Re(G)$ and G are homomorphic and $\eta_g \eta_{g'} = \eta_{gg'}$ for any $g, g' \in G$. Let H be a subgroup of G. It is a well-known fact that the set of cosets of H in G provides a partition of G as $G = Hg_1 + Hg_2 + \ldots + Hg_m$, where $g_1 = I$, the identity element of G and $g_i \in G$. The set of $\{g_1, g_2, \ldots, g_m\}$ is called a transversal. Consider the set of cosets $\{Hg_1, Hg_2, \ldots, Hg_m\}$. Following **Shinsaku Fujita** [3], for any $g \in G$, the set of permutations,

$$\bar{\eta}_g = \begin{pmatrix} Hg_1 & Hg_2 & \ldots & Hg_m \\ Hg_1 g & Hg_2 g & \ldots & Hg_m g \end{pmatrix},$$

constructs a permutation representation of G, which is called a ***coset representation*** of G by H and notified as $\Re(G/H)$. The degree of $\Re(G/H)$ is $m = [G:H]$, where $|G|$ is the number of elements in G. Obviously, the coset representation $\Re(G/H)$ I s transitive, *i.e.* has one orbit.

The ***Burnside's theorem*** states that any permutation representation $\Re(G)$ of a finite group G acting on X can be reduced into transitive CRs in accord with equation $\Re(G) = \sum_{i=1}^{s} \alpha_i \Re(G/G_i)$, wherein the multiplicity α_i is a non- negative integer obtained by solving equations

$$\mu_j = \sum_{i=1}^{s} \alpha_i M_{ij}, \ (1 \le j \le s). \qquad (1)$$

Here μ_j is the number of fixed points of G_j in $\Re(G)$ named mark of G_j, and the symbol M_{ij} denotes the mark of G_j in $\Re(G/G_i)$. Following Burnside, the matrix $M(G) = [M_{ij}]$ is called the ***table of mark*** or ***mark table*** of G. The matrix $MC(G)$ obtained from $M(G)$ in which we select rows and columns corresponding to the cyclic subgroups of G is called the ***markaracter table*** of G. Shinsaku Fujita in some of his leading papers [4-14], introduced the term markaracter to discuss marks for permutation representations and characters for linear representations in a common basis.

Throughout this paper our notation is standard and taken mainly from [15, 16]. We encourage the reader to consult papers by Balasubramanian [16,17], Kerber [18] and Pfeiffer [2] and references therein for background material as well as basic computational techniques, see also [19–21].

3. COMPUTING MARKARACTER TABLE OF SOME GROUPS

In this section we obtain some results about markaracter tables. Let p be a prime number and q be a positive integer such that$q|p$-1. Define the group $F_{p,q}$ to be presented by

$$F_{p,q}= <a,b,a^p=b^q=1, b^{-1}ab=a^u>$$

where u isan element of order q in multiplicative group Z_p^*. It is easy to see that $F_{p,q}$ is a non-abelian group of order pq.

Theorem 4. (Lagrange's Theorem) For any finite group G, the order of every subgroup H of G divides the order of G.

Let G be a group with mark table $M(G)$ with non-conjugate subgroups G_1, G_2, …, G_n. Since $M(G)$ is a lower triangular matrix, it is non-singular and so $det(M(G)) \neq 0$. On the other hand, according to Lemma 3, one can see that

$$\det(M(G)) = \prod_{i=1}^{n} M_{ii} = \prod_{i=1}^{n} [N_G(G_i) : G_i].$$

If $det(M(\mathrm{G})) = p$, then one can prove that G is isomorphic with cyclic group Z_p. Let G be a group of order n, if G has only one subgroup H (up to isomorphism), then regarding $[G:H] = n/m$, H is normal subgroup of G of order m. Hence, $M_{22} = n/m$ and so $det(M(G)) = n^2/m$. If m is not prime, then according to Lagrange's Theorem, H and so G has a subgroup of order a prime p that divides $|H|$, a contradiction. Hence, both m and n/m are primes and so $|G| = pq$, where p,q are prime numbers. Again by Lagrange's Theorem, we can prove easily that $p=q$ and so $|G| = p^2$. Because H is normal subgroup of order p, G is isomorphic with cyclic group Z_{p^2} and so $\det(M(G)) = p^3$. Thus, we proved the following theorem.

Theorem 5. Let G be a finite group and p,q be two distinct prime numbers. Then

i) $det(M(G)) = p$ *if and only if* $G \cong Z_p$.

ii) There is no group with $det(M(G)) = pq$.

iii) $det(M(G)) = p^3$ *if and only if* $G \cong Z_{p^2}$.

iv) There is no group with $det(M(G)) = p^4$.

Theorem 6. The table of marks of group $F_{p,q}$ is as reported in Table 1. Moreover, $det(M(G)) = pq^2$ if and only if $G \cong F_{p,q}$ and $det(M(G)) = p^2q^2$ if and only if $G \cong Z_{p^2}$.

Proof. It is easy to see that all non-conjugate subgroups of $G = F_{p,q}$ are $G_1 = ()$, $G_2 = Q$, $G_3 = P$ and $G_4 = G$, in which $|Q| = q$ and $|P| = p$. By Sylow theorem one can see that $P \lhd G$. So, by using Lemma 3, we have $M_{12} = p$, $M_{22} = 1$ and $M_{32} = M_{42} = 0$. On the other hand, $Q \not\lhd G$, because G is non-abelian, hence $M_{23} = M_{43} = 0$ and $M_{13} = M_{33} = 0$.

$M(F_{p,q})$	G_1	G_2	G_3	G_4
$G(/G_1)$	pq	0	0	0
$G(/G_2)$	p	1	0	0
$G(/G_3)$	q	0	q	0
$G(/G_4)$	1	1	1	1

$M(Z_{p^2})$	G_1	G_2	G_3	G_4
$G(/G_1)$	pq	0	0	0
$G(/G_2)$	p	p	0	0
$G(/G_3)$	q	0	q	0
$G(/G_4)$	1	1	1	1

Table 1.(*a*) The table of marks of group $F_{p,q}$ and (*b*) The table of marks of group Z_{p^2}.

Fujita in some of his papers computed the markaracter table of cyclic groups. Here, we demonstrate how to compute the markaracter table of some abelian groups.

Theorem 7. Let G and H be groups acting on sets X and Y, respectively. Then

$$|\mathrm{Fix}_{X\times Y}(U\times V)| = |\mathrm{Fix}_X(U)| \times |\mathrm{Fix}_Y(V)|,$$

where $U \le G$, $V \le H$ and $\mathrm{Fix}_X(U) = \{x \in X \mid xg = x;\ \forall g \in U\}$.

Proof. We have:

$$\begin{aligned}
|\mathrm{Fix}_{X\times Y}(U \times V)| &= |\{(x,y) \mid (x,y)(g,h) = (x,y);\ \forall\ (g,h) \in U\times V\}| \\
&= |\{(x,y) \mid (xg,yh) = (x,y);\ \forall\ (g,h) \in U\times V\}| \\
&= |\{(x,y) \mid xg = x \,\&\, yh = y;\ \forall g \in U \,\&\, \forall h \in \mathrm{V}\}| \\
&= |\{(x,y) \mid x \in \mathrm{Fix}_X(U)\ \&y \in \mathrm{Fix}_Y(V)\}| \\
&= |\mathrm{FixX(U)}| \times |\mathrm{FixY(V)}|.
\end{aligned}$$

Corollary 8 [22]. Let G and H be groups of co-prime orders acting on sets X and Y, respectively. If MC(G) = [a_{ij}] and MC(H) = [b_{ij}], then MC(G × H) = [c_{rs}], where $c_{rs} = a_{i_r i_s} b_{j_r j_s}$ and $G_{i_r} \times H_{j_r}$ G(/ $G_{i_s} \times H_{j_s}$) are the rth column and sth row of MC(G × H), respectively.

For any two arbitrary matrices A and B, we have the ***direct product*** or ***Kronecker product*** $A \otimes B$ defined as

$$\begin{bmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mn}B \end{bmatrix}.$$

Note that if A is m-by-n and B is p-by-r then $A \otimes B$ is an mp-by-nr matrix. This multiplication is not usually commutative. It is an easy task to show that in Corollary 8, $M(G \times H)$ is the Kronecker product $M(G) \otimes M(H)$. We now apply Lemma 3 to find another method for computing this table. To simplify our argument, in the following example, we only compute the mark table of a cyclic group of order $p^n q^m$.

Example 2. Let G be a cyclic group of order $p^n q^m$. It is a well-known fact that G is isomorphic to $H \times K$ in which H and K are subgroups of G of order p^n and q^m, respectively. Suppose $H_1, H_2, \ldots, H_{n+1}$ and $K_1, K_2, \ldots, K_{m+1}$ are all subgroups of H and K, respectively. One can see that $MC(H) = [a_{ij}]$ and $MC(K) = [b_{ij}]$, where

$$a_{ij} = \begin{cases} p^{n-j+1} & j \le i \\ 0 & otherwise \end{cases} \text{ and } b_{ij} = \begin{cases} q^{m-j+1} & j \le i \\ 0 & otherwise \end{cases}.$$

Then $MC(H \times K) = [c_{rs}]$, in which

$$c_{rs} = \begin{cases} p^{n-j_r+1} q^{m-j_s+1} & j_r \le i_r, j_s \le i_s \\ 0 & otherwise \end{cases}.$$

The dihedral group D_{2n} is the symmetry group of an n-sided regular polygon for $n > 1$. These groups are one of the most important classes of finite groups currently applicable in chemistry. For example D_6, D_8, D_5 and D_{12} point groups are dihedral groups. One group presentation for D_{2n} is $\langle x, y \mid x^2 = y^n = 1, (xy)^n = 1 \rangle$.

Theorem 9 [22]. Suppose $G = D_{2n}$ is the dihedral group of order $2n$. Then

$$1 = G_1, \langle b \rangle = G_2, \langle ab \rangle = G_3, \langle a^{n/2} \rangle = G_4, \langle a^{v_5} \rangle = G_5, \langle a^{v_6} \rangle = G_6,$$

$$\ldots, \langle a^{v_{t+1}} \rangle = \langle a \rangle = G_{t+2}$$

are all cyclic non-conjugate subgroups of D_n such that v_i divides n and t is the number of divisors of n. Moreover the markaracter table of G is as reported in Table 2.

Proof. Suppose $MC(G) = [a_{ij}]$ is markaracter table of D_{2n}. We first assume n is even. Then the conjugacy classes of D_{2n} are
$\{1\}$, $\{a^{n/2}\}$, $\{a^r,a^{-r}\}$ $(1 \le r \le n/2)$, $\{a^sb \mid 0 \le s \le n-1 \ \& \ 2 \mid s\}$, $\{a^sb \mid 0 \le s \le n-1 \ \& \ 2 \nmid s\}$.

Hence up to conjugacy there are three subgroups of order 2, $G_2 = \langle b \rangle$, $G_3 = \langle ab \rangle$, $G_4 = \langle a^{n/2} \rangle$ and $t = d(n)$ cyclic subgroups whose orders divide n, say G_5, …, $G_{t+2} = \langle a \rangle$. By using Lemma 3, $a_{ij} = |\{G_ig \mid G_j \subseteq g^{-1}G_ig\}|$ and so $a_{ii} = |N_G(G_i)| / |G_i|$. Clearly, $N_G(\langle b \rangle) = \{1, b, a^{n/2}, a^{n/2}b\}$, $N_G(\langle a^{n/2} \rangle) = G$ and $N_G(\langle ab \rangle) = \{1, ab, a^{n/2}, a^{1+n/2}b\}$. So $a_{22} = a_{33} = 2$ and $a_{44} = n$. Suppose $j \mid n$. By an elementary fact in finite groups $o(a^j) = n/j$. Since every subgroup of $\langle a \rangle$ is normal in G, $a_{ij} = 2n/(n/j) = 2j$. If $v_j \mid v_i$ then $G_j \subseteq G_i$ and so $a_{ij} = 2j$, as desired. We now assume that n is odd. Then the conjugacy classes of D_{2n} are $\{1\}$, $\{a^r,a^{-r}\}$ $(1 \le r \le (n-1)/2)$, $\{a^sb \mid 0 \le s \le n-1\}$ and up to conjugacy there is one only subgroup of order 2 and $d(n)$ cyclic subgroups whose orders divide n. Now a similar argument as above, complete the proof.

$M(D_{2n})$	G_1	G_2	G_3	G_4	$G_i = \langle a^{v_i} \rangle$ $(5 \le i \le t+2)$
$G/\langle\rangle$	$2n$	0	0	0	0
G/G_2	N	2	0	0	0
G/G_3	N	0	2	0	0
G/G_4	N	0	0	n	0
G/G_i $(5 \le i \le t+2)$	$2j$	0	0	α	γ

Table 2(*a*). The markaracter table of D_{2n}, where n is even.

$M(D_{2n})$	G_1	G_2	$G_j = \langle x^i \rangle$ $(3 \le j \le t+2)$
$G/\langle\rangle$	$2n$	0	0
G/G_2	n	1	0
G/G_j $(3 \le j \le t+2)$	$2j$	0	α

Table 2(*b*). The markaracter table of D_{2n}, where n is odd.

$$\text{where } \alpha = \begin{cases} 2j & v_j \mid \frac{n}{2} \\ 0 & Otherwise \end{cases} \text{ and } \gamma = \begin{cases} 2j & v_j \mid v_i \\ 0 & Otherwise \end{cases}.$$

4. APPLICATION IN CHEMISTRY

A bijection σ on vertices set of graph Γ is named an automorphism of graph, if it preserves the edge set. In other words, σ is an automorphism if $e = uv$ is an edge, then $\sigma(e) = \sigma(u)\sigma(v)$ is an edge of E. Let $Aut(\Gamma) = \{\alpha: V \to V, \alpha \text{ is bijection}\}$, then $Aut(\Gamma)$ under the composition of mappings forms a group.

The adjacency matrix $A(\Gamma)$ of graph $\Gamma$with vertex set $V(\Gamma) = \{v_1, v_2, \ldots, v_n\}$ is the $n \times n$ symmetric matrix $[a_{ij}]$ such that $a_{ij} = 1$ if v_i and v_j are adjacent and 0, otherwise. The ***Euclidean matrix*** of a chemical graph to find its symmetry. Here the Euclidean matrix of a molecular graph Γ is a matrix $D(\Gamma) = [d_{ij}]$, where for $i \neq j$, d_{ij} is the Euclidean distance between the nuclei i and j. In this matrix d_{ii} can be taken as zero if all the nuclei are equivalent. Otherwise, one may introduce different weights for different nuclei. Suppose σ is a permutation on n atoms of the molecule under consideration. Then the permutation matrix P_σ is defines as $P_\sigma = [x_{ij}]$, where $x_{ij} = 1$ if $i = \sigma(j)$ and 0 otherwise. It is easy to see that $P_\sigma P_\tau = P_{\sigma\tau}$, for any two permutations σ and τ on n objects, and so the set of all $n \times n$ permutation matrices is a group isomorphic to the symmetric group S_n on n symbols. For computing the symmetry of a molecule, it is sufficient to solve the matrix equation $P^tEP = E$, where E is the Euclidean matrix of the molecule under consideration and P varies on the set of all permutation matrices with the same dimension as E.

By having the markaracter table of symmetry group of a graph, we can compute the full automorphism group of underlying graph by an algebraic way. Consider the following example. The full automorphism group of a graph is one of the most important problem in graph theory and this is the first attempt to solve this problem by using the mark table.

Example 3. Consider the skeleton of naphthalene, Figure 3. The generators of its symmetry group are λ and ω, where $\lambda = (1, 9)(2, 10)(3, 7)(4, 8)$ and $\omega = (1, 2)(3, 4)(5, 6)(7, 8)(9, 10)$. The subgroups of G are $G_1 = <()>$, $G_2 = <\lambda>$, $G_3 = <\omega>$, $G_4 = <\lambda\omega>$ and $G_5 = G$. This group is isomorphic with $Z_2 \times Z_2$, where Z_2 is a group of order 2. Since every group of order 4 is abelian and then $Z_2 \times Z_2$, by using Corollary 4, for any subgroup G_i of $Z_2 \times Z_2$, $M_{ij} = 0$ or $|Z_2 \times Z_2|/|G_i|$. But for the pure subgroup H of $Z_2 \times Z_2$, $|H| = 2$. This implies the entries of mark table are 1, 2 and 4. By Theorem 2, $M_{11} = 4$ and $M_{i1} = 0$ for $2 \leq i \leq 4$. Also $M_{4j} = 1$ for $1 \leq j \leq 4$. Since all subgroups in Abelian group are normal, by using Corollary 4, we have

$M_{12} = M_{22} = 2$ and $M_{32} = M_{42} = 0$. Using again Corollary 4, it is easy to see that $M_{13} = M_{33} = 2$ and $M_{23} = M_{43} = 0$. In Tables 1 and 2, the mark table and markaracter table of this group are computed. On the other hand, the number of (μ_j) of fixed points are obtained by a geometrical examination of Eq.(1):

$$(10,2,0,0,0)=(\alpha_{G_1},\ \alpha_{G_2},\ \alpha_{G_3},\ \alpha_{G_4},\ \alpha_{G_5})\times\begin{pmatrix}4&0&0&0&0\\2&2&0&0&0\\2&0&2&0&0\\2&0&0&2&0\\1&1&1&1&1\end{pmatrix}.$$

So, by solving these equations we have $\alpha_{G_5}=\alpha_{G_4}=\alpha_{G_3}=0$, $\alpha_{G_1}=2$, $\alpha_{G_2}=1$ and $P_G = 2G(/G_1)+G(/G_2)$. This implies sub-orbits of X areX_{11}={1, 2, 9, 10}, X_{21}={5, 6}, X_{12}={3, 4, 7, 8}.

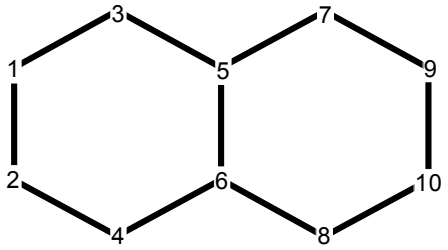

Figure 3. The skeleton of naphthalene.

$M(Z_2\times Z_2)$	G_1	G_2	G_3	G_4	G_5
$G(/G_1)$	4	0	0	0	0
$G(/G_2)$	2	2	0	0	0
$G(/G_3)$	2	0	2	0	0
$G(/G_4)$	2	0	0	2	0
$G(/G_5)$	1	1	1	1	1

Table 3. Mark table of the point group $Z_2\times Z_2$.

$MC(Z_2 \times Z_2)$	G_1	G_2	G_3	G_4
$G(/G_1)$	4	0	0	0
$G(/G_2)$	2	2	0	0
$G(/G_3)$	2	0	2	0
$G(/G_4)$	2	0	0	2

Table 4. Markaracter table of the point group $Z_2 \times Z_2$.

Using a similar discussion, the generators of the point group of antheracene skeleton (Figure 4) are δ and γ, where

$$\gamma = (1, 13)(2, 14)(3, 11)(4, 12)(5, 9)(6, 10),$$

$$\eta = (1, 2)(3, 4)(5, 6)(7, 8)\ (9, 10)(11, 12)(13, 14).$$

The subgroups of G are $G_1 = <()>$, $G_2 = <\gamma>$, $G_3 = <\eta>$, $G_4 = <\gamma\eta>$ and $G_5 = G$. Also, the mark table and markaracter table of this group are the same of naphthalene. Similarly, one can see that the sub-orbits of X are X_{11}={1,2,13,14}, X_{21}={7,8}, X_{22} = {5,6,9,10} and X_{12}={3,4,11,12}.

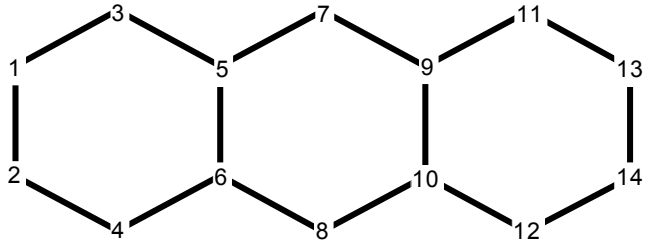

Figure 4. The skeleton of antheracene.

In generally, consider the graph of benzenoid chain with exactly n hexagons, Figure 5. Its point group is isomorphic with group $Z_2 \times Z_2$ generated by α and β where

$$\alpha = (1,3)(2,4)\cdots(4n-4,4n-2)(4n-3,4n-1),$$

$$\beta = (1,2)(3,4)\cdots(4n-1,4n)(4n+1,4n+2).$$

This implies the mark table and markaracter table of a benzenoid chain with exactly n hexagons are similar to antheracene and naphthalene.

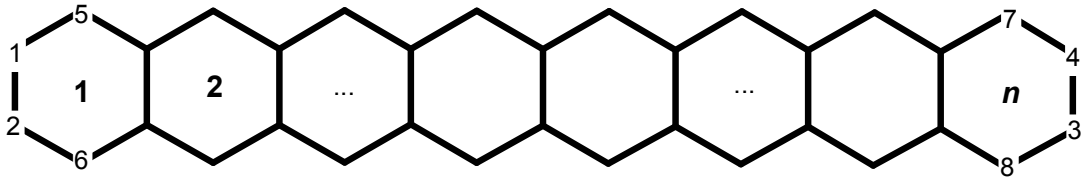

Figure 5. The skeleton of a benzenoid chain with *n* hexagons.

REFERENCES

1. W. Burnside, Theory of Groups of Finite Order, The University Press, Cambridge, 1897.
2. G. Pfeiffer, The subgroups of M_{24}, or how to compute the table of marks of a finite group, Exp. Math. 6 (3) (1997) 247–270.
3. S. Fujita, Markaracter tables and Q-conjugacy character tables for cyclic groups. An application to combinatorial enumeration, Bull. Chem. Soc. Jpn. 71 (1998) 1587–1596.
4. S. Fujita, Maturity of finite groups. An application to combinatorial enumeration of isomers, Bull. Chem. Soc. Jpn. 71 (1998) 2071–2080.
5. S. Fujita, Inherent automorphism and Q-conjugacy character tables of finite groups, An application to combinatorial enumeration of isomers, Bull. Chem. Soc. Jpn. 71 (1998) 2309–2321.
6. S. Fujita, Combinatorial enumeration of graphs, three-dimensional structures, and chemical compounds, Mathematical Chemistry Monographs: MCM 15, Kragujevac, 2013.
7. S. Fujita, Subduction of Q-conjugacy representations and characteristic monomials for combinatorial enumeration, Theor. Chem. Acc. 99 (1998) 224–230.
8. S. Fujita, Systematic enumeration of ferrocene derivatives by unit-subduced-cycle-index method and characteristic-monomial method, Bull. Chem. Soc. Jpn. 72 (1999) 2409–2416.
9. S. Fujita, A simple method for enumeration of non-rigid isomers. An application of characteristic monomials, Bull. Chem. Soc. Jpn. 72 (1999) 2403–2407.
10. S. Fujita, Möbius function and characteristic monomials for combinatorial enumeration, Theor. Chem. Acc. 101 (1999) 409–420.
11. S. Fujita, Characteristic monomials with chirality fittingness for combinatorial enumeration of isomers with chiral and achiral ligands, J. Chem. Inf. Comput. Sci. 4 (2000) 1101–1112.

12. S. Fujita, The unit-subduced-cycle-index methods and the characteristic-monomial method. Their relationship as group-theoretical tools for chemical combinatorics, J. Math. Chem. 30(3) (2001) 249–270.
13. S. Fujita, Symmetry and Combinatorial Enumeration in Chemistry, Springer-Verlag, Berlin-Heidelberg, 1991.
14. S. Fujita, Diagrammatical Approach to Molecular Symmetry and Enumeration of Stereoisomers, Mathematical Chemistry Monographs: MCM 4, Kragujevac, 2007.
15. . N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, FL., 1992.
16. K. Balasubramanian, "Combinatorics and Spectroscopy" in Chemical Group Theory. Techniques and Applications, Gordon and Breach Publications, Amsterdam,1995.
17. K. Balasubramanian, Recent applications of group theory to chemical physics in conceptual quantum chemistry: Models and applications, Croat. Chim. Acta 57 (1984) 1465–1492.
18. A. Kerber, Enumeration under finite group action, basic tools, results and methods, MATCH Commun. Math. Comput. Chem. 46 (2002) 151–198.
19. S. El-Basil, Prolegomenon on Theory and Applications of Tables of Marks, MATCH Commun. Math. Comput. Chem. 46 (2002) 7–23.
20. M. Ghorbani, Enumeration of hetero fullerenes: a survey, MATCH Commun. Math. Comput. Chem. 68 (2012) 381–414.
21. M. Ghorbani, Remarks on markaracter table of fullerene graphs, J. Comput. Theor. Nanosci. 11 (2014) 363–379.
22. A. R. Ashrafi and M. Ghorbani, A note on markaracter tables of finite groups, MATCH Commun. Math. Comput. Chem. 59 (2008) 595–603.