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Dominant representations and a markaracter table for a group of finite order

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Summary. The concept of markaracter is proposed to discuss marks and characters for a group of finite order on a common basis. Thus, we consider a non-redundant set of dominant subgroups and a non-redundant set of dominant representations (SDR), where coset representations concerning cyclic subgroups are named dominant representations (DRs). The numbers of fixed points corresponding to each DR are collected to form a row vecter called a dominant markaracter (mark-character). Such dominant markaracters for the SDR are collected as a markaracter table. The markaracter table is related to a subdominant markaracter table of its subgroup so that the corresponding row of the former table is constructed from the latter. The data of the markaracter table are in turn used to construct a character table of the group, after each character is regarded as a markaracter and transformed into a multiplicity vector. The concept of orbit index is proposed to classify multiplicity vectors; thus, the orbit index of each DR is proved to be equal to one, while that corresonding to an irreducible representation is equal to zero.

Key words: Dominant representation – Markaracter – Group – Orbit index

1. Introduction

Character tables for reducing linear representations into irreducible ones belong to the standard repertoire of chemical group theory. Since they are widely applied to various fields of chemistry, textbooks on chemical group theory [1]–[8] use many pages to introduce the concept and applications of character tables. On the other hand, the concept of mark tables for assigning permutation representations to coset representations, which has been developed by Burnside [9], has been unjustly neglected for a long time not only in chemical fileds but also in mathematics. Among several works using mark tables, Sheehan's enumeration of graphs [10], Kerber's contribution [11], Redfield's paper [12], our enumeration of digraphs [13], and our enumeration of polyhedra [14] can be mentioned for discussing mathematical applications. With respect to applications to chemistry, various methods for the enumeration of isomers are based on mark tables; *e.g.*, Hässelbarth's enumeration of isomers [15], Mead's work on a combination of mark tables and double cosets [16], our USCI (unit-subduced-cycle-index) approach [17, 18], our elementary superposition theorem [19], and Lloyd's mark version of the Redfield-Read superposition theorem [20]. Up to now, the tables of two types have been independently used in different fields, since they have been developed on the basis of different disciplines.

We have recently reported an application of coset representation to the construction of symmetry adapted functions [21], in which coset representations are reduced into irreducible representations by using character tables. This treatment implies a relationship between mark tables and character tables, since both the tables have thus been related to the same coset representations. Since such a relationship has not been discussed, it should be a target in order that we reach a deeper insight to group theory in both chemical and mathematical meanings.

On the other hand, we have presented an alternative formulation of Pólya's theorem by starting from our USCI approach [22], in which we use a correspondence between cyclic subgroups and conjugacy classes as a key concept. Although the original discussion on the correspondence has been restricted within perumtation representations, it can be easily extended to treat any groups of finite order. The correspondence can be combined with the fact that coset representations (and mark tables) are based on conjugate subgoups while irreducible representations (and charater tables) are based on conjugacy classes. This idea creates a working guideline that dominant representations (coset representations for cyclic subgroups) should have a crutial role to arrive at the goal. The present paper deals with detailed discusstions on the correspondence and the proposal of the concept of markaracter (mark-character), which allow us to treat marks and characters on a common basis.

2. Dominant subgroups

In order to have a brief perspective, Table 1 shows the terminology of the present approach on related concepts in comparison with those of the previous approaches. We here coin a term *markaracter* (mark-character) to integrate the terms "mark" and "character". The coinage is to clarify the fact that the present approach (markaracter approach) provides permutation representations and linear representations with a common basis.

Table 1. Terminology for concepts

Item	Mark approach	Character approach	Markaracter approach
representation	permutation representation	linear representation	linear (permutation) representation
basic representation	coset representation	irreducible representation	dominant representation
invariant	mark	character	markaracter
basic invariant	mark	irreducible character	dominant markaracter
table	mark table	character table	markaracter table
equivalency class	conjugate subgroups	conjugacy classes	conjugate cyclic subgroups

Let $\mathbf{G}$ be a group of finite order that has a non-redundant set of cyclic subgroups (SCSG):

$$SCSG_{\mathbf{G}} = \{\mathbf{G}_1, \mathbf{G}_2, \ldots, \mathbf{G}_s\} \quad (|\mathbf{G}_1| \leq |\mathbf{G}_2| \leq \cdots \leq |\mathbf{G}_s|), \tag{1}$$

where the group $\mathbf{G}_1$ is an identity and each subgroup is a representative selected from a respective set of conjugate cyclic subgroups. A group contained in the SCSG ic called a *dominant subgroup.* Note that the group $\mathbf{G}$ itself is not always a cyclic group.

We consider a *coset representation* (CR) by starting from a coset decomposition of the group $\mathbf{G}$ by each cyclic subgroup $\mathbf{G}_i$. The symbol $\mathbf{G}(/\mathbf{G}_i)$ is used in accord with our previous treatment. The CR, which is called a dominant representation (DR), may be written as permutation forms or as matrix representations. Thereby, we have a *non-redundant set of dominant representations* (SDR):

$$SDR_{\mathbf{G}} = \{\mathbf{G}(/\mathbf{G}_1), \mathbf{G}(/\mathbf{G}_2), \ldots, \mathbf{G}(/\mathbf{G}_s)\}. \tag{2}$$

The degree of each DR is representated by $|\mathbf{G}|/|\mathbf{G}_i|$ for $i = 1, 2, \ldots, s$. Note that the DRs in $SDR_{\mathbf{G}}$ are concerned with cyclic subgroups and selected from the corresponding non-redundunt set of CRs ($SCR_{\mathbf{G}}$) concerning cyclic and non-cyclic subgroups. Each DR of $SDR_{\mathbf{G}}$ ($\mathbf{G}(/\mathbf{G}_i)$) corresponds to a *dominant markaracter* that is a row vector whose elements are the number of fixed points when the DR is restricted within respective dominant subgroups. In the treatment of this section, the markaracter is identical with a fixed-point vector (FPV) described in our previous work [18] except that this is concerned with the SCR. Thus, a dominant markaracter is represented by

$$\begin{aligned} \boldsymbol{G}(/\boldsymbol{G}_i) &= (m_{i1}, m_{i2}, \ldots, m_{ii}, \ldots, m_{is}) \\ &= (m_{i1}, m_{i2}, \ldots, m_{ii}, 0, \ldots, 0) \;\; \text{for } i = 1, 2, \ldots, s \end{aligned} \tag{3}$$

which is uniquely determined once the $SDR_{\mathbf{G}}$ is selected. We use the slanted boldfaced symbol $\boldsymbol{G}(/\boldsymbol{G}_i)$ for designate such a markaracter. Each element of an FPV is the number of fixed points which is called a mark. On the other hand, each element of a markaracter is concerned with an invariant which includes a mark as a subconcept. Hence, the term "mark" is also used in the present paper although it involved an extended meaning.

Such dominant markaracters are collected to form a dominant markaracter table, which is simply called a *markaracter table* (MT). This is a lower triangular matrix as follows.

$$\widetilde{\mathrm{M}}_{\mathbf{G}} = (m_{ij}) = \begin{array}{c} \\ \boldsymbol{G}(/\boldsymbol{G}_1) \\ \boldsymbol{G}(/\boldsymbol{G}_2) \\ \vdots \\ \boldsymbol{G}(/\boldsymbol{G}_i) \\ \vdots \\ \boldsymbol{G}(/\boldsymbol{G}_s) \end{array} \begin{array}{c} \begin{array}{cccccccc} \downarrow \mathbf{G}_1 & \downarrow \mathbf{G}_2 & \cdots & \downarrow \mathbf{G}_i & \cdots & \downarrow \mathbf{G}_s \end{array} \\ \begin{pmatrix} m_{11} & & & & & \\ m_{21} & m_{22} & & & & \\ \vdots & \vdots & \ddots & & & \\ m_{i1} & m_{i2} & \cdots & m_{ii} & & \\ \vdots & \vdots & & \vdots & \ddots & \\ m_{s1} & m_{s2} & \cdots & m_{si} & \cdots & m_{ss} \end{pmatrix} \end{array}, \tag{4}$$

where zero elements above the main diagonal are omitted. A roman-character symbol with a tilde (*e.g.* $\widetilde{\mathrm{M}}_{\mathbf{G}}$) is used to designate such a markaracter table, when it is regarded as a square matrix.

Table 2 shows a markaracter table for the group $\mathbf{T}_d$. Note that the group $\mathbf{T}_d$ has a non-redundant set of dominant representations (SDR):

$$SDR_{\mathbf{T}_d} = \{\mathbf{T}_d(/\mathbf{C}_1), \mathbf{T}_d(/\mathbf{C}_2), \mathbf{T}_d(/\mathbf{C}_s), \mathbf{T}_d(/\mathbf{C}_3), \mathbf{T}_d(/\mathbf{S}_4)\}. \tag{5}$$

The table is regarded as a matrix, which is designated by the symbol $\widetilde{M}_{\mathbf{T}_d}$. The corresponding inverse matrix (Table 3) is also used in the present treatment.

Table 2. Dominant mark table for $\mathbf{T}_d$

$\widetilde{M}_{\mathbf{T}_d}$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_3$	$\mathbf{S}_4$
$\mathbf{T}_d(/\mathbf{C}_1)$	24	0	0	0	0
$\mathbf{T}_d(/\mathbf{C}_2)$	12	4	0	0	0
$\mathbf{T}_d(/\mathbf{C}_s)$	12	0	2	0	0
$\mathbf{T}_d(/\mathbf{C}_3)$	8	0	0	2	0
$\mathbf{T}_d(/\mathbf{S}_4)$	6	2	0	0	2

Table 3. Inverse matrix of the dominant markaracter table for $\mathbf{T}_d$

$\widetilde{M}^{-1}_{\mathbf{T}_d}$	$\mathbf{T}_d(/\mathbf{C}_1)$	$\mathbf{T}_d(/\mathbf{C}_2)$	$\mathbf{T}_d(/\mathbf{C}_s)$	$\mathbf{T}_d(/\mathbf{C}_3)$	$\mathbf{T}_d(/\mathbf{S}_4)$	sum
$\mathbf{C}_1$	$\frac{1}{24}$	0	0	0	0	$\frac{1}{24}$
$\mathbf{C}_2$	$-\frac{1}{8}$	$\frac{1}{4}$	0	0	0	$\frac{1}{8}$
$\mathbf{C}_s$	$-\frac{1}{4}$	0	$\frac{1}{2}$	0	0	$\frac{1}{4}$
$\mathbf{C}_3$	$-\frac{1}{6}$	0	0	$\frac{1}{2}$	0	$\frac{1}{3}$
$\mathbf{S}_4$	0	$-\frac{1}{4}$	0	0	$\frac{1}{2}$	$\frac{1}{4}$

The set of the dominant markaracters ($\mathbf{G}(/\mathbf{G}_i)$ for $i = 1, 2, \ldots, s$) is linearly independent and spans a vector space (V), which is called a *markaracter space*. Let consider a row vector involved in V:

$$\mathbf{X} = (x_1, x_2, \ldots, x_s). \tag{6}$$

This vector can be generated by counting fixed points for each cyclic subgroup when the group $\mathbf{G}$ acts on an object, giving a permutation representation. The vector $\mathbf{X}$ is represented by a linear combination of the vectors $\mathbf{G}(/\mathbf{G}_i)$ ($i = 1, 2, \ldots, s$) given by eq. 3. We thus obtain the following equation,

$$\mathbf{X} = \widetilde{\alpha}_1\mathbf{G}(/\mathbf{G}_1) + \widetilde{\alpha}_2\mathbf{G}(/\mathbf{G}_2) + \cdots \widetilde{\alpha}_s\mathbf{G}(/\mathbf{G}_s) = \sum_{i=1}^{s} \widetilde{\alpha}_i\mathbf{G}(/\mathbf{G}_i). \tag{7}$$

The coefficients are easily obtained by solving linear equations,

$$x_j = \sum_{i=1}^{s} \widetilde{\alpha}_i m_{ij} \qquad (j = 1, 2, \ldots, s). \tag{8}$$

or inverse linear equations,

$$\widetilde{\alpha}_i = \sum_{j=1}^{s} x_i \overline{m}_{ji} \qquad (i = 1, 2, \ldots, s). \tag{9}$$

These equations are summarized by the following theorem using matrix representations.

Theorem 1. *By defining a row vector,*

$$\widetilde{\mathbf{A}} = (\widetilde{\alpha}_1, \widetilde{\alpha}_2, \ldots, \widetilde{\alpha}_s), \tag{10}$$

the linear equations can be written as the following matrix expression:

$$\mathbf{X} = \widetilde{\mathbf{A}}\widetilde{\mathbf{M}}_{\mathbf{G}}, \tag{11}$$

or

$$\widetilde{\mathbf{A}} = \mathbf{X}\widetilde{\mathbf{M}}_{\mathbf{G}}^{-1}. \tag{12}$$

The vector $\widetilde{\mathbf{A}}$ is called a *multiplicity vector*, since it corresponds to the counterpart defined in our previous treatment [18]. When $\widetilde{\mathbf{A}}$ is generated from a dominant markaracter $\mathbf{G}(/\mathbf{G}_i)$ (for a cyclic $\mathbf{G}_i$), we call them a *dominant multiplicity vector* and use the slanted boldfaced symbol with a wide tilde $\widetilde{\mathbf{G}}(/\mathbf{G}_i)$ for designating them. Obviously, the multiplicity vectors $\widetilde{\mathbf{G}}(/\mathbf{G}_i)$ ($i = 1, 2, \ldots, s$) construct an orthonormal basis system.

It should be noted that *multiplicity vectors of the present approach may contain elements of rational number*, while previous multiplicity vectors contain elements of non-negative integer. This feature is illustrated in the following example.

Example 1. Let us consider a methane (or tetrahedron) skeleton. The four hydrogen atoms (vertices) construct an orbit governed by $\mathbf{T}_d(/\mathbf{C}_{3v})$. Since the dominant markaracter is $\mathbf{T}_d(/\mathbf{C}_{3v}) = (4, 0, 2, 1, 0)$, eq. 12 for this case is obtained as follows.

$$\widetilde{\mathbf{T}}_d(/\mathbf{C}_{3v}) = (4, 0, 2, 1, 0)\widetilde{\mathbf{M}}_{\mathbf{T}_d}^{-1} = (-\frac{1}{2}, 0, 1, \frac{1}{2}, 0). \tag{13}$$

On the other hand, the six edges construct an orbit governed by $\mathbf{T}_d(/\mathbf{C}_{2v})$. Since the dominant markaracter is $\mathbf{T}_d(/\mathbf{C}_{2v}) = (6, 2, 2, 0, 0)$, eq. 12 for this case is obtained as follows.

$$\widetilde{\mathbf{T}}_d(/\mathbf{C}_{2v}) = (6, 2, 2, 0, 0)\widetilde{\mathbf{M}}_{\mathbf{T}_d}^{-1} = (-\frac{1}{2}, \frac{1}{2}, 1, 0, 0). \tag{14}$$

Such symbols with a tilde are used to designate multiplicity vectors in the present paper. In a similar way, markaracters and multiplicity vectors are obtained for all of the coset representations of the group $\mathbf{T}_d$, as collected in Table 4. □

Since a mark table for $\mathbf{T}_d$ has been reported [18], a more convenient procedure is available. From the mark table, we select the columns corresponding to the cyclic subgroups of $\mathbf{T}_d$, giving a restricted mark table shown in the left part of Table 4, where the marks of each row are collected as a row vector (a markaracter) and the rows corresponding to the cyclic subgroups are shifted into the top of the table.

This example shows that the markaracter of each coset representation is transformed into a multiplicity vector based on the dominant multiplicity vectors ($\widetilde{\mathbf{T}}_d(/\mathbf{C}_1)$ to $\widetilde{\mathbf{T}}_d(/\mathbf{S}_4)$). In other words, it is represented by a linear combination of $\widetilde{\mathbf{T}}_d(/\mathbf{C}_1)$ to $\widetilde{\mathbf{T}}_d(/\mathbf{S}_4)$ as the orthonormal bases of the markaracter space.

Table 4. Restricted mark table and mulitiplicity vectors for $\mathbf{T}_d$

Markaracter		Multiplicity Vector
$\mathbf{T}_d(/\mathbf{C}_1) = (24,0,0,0,0)$	$\Longrightarrow$	$\widetilde{\mathbf{T}}_d(/\mathbf{C}_1) = (1,0,0,0,0)$
$\mathbf{T}_d(/\mathbf{C}_2) = (12,4,0,0,0)$	$\Longrightarrow$	$\widetilde{\mathbf{T}}_d(/\mathbf{C}_2) = (0,1,0,0,0)$
$\mathbf{T}_d(/\mathbf{C}_s) = (12,0,2,0,0)$	$\Longrightarrow$	$\widetilde{\mathbf{T}}_d(/\mathbf{C}_s) = (0,0,1,0,0)$
$\mathbf{T}_d(/\mathbf{C}_3) = (8,0,0,2,0)$	$\Longrightarrow$	$\widetilde{\mathbf{T}}_d(/\mathbf{C}_3) = (0,0,0,1,0)$
$\mathbf{T}_d(/\mathbf{S}_4) = (6,2,0,0,2)$	$\Longrightarrow$	$\widetilde{\mathbf{T}}_d(/\mathbf{S}_4) = (0,0,0,0,1)$
$\mathbf{T}_d(/\mathbf{C}_{2v}) = (6,2,2,0,0)$	$\Longrightarrow$	$\widetilde{\mathbf{T}}_d(/\mathbf{C}_{2v}) = (-\frac{1}{2},\frac{1}{2},1,0,0)$
$\mathbf{T}_d(/\mathbf{D}_2) = (6,6,0,0,0)$	$\Longrightarrow$	$\widetilde{\mathbf{T}}_d(/\mathbf{D}_2) = (-\frac{1}{2},\frac{3}{2},0,0,0)$
$\mathbf{T}_d(/\mathbf{C}_{3v}) = (4,0,2,1,0)$	$\Longrightarrow$	$\widetilde{\mathbf{T}}_d(/\mathbf{C}_{3v}) = (-\frac{1}{2},0,1,\frac{1}{2},0)$
$\mathbf{T}_d(/\mathbf{D}_{2d}) = (3,3,1,0,1)$	$\Longrightarrow$	$\widetilde{\mathbf{T}}_d(/\mathbf{D}_{2d}) = (-\frac{1}{2},\frac{1}{2},\frac{1}{2},0,\frac{1}{2})$
$\mathbf{T}_d(/\mathbf{T}) = (2,2,0,2,0)$	$\Longrightarrow$	$\widetilde{\mathbf{T}}_d(/\mathbf{T}) = (-\frac{1}{2},\frac{1}{2},0,1,0)$
$\mathbf{T}_d(/\mathbf{T}_d) = (1,1,1,1,1)$	$\Longrightarrow$	$\widetilde{\mathbf{T}}_d(/\mathbf{T}_d) = (-\frac{1}{2},0,\frac{1}{2},\frac{1}{2},\frac{1}{2})$

3. Elements of markaracter tables

Each element of a markaracter table is called a *mark* in the present approach. The term "mark" involves the term "mark" of the previous mark approach [18] and the term "trace" of the character approach under appropriate conditions. Such usage may provide no confusion.

Marks can be evaluated by making a coset representation from a multiplication table of a group at issue. This method is essentially equivalent to the method described in Chapter 5 of Ref. [18] for treating usual mark tables. The purpose of this section is to consider the meaning of each value appearing in such a markaracter table.

Theorem 2. *Let* $\mathbf{G}$ *be a group of finite order. Suppose that* $\mathbf{G}_i$ *and* $\mathbf{G}_j$ *are cyclic subgroups of* $\mathbf{G}$ *and that* $\mathbf{G}_j$ *and its conjugate groups are not the subgroup of* $\mathbf{G}_i$ *satisfying* $|\mathbf{G}_j| \leq |\mathbf{G}_i|$. *Then, the mark for* $\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j$ *is equal to zero,* i.e., $m_{ij} = 0$

Proof. Let us consider a coset decomposition,

$$\mathbf{G} = \mathbf{G}_i t_1 + \mathbf{G}_i t_2 + \cdots + \mathbf{G}_i t_r, \tag{15}$$

where $t_1 = I$ (itentity). Assume that a coset $\mathbf{G}_i t_k$ is fixed on the action of $\forall g (\in \mathbf{G}_j)$. Since the stabilizer of $\mathbf{G}_i t_k$ is $t_k^{-1}\mathbf{G}_i t_k$, we have $g \in t_k^{-1}\mathbf{G}_i t_k$. This allows us to select $\exists g_i (\in \mathbf{G}_i)$ to satisfy $g = t_k^{-1} g_i t_k$, or inversely $g_i = t_k g t_k^{-1}$. Since g moves over $\mathbf{G}_j$, we obtain

$$t_k^{-1}\mathbf{G}_j t_k = \{g_i\} \subset \mathbf{G}_i \tag{16}$$

This contradicts the assumption. Any representative t_k can be selected from the transversal associated with the coset decomposition. Hence, such fixed points (cosets) are absent. In other words, the mark for $\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j$ is equal to zero, *i.e.*, $m_{ij} = 0$ □

The following theorem gives the diagonal entries of a markaracter table. This theorem also holds for a non-cyclic subgroup.

Theorem 3. *Let* $\mathbf{G}_i$ *be a cyclic subgroup of* $\mathbf{G}$ *of finite order. Then, the mark for* $\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_i$ *(*m_{ii}*) is represented as follows.*

$$m_{ii} = \frac{|\mathbf{N_G}(\mathbf{G}_i)|}{|\mathbf{G}_i|}, \tag{17}$$

where $\mathbf{N_G}(\mathbf{G}_i)$ *is the normalizer of* $\mathbf{G}_i$ *within the group* $\mathbf{G}$.

Proof. Let us consider a coset representation of the normalizer $\mathbf{N_G}(\mathbf{G}_i)$ by $\mathbf{G}_i$.

$$\mathbf{N_G}(\mathbf{G}_i) = \mathbf{G}_i t_1 + \mathbf{G}_i t_2 + \cdots + \mathbf{G}_i t_r, \tag{18}$$

where $t_1 = I$ and r is equal to the number of the conjugate subgroups of $\mathbf{G}_i$ within $\mathbf{G}$, *i.e.*,

$$r = \frac{|\mathbf{N_G}(\mathbf{G}_i)|}{|\mathbf{G}_i|}. \tag{19}$$

By using eq. 18, a coset decomposition of $\mathbf{G}$ by $\mathbf{G}_i$ can be written as follows,

$$\begin{aligned} \mathbf{G} &= \mathbf{N_G}(\mathbf{G}_i)s_1 + \mathbf{N_G}(\mathbf{G}_i)s_2 + \cdots + \mathbf{N_G}(\mathbf{G}_i)t_p \\ &= \mathbf{G}_i s_{11} + \mathbf{G}_i s_{21} + \cdots + \mathbf{G}_i s_{r1} \\ &\quad + \mathbf{G}_i s_{12} + \mathbf{G}_i s_{22} + \cdots + \mathbf{G}_i s_{r2} + \cdots \end{aligned} \tag{20}$$

where $s_1 = I$, $s_{k\ell} = t_k s_\ell$ and

$$p = \frac{|\mathbf{G}|}{|\mathbf{N_G}(\mathbf{G}_i)|}. \tag{21}$$

The following cosets appearing in eq. 20,

$$\mathbf{G}_i s_{11} (= \mathbf{G}_i t_1), \quad \mathbf{G}_i s_{21} (= \mathbf{G}_i t_2), \cdots, \mathbf{G}_i s_{r1} (= \mathbf{G}_i t_r), \tag{22}$$

are respectively fixed by

$$s_{11}^{-1}\mathbf{G}_i s_{11} = s_{21}^{-1}\mathbf{G}_i s_{21} = \cdots = s_{r1}^{-1}\mathbf{G}_i s_{r1} (= \mathbf{G}_i). \tag{23}$$

These are identical with $\mathbf{G}_i$, since the cosets represented by eq. 22 appears in the coset representation (eq. 18) and $\mathbf{N_G}(\mathbf{G}_i)$ is the normalizer of $\mathbf{G}_i$. This means that the cosets (eq. 22) are fixed under the action of $g \in \mathbf{G}_i$. Moreover, g can be proved not to fix the remaining cosets appearing in eq. 20, whose stabilizers are the respective subgroups conjugate to $\mathbf{G}_i$. Hence, eq. 17 is equal to the mark m_{ii} of $\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_i$, *i.e.*,

$$m_{ii} = r = \frac{|\mathbf{N_G}(\mathbf{G}_i)|}{|\mathbf{G}_i|}. \tag{24}$$

□

Theorem 4. *Let* $\mathbf{G}_j$ *be a cyclic subgroup of* $\mathbf{G}_i$, *which is in turn a cyclic subgroup of* $\mathbf{G}$ *of finite order.*

1. *The cyclic group* $\mathbf{G}_i$ *contains only one cyclic subgroup whose order is equal to a divisor of* $|\mathbf{G}_i|$.
2. *The nomalizer* $\mathbf{N_G}(\mathbf{G}_j)$ *is identical with the normalizer* $\mathbf{N_G}(\mathbf{G}_i)$.

Proof.

1. Abbreviated.

2. Assume that $g^{-1}\mathbf{G}_j g \neq \mathbf{G}_j$ for $\exists g \in \mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)$. Obviously, we have $g \notin \mathbf{G}_j$. Moreover, the preceding proposition indicates that $g \notin \mathbf{G}_i$. This means that, in $\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)$, $\mathbf{G}_i$ containing $\mathbf{G}_j$ is distinct but conjugate to $g^{-1}\mathbf{G}_i g$ containing $g^{-1}\mathbf{G}_j g$, *i.e.* $g^{-1}\mathbf{G}_i g \neq \mathbf{G}_i$. This contradicts the assumption that g is an element of the normalizer $\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)$. □

Theorem 5. *Let $\mathbf{G}_j$ be a cyclic subgroup of $\mathbf{G}_i$, which is in turn a cyclic subgroup of $\mathbf{G}$ of finite order. Then, the mark for $\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j$ (m_{ij}) is equal to that for $\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_i$ (m_{ii}), which is represented as follows.*

$$m_{ij} = m_{ii} = \frac{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)|}{|\mathbf{G}_i|}, \tag{25}$$

where $\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)$ is the normalizer of $\mathbf{G}_i$ within the group $\mathbf{G}$.

Proof. Since $\mathbf{G}_i$ and $\mathbf{G}_i$ have the common normalizer $\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)$, the equation, $t_k^{-1}\mathbf{G}_i t_k = \mathbf{G}_i \iff t_k^{-1}\mathbf{G}_j t_k = \mathbf{G}_j$, holds true for any t_k of eq. 18. This means that the mark for $\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j$ (m_{ij}) is equal to that for $\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_i$ (m_{ii}). Note that $t_k^{-1}\mathbf{G}_i t_k$ is only one cyclic subgroup of $t_k^{-1}\mathbf{G}_j t_k$ whose order is equal to $|\mathbf{G}_j|$. Hence, eq. 17 gives eq. 25 to be proved. □

We easily obtain the following theorem that is concerned with an identity group $\mathbf{G}_1$ $(= \mathbf{C}_1)$.

Theorem 6. *Let $\mathbf{G}_i$ be a cyclic subgroup of $\mathbf{G}$ of finite order. Then, the mark for $\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_1$ (m_{i1}) is represented by*

$$m_{i1} = \frac{|\mathbf{G}|}{|\mathbf{G}_i|}. \tag{26}$$

In the light of Theorems 2–6, the elements of a dominant markaracter (eq. 3) are evaluated, giving a markaracter table. The following equation is derived from Theorem 3 and 6,

$$\frac{m_{i1}}{m_{ii}} = \frac{|\mathbf{G}|}{|\mathbf{G}_i|} \times \frac{|\mathbf{G}_i|}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)|} = \frac{|\mathbf{G}|}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)|}, \tag{27}$$

which is equal to the number of subgroups conjugate to $\mathbf{G}_i$ within the group $\mathbf{G}$.

4. Modified mark tables vs. markaracter tables

The purpose of this section is to show that the elements of a dominant markaracter table appear in the corresponding mark table and that the elements of its inverse also appear in the inverse of the mark table.

First, we define a *concurrent interchange* of an inverse pair (a matrix and its inverse) as an operation that involves interchange between the i-th row and the j-th row and between the i-th column and the j-th column for the matrix as well as simultaneous interchange between the i-th row and the j-th row and between the i-th column and the j-th column for the inverse matrix. Obviously, a pair of a matrix and its inverse is also an inverse pair after such concurrent interchanges.

Let us then consider concurrent interchanges of an inverse pair of a mark table $M_{\mathbf{G}}$ and its inverse $M_{\mathbf{G}}^{-1}$. We shall prove that the pair of $M_{\mathbf{G}}$ and $M_{\mathbf{G}}^{-1}$ remains a pair of lower triangular matrices after concurrent interchanges. For this purpose, we have a theorem concerning zero elements in a mark table.

Theorem 7. *Let* $\mathbf{G}$ *be a group of finite order. Suppose that* $\mathbf{G}_i$ *is a cyclic subgroup of* $\mathbf{G}$ *and that* $\mathbf{G}_j$ *is a non-cyclic subgroup of* $\mathbf{G}$*(*$\mathbf{G}_i \leq \mathbf{G}_j$*). Then, the mark for* $\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j$ *is equal to zero.*

Proof. Let us consider a coset representation represented by eq. 15. Assume that a coset $\mathbf{G}_i t_k$ is fixed on the action of $\forall g(\in \mathbf{G}_j)$. Since the stabilizer of $\mathbf{G}_i t_k$ is $t_k^{-1}\mathbf{G}_i t_k$, we have $g \in t_k^{-1}\mathbf{G}_i t_k$. Since g moves over $\mathbf{G}_j$, we obtain

$$\mathbf{G}_j \subset t_k^{-1}\mathbf{G}_i t_k. \tag{28}$$

Since $\mathbf{G}_i$ is cyclic, its conjugate subgroup $t_k^{-1}\mathbf{G}_i t_k$ also cyclic. Hence, eq. 28 indicates that $\mathbf{G}_j$ should be cyclic, because a subgroup of a cyclic group is also cyclic in general. This contradicts the assumption. Any representative t_k can be selected from the transversal associated with the coset decomposition. It follows that such fixed points (cosets) are absent. Namely, the mark for $\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j$ is equal to zero. □

Theorem 7 allows us to carry out consecutive concurrent interchanges of a pair of a mark table $M_{\mathbf{G}}$ and its inverse $M_{\mathbf{G}}^{-1}$ so that the resulting matrices (a *modified mark table* and its inverse) are also lower triangular matrices, where the elements corresponding to cyclic subgroups are gathered into the upperleft parts of the respective matrices. The parts are selected to be a dominant markaracter table and its inverse, since any upperleft square of a lower triangular matrix is inverse to the corresponding part of its inverse matrix.

In accord with the consecutive concurrent interchanges, the corresponding $SCR_{\mathbf{G}}$ is transformed into a *modified set of coset representations* (MSCR),

$$MSCR_{\mathbf{G}} = \{\mathbf{G}(/\mathbf{G}_1), \mathbf{G}(/\mathbf{G}_2), \ldots, \mathbf{G}(/\mathbf{G}_s), \mathbf{G}(/\mathbf{G}_{s+1}), \ldots, \mathbf{G}(/\mathbf{G}_t)\}, \tag{29}$$

where the CRs $\mathbf{G}(/\mathbf{G}_i)$ for $i = 1$ to s are identical with those of $SDR_{\mathbf{G}}$ (eq. 2) and the remaining CRs are concerned with non-cyclic subgroups of $\mathbf{G}$.

For illustrating this treatment, Tables 5 and 6 show a modified mark table and its inverse that are generated by the concurrent interchanges of the mark table for $\mathbf{D}_{3h}$ [18]. The upperleft squares (a markaracter table and its inverse for $\mathbf{D}_{3h}$) are respectively designated by dividing with a vertical and a horizontal line. Note that the original position of the row $\mathbf{D}_{3h}(/\mathbf{C}_{3h})$ is between the rows $\mathbf{D}_{3h}(/\mathbf{C}_{3v})$ and $\mathbf{D}_{3h}(/\mathbf{D}_3)$ in the mark table reported in Appendix A.2 of Ref. [18].

Table 5. Modified mark table for $\mathbf{D}_{3h}$

$M_{\mathbf{D}_{3h}}$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}'_s$	$\mathbf{C}_3$	$\mathbf{C}_{3h}$	$\mathbf{C}_{2v}$	$\mathbf{C}_{3v}$	$\mathbf{D}_3$	$\mathbf{D}_{3h}$
$\mathbf{D}_{3h}(/\mathbf{C}_1)$	12	0	0	0	0	0	0	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_2)$	6	2	0	0	0	0	0	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_s)$	6	0	2	0	0	0	0	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}'_s)$	6	0	0	6	0	0	0	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_3)$	4	0	0	0	4	0	0	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_{3h})$	2	0	0	2	2	2	0	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_{2v})$	3	1	1	3	0	0	1	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_{3v})$	2	0	2	0	2	0	0	2	0	0
$\mathbf{D}_{3h}(/\mathbf{D}_3)$	2	2	0	0	2	0	0	0	2	0
$\mathbf{D}_{3h}(/\mathbf{D}_{3h})$	1	1	1	1	1	1	1	1	1	1

Table 6. Inverse matrix of the modified mark table for $\mathbf{D}_{3h}$

$M^{-1}_{\mathbf{D}_{3h}}$	$\mathbf{D}_{3h}(/\mathbf{C}_1)$	$\mathbf{D}_{3h}(/\mathbf{C}_2)$	$\mathbf{D}_{3h}(/\mathbf{C}_s)$	$\mathbf{D}_{3h}(/\mathbf{C}'_s)$	$\mathbf{D}_{3h}(/\mathbf{C}_3)$	$\mathbf{D}_{3h}(/\mathbf{C}_{3h})$	$\mathbf{D}_{3h}(/\mathbf{C}_{2v})$	$\mathbf{D}_{3h}(/\mathbf{C}_{3v})$	$\mathbf{D}_{3h}(/\mathbf{D}_3)$	$\mathbf{D}_{3h}(/\mathbf{D}_{3h})$	sum
$\mathbf{C}_1$	$\frac{1}{12}$	0	0	0	0	0	0	0	0	0	$\frac{1}{12}$
$\mathbf{C}_2$	$-\frac{1}{4}$	$\frac{1}{2}$	0	0	0	0	0	0	0	0	$\frac{1}{4}$
$\mathbf{C}_s$	$-\frac{1}{4}$	0	$\frac{1}{2}$	0	0	0	0	0	0	0	$\frac{1}{4}$
$\mathbf{C}'_s$	$-\frac{1}{12}$	0	0	$\frac{1}{6}$	0	0	0	0	0	0	$\frac{1}{12}$
$\mathbf{C}_3$	$-\frac{1}{12}$	0	0	0	$\frac{1}{4}$	0	0	0	0	0	$\frac{1}{6}$
$\mathbf{C}_{3h}$	$\frac{1}{12}$	0	0	$-\frac{1}{6}$	$-\frac{1}{4}$	$\frac{1}{2}$	0	0	0	0	$\frac{1}{6}$
$\mathbf{C}_{2v}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	0	0	1	0	0	0	0
$\mathbf{C}_{3v}$	$\frac{1}{4}$	0	$-\frac{1}{2}$	0	$-\frac{1}{4}$	0	0	$\frac{1}{2}$	0	0	0
$\mathbf{D}_3$	$\frac{1}{4}$	$-\frac{1}{2}$	0	0	$-\frac{1}{4}$	0	0	0	$\frac{1}{2}$	0	0
$\mathbf{D}_{3h}$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	0

5. Markaracter tables and conjugacy classes

The purpose of this section is to indicate that markaracter tables proposed in the present paper are closely related to character tables. This requires the relationship between conjugate cyclic subgroups and conjugacy classes.

Theorem 8. *Let* $\mathbf{G}$ *be a group of finite order. Select an element* g *(*$\in \mathbf{G}$*) as a generator and construct a cyclic group* $\langle g \rangle$,

$$\mathbf{G}_i = \langle g \rangle = \{g, g^2, \ldots, g^r, \ldots, g^n (= I)\}. \tag{30}$$

1. *Let* r *be a divisor of* n *satifying* $1 < r < n$. *Then the cyclic group* $\langle g^r \rangle$ *generated by* g^r *is a subgroup of* $\mathbf{G}_i$ *(Case 1).*
2. *Let* r *and* n *be coprime, satifying* $1 < r < n$. *Then the cyclic group* $\langle g^r \rangle$ *generated by* g^r *is identical with* $\mathbf{G}_i$ *(Case 2).*
3. *Whether* g^r *belongs to Case 1 or 2, the inverse element* g^{-1} *generates the same group as* $\langle g^r \rangle$.

Proof.

1. We have $n = mr$ where m is a positive integer. Hence the group at issue,

$$\langle g^r \rangle = \{g^r, g^{2r}, \ldots, g^{kr}, \ldots, g^{mr} (= I)\}, \tag{31}$$

satisfies $g^{mr} = g^n = I$. This means that the group $\langle g^r \rangle$ is a cyclic group of order m. Since the elements of $\langle g^r \rangle$ are involved in $\langle g \rangle$, the group $\langle g^r \rangle$ is a subgroup of $\langle g \rangle$.

2. Since n and r are coprime, the number nr is the least common multiple. Hence the group at issue,

$$\langle g^r \rangle = \{g^r, g^{2r}, \ldots, g^{kr}, \ldots, g^{nr} (= I)\}, \tag{32}$$

satisfies $g^{nr} = (g^n)^r = I$. Suppose that an integer k satisfies $1 < k \leq n$ and $g^{kr} = I$. This means that kr is a multiple of n because $g^n = I$. Since r and n are coprime, k should be a multiple of n. The presumption $1 < k \leq n$ provides the equality $n = r$. Thus, the groups $\langle g \rangle$ and $\langle g^r \rangle$ have the same order and contain a common element g^r. Hence, they are concluded to be identical.

3. Since we have $g^{-nr} = (g^n)^{-r} = I$ and $g^{kr}g^{-kr} = I$, the group $\langle g^{-r}\rangle$:

$$\langle g^{-r}\rangle = \{g^{-r}, g^{-2r}, \ldots, g^{-kr}, \ldots, g^{nr}(= I)\} \tag{33}$$

is identical with $\langle g^{r}\rangle$ for Case 2. Case 1 can be similarly proved. □

The proof of Theorem 8 is essetially equivalent to the procedure described for Lemma 2 in Ref. [22], though the latter has been concerned with concrete cycle structures.

It should be noted that g^r and g^{-r} contained in a cyclic group $\mathbf{G}$ belong to different conjugacy classes but they belong to the same subgroup $\langle g^r\rangle$ (= $\langle g^{-r}\rangle$), where each element of the cyclic group $\mathbf{G}$ constructs a conjugacy class. Thus, there are cases in which two (or more) conjugacy classes correspond to a cyclic subgroup $\mathbf{G}_i$ as well as cases in which they correspond to each other in one-to-one fashion. In order to treat these cases, we define a *dominant class* as a disjoint set of conjugacy classes that correspond to the same dominant subgroup.

Theorem 9. *Suppose that the cyclic subgroup* $\mathbf{G}_i$ *defined in Theorem 8 involves an SCSG:*

$$SCSG_{\mathbf{G}_i} = \{\mathbf{G}_1^{(i)}, \mathbf{G}_2^{(i)}, \ldots, \mathbf{G}_t^{(i)}\} \tag{34}$$

$$(|\mathbf{G}_1^{(i)}| \leq |\mathbf{G}_2^{(i)}| \leq \cdots \leq |\mathbf{G}_t^{(i)}|), \tag{35}$$

Let N be the number of elements contained in a dominant class $\mathbf{K}$ *which is concerned with the subgroup* $\mathbf{G}_i$*. These elements are involved in* $\mathbf{G}_i - \bigcup_{\ell=1}^{t-1} \mathbf{G}_\ell^{(i)}$*, where the group corresponding to $\ell = t$ is excluded because* $\mathbf{G}_i = \mathbf{G}_\ell^{(t)}$.

$$N = |\mathbf{G}_i - \bigcup_{\ell=1}^{t-1} \mathbf{G}_\ell^{(i)}| = \varphi(|\mathbf{G}_i|), \tag{36}$$

where $\varphi(|\mathbf{G}_i|)$ *represents Euler's function for interger* $|\mathbf{G}_i|$.

Proof. The elements of $\mathbf{G}_i$ are classified into either one of the cases described above. The elements of Case 1 are involved in $\bigcup_{\ell=1}^{t-1} \mathbf{G}_\ell^{(i)}$, since the cyclic group $\mathbf{G}_i$ contains only one subgroup whose order is equal to each divisor of $|\mathbf{G}_i|$. Hence the elements of Case 2 are concluded to belong to the set $\mathbf{G}_i - \bigcup_{\ell=1}^{t-1} \mathbf{G}_\ell^{(i)}$. It follows that

$$N = |\mathbf{G}_i - \bigcup_{\ell=1}^{t-1} \mathbf{G}_\ell^{(i)}| = \varphi(|\mathbf{G}_i|), \tag{37}$$

□

Theorem 10. *Let* $\mathbf{G}$ *be a group of finite order and* $\mathbf{K}'$ *a conjugacy class of* $\mathbf{G}$*. Select elements g_1 and g_2 ($\in$* $\mathbf{K}'$*) as generators and construct cyclic groups $\langle g_1\rangle$ and $\langle g_2\rangle$. Then $\langle g_1\rangle$ and $\langle g_2\rangle$ are conjugate in the group* $\mathbf{G}$.

Proof. Let us consider $\langle g_1\rangle = \mathbf{G}_i$ generated by g_1 ($\in \mathbf{K}'$):

$$\mathbf{G}_i = \langle g_1\rangle = \{g_1, g_1^2, \ldots, g_1^r, \ldots, g_1^n(= I)\} \tag{38}$$

Since the elements g_1 and g_2 are conjugate, we can write $g_2 = g^{-1}g_1g(g \in \mathbf{G})$. Thereby, we have

$$g_2^r = \underbrace{g^{-1}g_1g \cdot g^{-1}g_1g \cdots g^{-1}g_1g}_{r} = g^{-1}g_1^r g, \tag{39}$$

wherein $r = 1, 2, \ldots, n$ and $g_2^n = g^{-1}g_n^r g = I$. It follows that the group,

$$\mathbf{G}_j = \langle g_2 \rangle = \{g_2, g_2^2, \ldots, g_2^r, \ldots, g_2^n (= I)\} = g^{-1}\mathbf{G}_i g, \tag{40}$$

is conjugate to $\mathbf{G}$. □

Let us consider a case, $\mathbf{G}_j = g^{-1}\mathbf{G}_i g = \mathbf{G}_i$, in eq. 40 as a special one. This means that an appropriate g_1^r appearing in eq. 38 is equal to g_2 ($\in \mathbf{G}_j$). This selection corresponds to the case 2 of Theorem 8. This discussion can be summarized as a corollary.

Corollary 1. *In Theorem 10, let g_2 be an element of $\langle g_1 \rangle$,* i.e., $g_2 = g_1^r$. *Then $|\mathbf{G}_i|$ ($=|\langle g_1 \rangle|$) and r are coprime.*

Since any representative is selected from conjugate subgroups in the present approach, Theorem 10 permits us to select a *representative cyclic subgroup* $\mathbf{G}_i$ that corresponds to a conjugacy class $\mathbf{K}'$, more precisely to a dominant class containing $\mathbf{K}'$. The subgroup $\mathbf{G}_i$ is definitely determined when conjugate subgroups are regarded as being equivalent.

Theorem 11. *Let $\mathbf{G}_i$ be a representative cyclic subgroup corresponding to a dominant class $\mathbf{K}$ of $\mathbf{G}$. The number ($n_{\mathbf{K}}$) of the elements contained in the class $\mathbf{K}$ is represented by*

$$n_{\mathbf{K}} = \frac{|\mathbf{G}|\varphi(|\mathbf{G}_i|)}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)|}, \tag{41}$$

wherein $\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)$ is the normalizer of $\mathbf{G}_i$ within the group $\mathbf{G}$.

Proof. In the light of Theorem 10, the element of $\mathbf{K}$ can be classified into m conjugated subgroups,

$$\mathbf{G}_i, \quad g_2^{-1}\mathbf{G}_i g_2, \quad g_3^{-1}\mathbf{G}_i g_3, \quad \ldots, \quad g_m^{-1}\mathbf{G}_i g_m, \tag{42}$$

where each subgroup contains the same number of elements of $\mathbf{K}$. Since Theorem 8 gives the number N for each of the conjugate subgroups, we have

$$Nm = n_{\mathbf{K}}. \tag{43}$$

On the other hand, the number m is evaluated by the equation,

$$m = \frac{|\mathbf{G}|}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)|}. \tag{44}$$

Equations 43 and 44 yield

$$n_{\mathbf{K}} = Nm = \frac{|\mathbf{G}|\varphi(|\mathbf{G}_i|)}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)|}. \tag{45}$$

□

Theorem 12. *Suppose that a cyclic group* $\mathbf{G}$ *of finite order is divided into a set of s dominant classes,*

$$\mathbf{K}_1, \mathbf{K}_2, \ldots, \mathbf{K}_s \tag{46}$$

and that the corresponding cyclic subgroups construct an an SCSG:

$$SCSG_{\mathbf{G}} = \{\mathbf{G}_1, \mathbf{G}_2, \ldots, \mathbf{G}_s\} \quad (|\mathbf{G}_1| \leq |\mathbf{G}_2| \leq \cdots \leq |\mathbf{G}_s|), \tag{47}$$

Then we have

$$\sum_{i=1}^{s} \frac{\varphi(|\mathbf{G}_i|)}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)|} = 1. \tag{48}$$

Proof. By using Theorem 11, the number of elements contained in $\mathbf{K}_i$ is represented by

$$n_{\mathbf{K}_i} = \frac{|\mathbf{G}|\varphi(|\mathbf{G}_i|)}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)|}. \tag{49}$$

These are summed up over all of the conjugacy classes, giving the order of $\mathbf{G}$, *i.e.*,

$$|\mathbf{G}| = \sum_{i=1}^{s} n_{\mathbf{K}_i} = \sum_{i=1}^{s} \frac{|\mathbf{G}|\varphi(|\mathbf{G}_i|)}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_i)|}. \tag{50}$$

When the both sides of the equation are divided by $|\mathbf{G}|$, we obtain eq. 48 to be proved. □

6. Orbit indices

In order to characterize multiplicity vectors defined above, we further introduce orbit indices.

Definition 1. *The orbit index of a multiplicity vector is defined by the equation,*

$$\widetilde{\Delta} = \sum_{i=1}^{s} \widetilde{\alpha}_i, \tag{51}$$

where each $\widetilde{\alpha}_i$ *is calculated by eq. 7.*

From each $\widetilde{\alpha}_i$ appearing in eq. 9, the orbit index is calculated as follows, since two summantion processes can be inversed.

Theorem 13.

$$\widetilde{\Delta} = \sum_{i=1}^{s} \widetilde{\alpha}_i = \sum_{i=1}^{s}\sum_{j=1}^{s} x_j \overline{m}_{ji} = \sum_{j=1}^{s} x_j \left(\sum_{i=1}^{s} \overline{m}_{ji}\right) \tag{52}$$

$$= \sum_{j=1}^{s} \frac{x_j \varphi(|\mathbf{G}_j|)}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_j)|}. \tag{53}$$

Equation 53 is derived from Theorem 16.2 of the book [18], since the subgroups $\mathbf{G}_j$ are cyclic, *i.e.*,

$$\sum_{i=1}^{s} \overline{m}_{ji} = \frac{\varphi(|\mathbf{G}_j|)}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_j)|} \quad (j = 1, 2, \ldots, s) \tag{54}$$

where $\varphi(|\mathbf{G}_j|)$ represents Euler's function and $\mathbf{N}_{\mathbf{G}}(\mathbf{G}_j)$ is the normalizer of $\mathbf{G}_j$ within the group $\mathbf{G}$.

Let us consider $MSCR_{\mathbf{G}}$ shown in eq. 29. Let a row vector $\mathbf{X}$ be a vector of a fixed-point vector space which is associated with the modified mark table of $\mathbf{G}$,

$$\mathbf{X} = (x_1, x_2, \ldots, x_s, x_{s+1}, \ldots, x_t), \tag{55}$$

where the top s elements are equal to those of a vector of a dominant fixed-point vector space. Corollary 5.2 (Ref. [18]) described for $SCR_{\mathbf{G}}$ can be modified to give the total number (Δ) of orbits,

$$\Delta = \sum_{j=1}^{t} x_j \left(\sum_{i=1}^{t} \overline{m}_{ji} \right) \tag{56}$$

Since the modified mark table is generated by the concurrent interchange, we are able to obtain the following equation.

$$\sum_{i=1}^{t} \overline{m}_{ji} = \begin{cases} \sum_{i=1}^{s} \overline{m}_{ji} & \text{for cyclic } \mathbf{G}_j, \quad (57a) \\ 0 & \text{for non-cyclic } \mathbf{G}_j, \quad (57b) \end{cases}$$

where the latter zero value is based on Theorem 16.2 of the book [18]. This result allows us to equalize eqs. 52 and 56, *i.e.*,

$$\Delta = \sum_{j=1}^{t} x_j \left(\sum_{i=1}^{t} \overline{m}_{ji} \right) = \sum_{j=1}^{s} x_j \left(\sum_{i=1}^{s} \overline{m}_{ji} \right) = \widetilde{\Delta} \tag{58}$$

It should be noted that the elements of $\mathbf{X}$ (x_{s+1} to x_t in eq. 55) have no effects on the value of Δ. Hence, we arrive at a simple but important theorem.

Theorem 14. *An orbit index is an invariant during the transformation between a fixed-point vector space and a markaracter space,* i.e.,

$$\widetilde{\Delta} = \Delta \tag{59}$$

When a row vector $\mathbf{X}$ is selected from a modified mark table of $\mathbf{G}$, the top s elements of eq. 55 (x_1 to x_s) are equal to those for the corresponding dominant markaracter table. Since the $\mathbf{X}$ is associated with one orbit, we arrive at the following theorem.

Theorem 15. *When a row vector $x_j = \sum_{i=1}^{s} \widetilde{\alpha}_i m_{ij}$ is obtained for one coset representation $\mathbf{G}(/\mathbf{G}_j)$, the orbit index is expressed by the following equation.*

$$\widetilde{\Delta} = \sum_{i=1}^{s} \widetilde{\alpha}_i = \sum_{i=1}^{s} \sum_{j=1}^{s} x_j \overline{m}_{ji} = \sum_{j=1}^{s} x_j \left(\sum_{i=1}^{s} \overline{m}_{ji} \right) = \Delta = 1, \tag{60}$$

where the subgroup $\mathbf{G}_j$ is not always cyclic, but all of the subgroups $\mathbf{G}_i$ are cyclic.

The theorem gives a necessary condition for assigning a sum of dominant representations (DRs) to a coset representation. It is exemplified by inspection of the multiplicity vectors collected in Table 4.

7. Subdominant markaracter tables

We have discussed the consecutive concurrent interchange of a mark table (and its inverse) to produce a markaracter table (and its inverse). The operation is based on Theorem 7. In the light of the corresponding theorem (Theorem 2), the same procedure can be applied to the resulting (dominant) markaracter table (and its inverse), giving a subdominant markaracter table (and its inverse).

Let $\mathbf{G}_j$ be a subgroup of $\mathbf{G}$ which is a group of finite order. Note that $\mathbf{G}_j$ and $\mathbf{G}$ are cyclic or non-cyclic. The group $\mathbf{G}_j$ has a non-redundant set of cyclic subgroups, *i.e.*,

$$SCSG_{\mathbf{G}_j} = \{\mathbf{G}_1^{(j)}, \mathbf{G}_2^{(j)}, \ldots, \mathbf{G}_r^{(j)}\} \tag{61}$$

Let us select CRs of $\mathbf{G}$ corresponding to the $SCSG_{\mathbf{G}_j}$. They construct a *non-redundant set of subdominant representations* (SSDR), *i.e.*,

$$SSDR_{\mathbf{G}\downarrow\mathbf{G}_j} = \{\mathbf{G}\downarrow\mathbf{G}_j(/\mathbf{G}_1^{(j)}), \mathbf{G}\downarrow\mathbf{G}_j(/\mathbf{G}_2^{(j)}), \ldots, \mathbf{G}\downarrow\mathbf{G}_j(/\mathbf{G}_r^{(j)})\}. \tag{62}$$

The CRs contained in the SSDR are called subdominant representations. It should be noted that each CR is selected from $SDR_{\mathbf{G}}$. Hence, the degree of each CR is representated by $|\mathbf{G}|/|\mathbf{G}_k^{(j)}|$ for $k = 1, 2, \ldots, r$.

Each CR of $SSDR_{\mathbf{G}}$ (*i.e.*, $\mathbf{G}\downarrow\mathbf{G}_j(/\mathbf{G}_k^{(j)})$) corresponds to a subdominant markaracter, the elements of which are selected from the corresponding markaracter table. This process is permitted on the basis of Theorem 2. Thus, we have a subdominant markaracter,

$$\begin{aligned} \mathbf{G}\downarrow\mathbf{G}_j(/\mathbf{G}_k^{(j)}) &= (m_{k1}^{(j)}, m_{k2}^{(j)}, \ldots, m_{kk}^{(j)}, \ldots, m_{kr}^{(j)}) \\ &= (m_{k1}^{(j)}, m_{k2}^{(j)}, \ldots, m_{kk}^{(j)}, 0, \ldots, 0) \quad \text{for } k = 1, 2, \ldots r, \end{aligned} \tag{63}$$

which is uniquely determined once the $SSDR_{\mathbf{G}}$ is selected. Note that j is tentatively fixed.

Such subdominant markaracters are collected to form a subdominant markaracter table (SDMT), which is lower triangular because of Theorem 2.

$$\widetilde{\widetilde{\mathbf{M}}}_{\mathbf{G}\downarrow\mathbf{G}_j} = (m_{jk}^{(j)}) =$$

$$\begin{array}{c} \\ \mathbf{G}\downarrow\mathbf{G}_j(/\mathbf{G}_1^{(j)}) \\ \mathbf{G}\downarrow\mathbf{G}_j(/\mathbf{G}_2^{(j)}) \\ \vdots \\ \mathbf{G}\downarrow\mathbf{G}_j(/\mathbf{G}_k^{(j)}) \\ \vdots \\ \mathbf{G}\downarrow\mathbf{G}_j(/\mathbf{G}_r^{(j)}) \end{array} \begin{array}{c} \begin{array}{cccccc} \downarrow\mathbf{G}_1^{(j)} & \downarrow\mathbf{G}_2^{(j)} & \cdots & \downarrow\mathbf{G}_k^{(j)} & \cdots & \downarrow\mathbf{G}_s^{(j)} \end{array} \\ \left(\begin{array}{cccccc} m_{11}^{(j)} & & & & & \\ m_{21}^{(j)} & m_{22}^{(j)} & & & & \\ \vdots & \vdots & \ddots & & & \\ m_{k1}^{(j)} & m_{k2}^{(j)} & \cdots & m_{kk}^{(j)} & & \\ \vdots & \vdots & & \vdots & \ddots & \\ m_{r1}^{(j)} & m_{r2}^{(j)} & \cdots & m_{rk}^{(j)} & \cdots & m_{rr}^{(j)} \end{array} \right) \end{array} \tag{64}$$

where the elements of subdominant markaracter are called *marks*, omitting zeros above the main diagonal. The set of subdominant markaracter defined by eq. 63 spans a *subdominant markaracter space* of order r.

The construction of the subdominant markaracter table corresponds to the evaluation of each mark during $[\mathbf{G}\downarrow\mathbf{G}_j(/\mathbf{G}_k^{(j)})]\downarrow\mathbf{G}_\ell^{(j)}$, where $k = 1, 2, \ldots, r$ and $\ell = 1, 2, \ldots, r$. Theorem 2 (concurrent interchanges constructing a subdominant markaracter table from a markaracter table) means that the process can alternatively be interpreted; thus, we directly consider subduced representations of CRs, $\mathbf{G}(/\mathbf{G}_k^{(j)}) \downarrow \mathbf{G}_\ell^{(j)}$, after which the elements concerning $\mathbf{G}_j$ (*i.e.* $k = 1, 2, \ldots, r$ and $\ell = 1, 2, \ldots, r$) are gathered. The two notations, $[\mathbf{G} \downarrow \mathbf{G}_j(/\mathbf{G}_k^{(j)})] \downarrow \mathbf{G}_\ell^{(j)}$ (selection and subduction) *vs.* $\mathbf{G}(/\mathbf{G}_k^{(j)}) \downarrow \mathbf{G}_\ell^{(j)}$ (subduction and selection), express the conceptual difference between their procedures, but give the same subdominant markaracter table.

Table 7 shows a subdominant markaracter table for the process $\mathbf{T}_d \downarrow \mathbf{C}_{3v}$. Note that the process $\mathbf{T}_d \downarrow \mathbf{C}_{3v}$ corresponds to a a non-redundant set of subdominant representations (SSDR):

$$SSDR_{\mathbf{T}_d\downarrow\mathbf{C}_{3v}} = \{\mathbf{T}_d \downarrow \mathbf{C}_{3v}(/\mathbf{C}_1), \mathbf{T}_d \downarrow \mathbf{C}_{3v}(/\mathbf{C}_s), \mathbf{T}_d \downarrow \mathbf{C}_{3v}(/\mathbf{C}_3)\} \tag{65}$$

The corresponding inverse matrix (Table 3) is also used in the present treatment.

Table 7. Subdominant markaracter table for $\mathbf{T}_d \downarrow \mathbf{C}_{3v}$

$\widetilde{\widetilde{\mathrm{M}}}_{\mathbf{T}_d\downarrow\mathbf{C}_{3v}}$	$\mathbf{C}_1$	$\mathbf{C}_s$	$\mathbf{C}_3$
$\mathbf{T}_d \downarrow \mathbf{C}_{3v}(/\mathbf{C}_1)$	24	0	0
$\mathbf{T}_d \downarrow \mathbf{C}_{3v}(/\mathbf{C}_s)$	12	2	0
$\mathbf{T}_d \downarrow \mathbf{C}_{3v}(/\mathbf{C}_3)$	8	0	2

Table 8. Inverse matrix of the subdominant mMarkaracter table for $\mathbf{T}_d \downarrow \mathbf{C}_{3v}$

$\widetilde{\widetilde{\mathrm{M}}}^{-1}_{\mathbf{T}_d\downarrow\mathbf{C}_{3v}}$	$\mathbf{T}_d \downarrow \mathbf{C}_{3v}(/\mathbf{C}_1)$	$\mathbf{T}_d \downarrow \mathbf{C}_{3v}(/\mathbf{C}_s)$	$\mathbf{T}_d \downarrow \mathbf{C}_{3v}(/\mathbf{C}_3)$	sum
$\mathbf{C}_1$	$\frac{1}{24}$	0	0	$\frac{1}{24}$
$\mathbf{C}_s$	$-\frac{1}{4}$	$\frac{1}{2}$	0	$\frac{1}{4}$
$\mathbf{C}_3$	$-\frac{1}{6}$	0	$\frac{1}{2}$	$\frac{1}{3}$

On the other hand, we consider a non-redundant set of dominant representations (SDR) for the group $\mathbf{G}_j$:

$$SDR_{\mathbf{G}_j} = \{\mathbf{G}_j(/\mathbf{G}_1^{(j)}), \mathbf{G}_j(/\mathbf{G}_2^{(j)}), \ldots, \mathbf{G}_j(/\mathbf{G}_r^{(j)})\}, \tag{66}$$

The degree of each CR is representated by $|\mathbf{G}_j|/|\mathbf{G}_k^{(j)}|$ for $k = 1, 2, \ldots, r$.

Table 9 shows a (dominant) markaracter table for the group $\mathbf{C}_{3v}$. Note that the group $\mathbf{C}_{3v}$ has a a non-redundant set of dominant representations (SDR):

$$SDR_{\mathbf{C}_{3v}} = \{\mathbf{C}_{3v}(/\mathbf{C}_1), \mathbf{C}_{3v}(/\mathbf{C}_s), \mathbf{C}_{3v}(/\mathbf{C}_3)\} \tag{67}$$

The corresponding inverse matrix (Table 10) is also used in the present treatment.

The subdominant markaracter represented by eq. 63, *i.e.*, $\mathbf{G} \downarrow \mathbf{G}_j(/\mathbf{G}_k^{(j)})$, is concerned with the CR $\mathbf{G}(/\mathbf{G}_k^{(j)})$. On the other hand, the corresponding dominant markaracter $\mathbf{G}_j(/\mathbf{G}_k^{(j)})$ is concerned with the CR $\mathbf{G}_j(/\mathbf{G}_k^{(j)})$. In the light of Lemma 7.2 and eq. 7.11 of Ref. [18], these two CRs are related to each other by the induction,

$$\mathbf{G}_j(/\mathbf{G}_k^{(j)}) \uparrow \mathbf{G}(/\mathbf{G}_j) = \mathbf{G}(/\mathbf{G}_k^{(j)}). \tag{68}$$

Table 9. Markaracter table for $\mathbf{C}_{3v}$

$\widetilde{\mathbf{M}}_{\mathbf{C}_{3v}}$	$\mathbf{C}_1$	$\mathbf{C}_s$	$\mathbf{C}_3$
$\mathbf{C}_{3v}(/\mathbf{C}_1)$	6	0	0
$\mathbf{C}_{3v}(/\mathbf{C}_s)$	3	1	0
$\mathbf{C}_{3v}(/\mathbf{C}_3)$	2	0	2

Table 10. Inverse matrix of the markaracter table for $\mathbf{C}_{3v}$

$\widetilde{\mathbf{M}}^{-1}_{\mathbf{C}_{3v}}$	$\mathbf{C}_{3v}(/\mathbf{C}_1)$	$\mathbf{C}_{3v}(/\mathbf{C}_s)$	$\mathbf{C}_{3v}(/\mathbf{C}_3)$	sum
$\mathbf{C}_1$	$\frac{1}{6}$	0	0	$\frac{1}{6}$
$\mathbf{C}_s$	$-\frac{1}{2}$	1	0	$\frac{1}{2}$
$\mathbf{C}_3$	$-\frac{1}{6}$	0	$\frac{1}{2}$	$\frac{1}{3}$

This relationship is represented in the present approach by the following correspondence:

Theorem 16. *A dominant multiplicity vector, $\widetilde{\mathbf{G}} \downarrow \mathbf{G}_j(/\mathbf{G}_k^{(j)})$, corresponds to $\mathbf{G}(/\mathbf{G}_k^{(j)})$, while a multiplicty vector, $\widetilde{\mathbf{G}}_j(/\mathbf{G}_k^{(j)})$, corresponds to $\mathbf{G}_j(/\mathbf{G}_k^{(j)})$. In the light of the induction (eq. 68), we have the following expression.*

$$\widetilde{\mathbf{G}} \downarrow \mathbf{G}_j(/\mathbf{G}_k^{(j)}) = \widetilde{\mathbf{G}}_j(/\mathbf{G}_k^{(j)}) = (0, 0, \ldots, 0, \underbrace{1}_{\mathbf{G}_k^{(j)}}, 0, \ldots, 0). \tag{69}$$

whether fusions occur or not in the process of induction.

Proof. A row vector of the subdominant markaracter table satisfies

$$\mathbf{G} \downarrow \mathbf{G}_j(/\mathbf{G}_k^{(j)})\widetilde{\widetilde{\mathbf{M}}}^{-1}_{\mathbf{G}\downarrow\mathbf{G}_j} = \widetilde{\mathbf{G}} \downarrow \mathbf{G}_j(/\mathbf{G}_k^{(j)}) = (0, 0, \ldots, 0, \underbrace{1}_{\mathbf{G}_k^{(j)}}, 0, \ldots, 0). \tag{70}$$

On the other hand, the corresponding row vector of the dominant markaracter table satisfies

$$\mathbf{G}_j(/\mathbf{G}_k^{(j)})\widetilde{\mathbf{M}}^{-1}_{\mathbf{G}_j} = \widetilde{\mathbf{G}}_j(/\mathbf{G}_k^{(j)}) = (0, 0, \ldots, 0, \underbrace{1}_{\mathbf{G}_k^{(j)}}, 0, \ldots, 0). \tag{71}$$

Thus, they give the same unit row vector. □

Let us next consider the induction of $\mathbf{G}_j(/\mathbf{G}_j)$ to $\mathbf{G}$, *i.e.*,

$$\mathbf{G}_j(/\mathbf{G}_j) \uparrow \mathbf{G}(/\mathbf{G}_j) = \mathbf{G}(/\mathbf{G}_j). \tag{72}$$

Suppose that $\mathbf{G}(/\mathbf{G}_j)$ is associated to the following vector,

$$\begin{aligned} \mathbf{G} \downarrow \mathbf{G}_j(/\mathbf{G}_j)\widetilde{\widetilde{\mathbf{M}}}^{-1}_{\mathbf{G}\downarrow\mathbf{G}_j} &= \widetilde{\mathbf{G}} \downarrow \mathbf{G}_j(/\mathbf{G}_j) \\ = \sum_{k=1}^{r} \widetilde{\beta}_k \widetilde{\mathbf{G}} \downarrow \mathbf{G}_j(/\mathbf{G}_k^{(j)}) &= (\widetilde{\beta}_1, \widetilde{\beta}_2, \ldots, \widetilde{\beta}_r). \end{aligned} \tag{73}$$

computed by evaluating the terms in Eqs. (34)–(41) and then adding the contribution

$$\langle 0|\Delta \exp(-T)\exp(T)|0\rangle. \tag{45}$$

In Eq. (45), Δ is a composite operator

$$\Delta \equiv \mathscr{X} + r_0\mathscr{L}, \tag{46}$$

whose definition is motivated by pragmatism rather than physical significance. The most demanding programming is associated with the first task, as an existing ground state CC gradient program can be used to evaluate Eq. (45) by simply using matrix elements of Δ instead of the λ amplitudes. This is precisely the strategy that has been adopted in our implementation.

3 Guidelines for implementation

Although relatively simple conceptually, gradient equations such as Eq. (23) are not appropriate for numerical computations due to the inconvenience of evaluating $\partial f_{pq}/\partial\chi$ and $\partial\langle pq\|rs\rangle/\partial\chi$ explicitly. These quantities depend upon the first-order response of both the electronic Hamiltonian [in the atomic orbital basis] and the molecular orbital coefficients. Ideally, one seeks a formulation that avoids the latter since differentiated one- and two-electron integrals are readily calculated in the atomic orbital basis by standard Gaussian integral programs. An elegant means for eliminating the orbital response contribution was introduced more than a decade ago by Handy and Schaefer [57]. In this "z-vector" method – which is closely related to the approach used to eliminate the T amplitude response in CCSD and EOM-CCSD gradient theories – a linear equation involving the orbital rotation gradient and the self-consistent field orbital Hessian is solved. The resulting solution can be considered as part of a one-particle effective density d_q^p. Combining this with the perturbation dependence of the atomic orbitals allows Eq. (23) to be rewritten as

$$\frac{\partial E}{\partial\chi} = \sum_{pq} d_q^p f_{qp}^{(x)} + \sum_{pqrs} D_{rs}^{pq}\langle rs\|pq\rangle^{\chi} + I_{pq}S_{pq}^{\chi} \tag{47}$$

where S_{pq}^{χ} and $\langle rs\|pq\rangle^{\chi}$ are derivatives of the atomic orbital overlap and antisymmetrized two-electron integrals transformed to the unperturbed molecular orbital representation, $f_{pq}^{(x)}$ are Fock matrix elements evaluated with differentiated integrals and the unperturbed reference determinant density matrix, and the I_{pq} coefficients serve to enforce orthonormality of the perturbed molecular orbitals. The z-vector and I_{pq} coefficients depend parametrically on both the unperturbed Hamiltonian and matrix elements of D. Apart from a dependence on D [and therefore ρ and $\tilde{\rho}$], solution of the z-vector equations in EOM-CCSD gradient calculations requires no new theoretical insight or programming.

The paragraph above underscores a point that was emphasized throughout the previous section, namely that an existing CCSD gradient program already contains much of the code needed to calculate EOM-CCSD energy derivatives provided the strategy outlined here is followed. Specifically, the only significant additional programming tasks are: (1) evaluation of the ξ_a^i and ξ_{ab}^{ij} amplitudes; (2) solution of

Example 3. A subdominant markaracter is obtained to be $\mathbf{T}_d \downarrow \mathbf{D}_2(/\mathbf{C}_1) = (24, 0)$ and $\mathbf{T}_d \downarrow \mathbf{D}_2(/\mathbf{C}_2) = (12, 4)$. They are multiplied by $\tilde{\tilde{\mathbf{M}}}^{-1}_{\mathbf{T}_d\downarrow\mathbf{D}_2}$ to give

$$(24,0)\tilde{\tilde{\mathbf{M}}}_{\mathbf{T}_d\downarrow\mathbf{D}_2} = (24,0)\begin{pmatrix} \frac{1}{24} & 0 \\ -\frac{1}{8} & -\frac{1}{4} \end{pmatrix} = (1,0)$$

$$(12,4)\tilde{\tilde{\mathbf{M}}}_{\mathbf{T}_d\downarrow\mathbf{D}_2} = (12,4)\begin{pmatrix} \frac{1}{24} & 0 \\ -\frac{1}{8} & -\frac{1}{4} \end{pmatrix} = (0,1)$$

On the other hand, we have fused dominant markaracters, $\mathbf{D}_2(/\mathbf{C}_1) = (4, 0)$ and $\mathbf{D}_2(/\mathbf{C}_2) = (2, 2)$, by omitting the rows and columns for $\downarrow \mathbf{C}_2'$ and $\downarrow \mathbf{C}_2''$ of $\tilde{\mathbf{M}}_{\mathbf{D}_2}$,

$$\tilde{\mathbf{M}}_{\mathbf{D}_2} = \begin{array}{c} \\ \mathbf{D}_2(/\mathbf{C}_1) \\ \mathbf{D}_2(/\downarrow\mathbf{C}_2) \\ \mathbf{D}_2(/\downarrow\mathbf{C}_2') \\ \mathbf{D}_2(/\downarrow\mathbf{C}_2'') \end{array} \begin{array}{c} \begin{array}{cccc} \downarrow\mathbf{C}_1 & \downarrow\mathbf{C}_2 & \downarrow\mathbf{C}_2') & \downarrow\mathbf{C}_2'' \end{array} \\ \begin{pmatrix} 4 & 0 & 0 & 0 \\ 2 & 2 & 0 & 0 \\ 2 & 0 & 2 & 0 \\ 2 & 0 & 0 & 2 \end{pmatrix} \end{array} \tag{81}$$

We make the inverse of a fused dominant markaracter table, $\tilde{\tilde{\mathbf{M}}}^{-1\ddagger}_{\mathbf{D}_2}$, by modifying the inverse of a dominant markaracter table, $\tilde{\tilde{\mathbf{M}}}^{-1}_{\mathbf{D}_2}$.

$$\tilde{\tilde{\mathbf{M}}}^{-1}_{\mathbf{D}_2} = \begin{array}{c} \\ \downarrow\mathbf{C}_1 \\ \downarrow\mathbf{C}_2 \\ \downarrow\mathbf{C}_2' \\ \downarrow\mathbf{C}_2'' \end{array} \begin{array}{c} \begin{array}{cccc} \mathbf{D}_2(/\mathbf{C}_1) & \mathbf{D}_2(\mathbf{C}_2) & \mathbf{D}_2(\mathbf{C}_2') & \mathbf{D}_2(\mathbf{C}_2'') \end{array} \\ \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ -\frac{1}{4} & \frac{1}{2} & 0 & 0 \\ -\frac{1}{4} & 0 & \frac{1}{2} & 0 \\ -\frac{1}{4} & 0 & 0 & \frac{1}{2} \end{pmatrix} \end{array}$$

$$\Longrightarrow \quad \tilde{\tilde{\mathbf{M}}}^{-1\ddagger}_{\mathbf{D}_2} = \begin{array}{c} \\ \downarrow\mathbf{C}_1 \\ \downarrow\mathbf{C}_2 \end{array} \begin{array}{c} \begin{array}{cc} \mathbf{D}_2(/\mathbf{C}_1) & \mathbf{D}_2(\mathbf{C}_2) \end{array} \\ \begin{pmatrix} \frac{1}{4} & 0 \\ -\frac{1}{4} & \frac{1}{2} \end{pmatrix} \end{array}, \tag{82}$$

where the rows and columns for $\downarrow \mathbf{C}_2'$ and $\downarrow \mathbf{C}_2''$ are omitted. The fused dominant markaracters described above are multiplied by $\tilde{\tilde{\mathbf{M}}}^{-1\ddagger}_{\mathbf{D}_2}$ to give

$$(4,0)\tilde{\tilde{\mathbf{M}}}^{-1\ddagger}_{\mathbf{D}_2} = (4,0)\begin{pmatrix} \frac{1}{4} & 0 \\ -\frac{1}{4} & \frac{1}{2} \end{pmatrix} = (1,0)$$

$$(2,2)\tilde{\tilde{\mathbf{M}}}^{-1\ddagger}_{\mathbf{D}_2} = (2,2)\begin{pmatrix} \frac{1}{4} & 0 \\ -\frac{1}{4} & \frac{1}{2} \end{pmatrix} = (0,1)$$

Thus, Theorem 16 holds for such a case that fusions occur.

In contrast to Theorem 16, Theorem 17 should be modified in order to treat cases in which there occur fusions. Theorem 17 can easily be extended to these cases, since the contribution of respective fusions is linearly independent. Thus, we have Thereom 18.

Theorem 18. *When there occur fusions concerning* $\mathbf{G}_k^{(j)}$ *in the process of induction,*

$$(1, 1, \ldots, \underbrace{m}_{\mathbf{G}_k^{(j)}}, \ldots, 1)\widetilde{\mathbf{M}}_{\mathbf{G}_j}^{-1} = (\widetilde{\beta}_1, \widetilde{\beta}_2, \ldots, \widetilde{\beta}_r) \tag{83}$$

$$(y_1, y_2, \ldots, y_r)\widetilde{\widetilde{\mathbf{M}}}_{\mathbf{G}\downarrow\mathbf{G}_j}^{-1} = (\widetilde{\beta}_1, \widetilde{\beta}_2, \ldots, \widetilde{\beta}_r). \tag{84}$$

A vector such as $(1, 1, \ldots, m, \ldots, 1)$ is called a fused dominant markaracter. The integer m is the number of fused subgroups.

We examine two typical cases as examples, in which two or three subgroups are fused into one subgroup. First we consider a subdominant markaracter $\mathbf{T}_d \downarrow \mathbf{D}_2(/\mathbf{D}_2)$ in which three subgroups are fused into one subgroup.

Example 4. From a row vector, $\mathbf{D}_2(/\mathbf{D}_2) = (1, 1, 1, 1)$, we can construct a fused dominant markaracter, $\mathbf{D}_2(/\mathbf{D}_2)^\dagger = (1, 3)$, by adding the values corresponding to $\mathbf{C}_2$ and $\mathbf{C}_2''$, since these are fused in the process of the induction, $\mathbf{D}_2 \uparrow \mathbf{T}_d$. Thus we have

$$(1, 3)\widetilde{\mathbf{M}}_{\mathbf{D}_2}^{-1\ddagger} = (1, 3)\begin{pmatrix} \frac{1}{4} & 0 \\ -\frac{1}{4} & \frac{1}{2} \end{pmatrix} = (-\frac{1}{2}, \frac{3}{2}), \tag{85}$$

The resulting vector is multiplied with $\widetilde{\widetilde{\mathbf{M}}}_{\mathbf{T}_2\downarrow\mathbf{D}_2}$ to give

$$(-\frac{1}{2}, \frac{3}{2})\widetilde{\widetilde{\mathbf{M}}}_{\mathbf{T}_d\downarrow\mathbf{D}_2} = (-\frac{1}{2}, \frac{3}{2})\begin{pmatrix} 24 & 0 \\ 12 & 4 \end{pmatrix} = (6, 6). \tag{86}$$

Thus, we obtain $\widetilde{\mathbf{T}}_d \downarrow \mathbf{D}_2(/\mathbf{D}_2) = (-\frac{1}{2}, \frac{3}{2})$ and $\mathbf{T}_d \downarrow \mathbf{D}_2(/\mathbf{D}_2) = (6, 6)$. These vectors yield $\mathbf{T}_d(/\mathbf{D}_2)$ and $\widetilde{\mathbf{T}}_d(/\mathbf{D}_2)$ by adding zero elements that correspond to $\mathbf{C}_s$ (the 3rd place), $\mathbf{C}_3$ (the 4th place) and $\mathbf{S}_4$ (the last place). Thus, we have $\widetilde{\mathbf{T}}_d(/\mathbf{D}_2) = (-\frac{1}{2}, \frac{3}{2}, 0, 0, 0)$ and $\mathbf{T}_{2d}(/\mathbf{D}_2) = (6, 6, 0, 0, 0)$, which are alternatively calculated as shown in Table 4. In a similar way, we obtain $\widetilde{\mathbf{T}}_d(/\mathbf{D}_{2d})$ and $\mathbf{T}_d(/\mathbf{D}_{2d})$, constructing alternatively Table 4. □

Next we consider a subdominant markaracter $\mathbf{D}_{2d} \downarrow \mathbf{D}_2(/\mathbf{D}_2)$ in which two subgroups are fused into one subgroup.

Example 5. From a row vector, $\mathbf{D}_2(/\mathbf{D}_2) = (1, 1, 1, 1)$, we can construct a fused dominant markaracter, $\mathbf{D}_2(/\mathbf{D}_2)^* = (1, 1, 2)$, by adding the values corresponding to $\mathbf{C}_2'$ and $\mathbf{C}_2''$, since these are fused in the process of the induction, $\mathbf{D}_2 \uparrow \mathbf{D}_{2d}$. We make the inverse of a fused dominant markaracter table, $\widetilde{\mathbf{M}}_{\mathbf{D}_2}^{-1*}$, by modifying the inverse of a dominant markaracter table, $\widetilde{\mathbf{M}}_{\mathbf{D}_2}^{-1}$,

$$\widetilde{\mathbf{M}}_{\mathbf{D}_2}^{-1} \Longrightarrow \widetilde{\mathbf{M}}_{\mathbf{D}_2}^{-1*} = \begin{array}{c} \\ \downarrow \mathbf{C}_1 \\ \downarrow \mathbf{C}_2 \\ \downarrow \mathbf{C}_2' \end{array} \begin{array}{c} \begin{array}{ccc} \mathbf{D}_2(/\mathbf{C}_1) & \mathbf{D}_2(\mathbf{C}_2) & \mathbf{D}_2(\mathbf{C}_2') \end{array} \\ \begin{pmatrix} \frac{1}{4} & 0 & 0 \\ -\frac{1}{4} & \frac{1}{2} & 0 \\ -\frac{1}{4} & 0 & \frac{1}{2} \end{pmatrix} \end{array}, \tag{87}$$

where the row of $\downarrow \mathbf{C}_2''$ is omitted. Thus we have

$$(1,1,2)\widetilde{\mathbf{M}}_{\mathbf{D}_2}^{-1*} = (1,1,2)\begin{pmatrix} \frac{1}{4} & 0 & 0 \\ -\frac{1}{4} & \frac{1}{2} & 0 \\ -\frac{1}{4} & 0 & \frac{1}{2} \end{pmatrix} = (-\frac{1}{2}, \frac{1}{2}, 1), \tag{88}$$

The resulting vector is multiplied by $\widetilde{\widetilde{\mathbf{M}}}_{\mathbf{D}_{2d}\downarrow\mathbf{D}_2}$ to give

$$(-\frac{1}{2}, \frac{1}{2}, 1)\widetilde{\widetilde{\mathbf{M}}}_{\mathbf{D}_{2d}\downarrow\mathbf{D}_2} = (-\frac{1}{2}, \frac{1}{2}, 1)\begin{pmatrix} 8 & 0 & 0 \\ 4 & 4 & 0 \\ 4 & 0 & 2 \end{pmatrix} = (2,2,2). \tag{89}$$

Thus, we obtain $\widetilde{\mathbf{D}}_{2d} \downarrow \mathbf{D}_2(/\mathbf{D}_2) = (-\frac{1}{2}, \frac{1}{2}, 1)$ and $\mathbf{D}_{2d} \downarrow \mathbf{D}_2(/\mathbf{D}_2) = (2,2,2)$. These vectors yield $\mathbf{D}_{2d}(/\mathbf{D}_2)$ and $\widetilde{\mathbf{D}}_{2d}(/\mathbf{D}_2)$ by adding zero values that correspond to $\mathbf{C}_s$ (the 3rd place) and $\mathbf{S}_4$ (the last place). Thus, we have $\widetilde{\mathbf{D}}_{2d}(/\mathbf{D}_2) = (-\frac{1}{2}, \frac{1}{2}, 1, 0, 0)$ and $\mathbf{D}_{2d}(/\mathbf{D}_2) = (2,2,2,0,0)$. □

8. Characters as markaracters

Throughout this section, we discuss a special case in which any cojugacy class corresponds to a dominant subgroup in one-to-one fashion. That is to say, any dominant class contains only one cojugacy class. For characterizing the special case, we have the following theorem,

Theorem 19. *Let $\mathbf{G}_i$ be a representative cyclic subgroup corresponding to a conjugacy class $\mathbf{K}'$ of $\mathbf{G}$ in one-to-one fashion. The character for $\mathbf{G}(/\mathbf{G}_i)$ uder the action of $g(\in \mathbf{K}')$ is equal to the dominant markaracter uder the action of $\langle g\rangle(= \mathbf{G}_j)$.*

Proof. Let us consider the coset decomposition represented by eq. 15. Consider that $g(\in \mathbf{K}')$ fixes a coset $\mathbf{G}_i t_k$. It follows that $g = t_k^{-1} h t_k$ (for $h \in \mathbf{G}_i$ and $h \in \mathbf{K}'$).

$$g^r = \underbrace{t_k^{-1} h t_k \cdot t_k^{-1} h t_k \cdots t_k^{-1} h t_k}_{r} = t_k^{-1} h^r t_k, \tag{90}$$

wherein $r = 1, 2, \ldots, n$ and $g^n = t_k^{-1} h^n t_k = I$. It follows that $\langle g\rangle = t_k^{-1}\mathbf{G}_i t_k$. This means that $\langle g\rangle$ fixes the coset $\mathbf{G}_i t_k$. □

Theorem 19 indicates that the present markaracter tables are closely related to character tables for coset representations described previously by us [21]. Thus, Theorem 19 allows us to regard markaracters as characters, since each dominant subgroup corresponds to a conjugacy class. Thus, we have reported the reduction of a coset representation into irreducible representations [21]. Note that dominant markaracters span a vector space and irreducible characters span another vector space. However, they can be equalized, since the two vector spaces contain in common a vector whose elements are all equal to 1. It follows that we can inversely regard characters as markaracters. The following example illustrates such an inverse point of view.

Example 6. The character table for $\mathbf{T}_d$ is multiplied by $\widetilde{\mathbf{M}}_{\mathbf{T}_d}^{-1}$ to afford a set of multiplicity vectors.

$$
\begin{array}{c}
 \\ A_1 \\ A_2 \\ E \\ T_1 \\ T_2
\end{array}
\begin{array}{c}
\begin{array}{ccccc} \downarrow \mathbf{C}_1 & \downarrow \mathbf{C}_2 & \downarrow \mathbf{C}_s & \downarrow \mathbf{C}_3 & \downarrow \mathbf{S}_4 \end{array} \\
\left(\begin{array}{ccccc}
1 & 1 & 1 & 1 & 1 \\
1 & 1 & -1 & 1 & -1 \\
2 & 2 & 0 & -1 & 0 \\
3 & -1 & -1 & 0 & 1 \\
3 & -1 & 1 & 0 & -1
\end{array}\right)
\end{array}
\widetilde{\mathbf{M}}_{\mathbf{T}_d}^{-1}
$$

$$
= \begin{array}{c}
 \\ \widetilde{A}_1 \\ \widetilde{A}_2 \\ \widetilde{E} \\ \widetilde{T}_1 \\ \widetilde{T}_2
\end{array}
\begin{array}{c}
\begin{array}{ccccc} \downarrow \mathbf{C}_1 & \downarrow \mathbf{C}_2 & \downarrow \mathbf{C}_s & \downarrow \mathbf{C}_3 & \downarrow \mathbf{S}_4 \end{array} \\
\left(\begin{array}{ccccc}
-\frac{1}{2} & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\
0 & \frac{1}{2} & 0 & -\frac{1}{2} & 0 \\
\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} \\
0 & 0 & \frac{1}{2} & 0 & -\frac{1}{2}
\end{array}\right)
\end{array}
\tag{91}
$$

The sum of each row of the resulting matrix (except the $\widetilde{A}_1$-row) is calculated to be zero.

The orthogonality relationship between two irreducible characters $\Gamma^a(\mathbf{K}_j)$ and $\Gamma^b(\mathbf{K}_j)$ is represented by

$$\frac{1}{|\mathbf{G}|}\sum_{j=1}^{s} n_{\mathbf{K}_j}\Gamma^a(\mathbf{K}_j)\Gamma^b(\mathbf{K}_j) = \delta_{ab} \tag{92}$$

where δ_{ab} is Kronecker's delta. It should be noted that the orthogonality of irreducible characters is concerned with each element of the group so that each term of eq. 92 concerning a conjugacy class involves the coefficient $n_{\mathbf{K}_j}/|\mathbf{G}|$. By means of Theorem 11, the left-hand side of eq. 92 is transformed into an equation concerning $\mathbf{G}$,

$$\frac{1}{|\mathbf{G}|}\sum_{j=1}^{s}\frac{|\mathbf{G}|\varphi(|\mathbf{G}_j|)}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_j)|}\Gamma^a(\mathbf{K}_j)\Gamma^b(\mathbf{K}_j) = \sum_{j=1}^{s}\frac{\varphi(|\mathbf{G}_j|)}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_j)|}\Gamma^a(\mathbf{G}_j)\Gamma^b(\mathbf{G}_j), \tag{93}$$

where the summation over $\mathbf{K}_j$ is changed into the summation over $\mathbf{G}_j$. This change agrees with the present treatment in which a character is regarded as a markaracter. We now arrive at a theorem which crorresponds to the orthogonality relationship of irreducible characters,

Theorem 20. *When two row vectors $\Gamma^a(\mathbf{G}_j)$ and $\Gamma^b(\mathbf{G}_j)$ are obtained for irreducible characters, we have*

$$\sum_{j=1}^{s}\frac{\varphi(|\mathbf{G}_j|)}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_j)|}\Gamma^a(\mathbf{G}_j)\Gamma^b(\mathbf{G}_j) = \delta_{ab}. \tag{94}$$

When we have $\Gamma^b(\mathbf{K}_j) = (1, 1, \ldots, 1)$ as a special case, this equation is transformed into

$$\sum_{j=1}^{s}\frac{\Gamma^a(\mathbf{G}_j)\varphi(|\mathbf{G}_j|)}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_j)|} = 0, \tag{95}$$

for $\Gamma^a(\mathbf{K}_j)$ other than $(1, 1, \ldots, 1)$. The left-hand side is equal to the orbit index described in Theorem 13. Thus, we have a theorem for classifying a multiplicity vector.

Theorem 21. *When a row vector $\Gamma(\mathbf{G}_j)$ is obtained for an irreducible character other than* $(1, 1, \ldots, 1)$, *the orbit index is expressed by the following equation.*

$$\widetilde{\Delta} = \sum_{j=1}^{s} \frac{\Gamma(\mathbf{G}_j)\varphi(|\mathbf{G}_j|)}{|\mathbf{N}_{\mathbf{G}}(\mathbf{G}_j)|} = 0. \qquad (96)$$

Markaracters can alternatively be considered to be generalized characters in the present case. The difference of two markaracters having the orbit index of one creates a markaracter having the orbit index of zero, which is a candidate for an irreducible character.

Example 7. From the data of Table 4, we obtain irreducible characters as follows.

$$\begin{aligned}
\mathbf{T}_d(/\mathbf{T}) - \mathbf{T}_d(/\mathbf{T}_d) &= (2,2,0,2,0) - (1,1,1,1,1) = (1,1,-1,1,-1) = A_2 \\
\mathbf{T}_d(/\mathbf{D}_{2d}) - \mathbf{T}_d(/\mathbf{T}_d) &= (3,3,1,0,1) - (1,1,1,1,1) = (2,2,0,-1,0) = E \\
\mathbf{T}_d(/\mathbf{C}_{3v}) - \mathbf{T}_d(/\mathbf{T}_d) &= (4,0,2,1,0) - (1,1,1,1,1) = (3,-1,1,0,-1) = T_2 \\
\mathbf{T}_d(/\mathbf{S}_4) - \mathbf{T}_d(/\mathbf{D}_{2d}) &= (6,2,0,0,2) - (3,3,1,0,1) = (3,-1,-1,0,1) = T_1
\end{aligned}$$

The corresponding multiplicity vectors are calculated also from the data of Table 4 as shown,

$$\begin{aligned}
\widetilde{\mathbf{T}}_d(/\mathbf{T}) - \widetilde{\mathbf{T}}_d(/\mathbf{T}_d) &= (-\frac{1}{2},\frac{1}{2},0,1,0) - (-\frac{1}{2},0,\frac{1}{2},\frac{1}{2},\frac{1}{2}) \\
&= (0,\frac{1}{2},-\frac{1}{2},\frac{1}{2},-\frac{1}{2}) = \widetilde{A}_2 \\
\widetilde{\mathbf{T}}_d(/\mathbf{D}_{2d}) - \widetilde{\mathbf{T}}_d(/\mathbf{T}_d) &= (-\frac{1}{2},\frac{1}{2},\frac{1}{2},0,\frac{1}{2}) - (-\frac{1}{2},0,\frac{1}{2},\frac{1}{2},\frac{1}{2}) \\
&= (0,\frac{1}{2},0,-\frac{1}{2},0) = \widetilde{E} \\
\widetilde{\mathbf{T}}_d(/\mathbf{C}_{3v}) - \widetilde{\mathbf{T}}_d(/\mathbf{T}_d) &= (-\frac{1}{2},0,1,\frac{1}{2},0) - (-\frac{1}{2},0,\frac{1}{2},\frac{1}{2},\frac{1}{2}) \\
&= (0,0,\frac{1}{2},0,-\frac{1}{2}) = \widetilde{T}_2 \\
\widetilde{\mathbf{T}}_d(/\mathbf{S}_4) - \widetilde{\mathbf{T}}_d(/\mathbf{D}_{2d}) &= (0,0,0,0,1) - (-\frac{1}{2},\frac{1}{2},\frac{1}{2},0,\frac{1}{2}) \\
&= (\frac{1}{2},-\frac{1}{2},-\frac{1}{2},0,\frac{1}{2}) = \widetilde{T}_1
\end{aligned}$$

These are identical with the respective rows of the matrix (eq. 91) obtained by an alternative method. □

9. Conclusion

For integrating two concepts of different categories, marks and characters, we have proposed the concept of markaracter and discussed mathematical foundations for chemical applications.

1. The correspondence between conjugate cyclic subgroups and conjugacy classes is discussed in terms of dominant classes.

2. We consider coset representations concerning cyclic subgroups, which are called dominant representations (DRs).
3. We construct a row vecter called a dominant markaracter (mark-character) by counting the numbers of fixed points corresponding to each DR. Such dominant markaracters for a non-redundant set of DRs are collected to form a markaracter table.
4. The markaracter table and its inverse are obtained from the usual mark table and its inverse. This procedure is based on concecutive concurrent interchanges of the lower triangular matrix.
5. The markaracter table is related to a subdominant markaracter table of its subgroup so that the corresponding row of the former table is constructed from the latter.
6. The data of the markaracter table are in turn used to construct a character table of the group, after each character is regarded as a markaracter and transformed into a multiplicity vector.
7. The concept of orbit index is proposed to classify multiplicity vectors; thus, the orbit index of each DR is proved to be equal to one. On the other hand, the orbit index of each irreducible representation is equal to zero, when conjugacy classes are equal to dominant classes.

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