Maturity of Finite Groups. An Application to Combinatorial Enumeration of Isomers

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The maturity of a finite group $\mathbf{G}$ is defined by examining how a dominant class ($\mathbf{Q}$-conjugacy class) corresponding to a cyclic subgroup $\mathbf{H}$ contains conjugacy classes. If the ingeter $q=|\mathbf{N}_\mathbf{G}(\mathbf{H})|/|\mathbf{C}_\mathbf{G}(\mathbf{H})|$ (called the maturity discriminant) is less than an Euler function $\varphi(|\mathbf{H}|)$, the group $|\mathbf{G}|$ is concluded to be unmatured concerning $\mathbf{H}$, where $\mathbf{N}_\mathbf{G}(\mathbf{H})$ and $\mathbf{C}_\mathbf{G}(\mathbf{H})$ respectively denote the normalizer and the centralizer of $\mathbf{H}$ within $\mathbf{G}$. A matured representation defined for a matured or an unmatured group is subduced into cyclic subgroups to give the corresponding monomials, which are applied to the combinatorial enumeration of isomers.

In order to develop new methods of combinatorial enumeration of isomers, we have clarified the relationship between character tables[1—8] and mark tables.[9—20] Thus, we have proposed markaracter tables which enable us to discuss characters and marks on a common basis.[21,22] However, the previous papers have dealt with one extreme case (e.g. $\mathbf{T}_d$) in which each dominant class contains only one conjugacy class[21] as well as with another extreme case (cyclic groups) in which each element of a dominant class is composed of one-membered conjugacy classes.[23] Although we have proposed a new method of combinatorial enumeration applicable to general cases (e.g. $\mathbf{T}$) in which a dominant class contains one or more of one- or more-membered conjugacy classes,[24] its theoretical foundations have not been reported. In the present paper, we shall formulate the first case (e.g. $\mathbf{T}_d$) as a matured group and the second case (a cyclic group) as a fully unmatured group; then, we shall treat the third case (the general cases) as unmatured groups. Such a formulation enables us to develop an improved method of combinatorial enumeration, which is simpler and more convenient than the previous one.

1 Maturity of Finite Groups. Theoretical Foundations

1.1 Matured and Unmatured Dominant Classes. Dominant classes can be defined as $\mathbf{Q}$-conjugacy classes.[23] Suppose that the elements of a finite group $\mathbf{G}$ are partitioned into s dominant classes $\mathbf{K}_i$ $(i=1,2,\cdots,s)$ that correspond to cyclic subgroups $\mathbf{G}_i$ $(i=1,2,\cdots,s)$ selected from a non-redundant set of cyclic subgroups (SCSG). When elements, h_1 and h_2, are conjugate within $\mathbf{G}$ (i.e., $\exists t \in \mathbf{G}$, $t^{-1}h_1t=h_2$) and $\langle h_1\rangle$ and $\langle h_2\rangle$ represent the cyclic subgroups generated respectively from h_1 and h_2, we easily obtain

$$t^{-1}\langle h_1\rangle t=\langle h_2\rangle, \tag{1}$$

since we have

$$t^{-1}h_1^rt=(t^{-1}h_1t)(t^{-1}h_1t)\cdots(t^{-1}h_1t)=h_2^r \tag{2}$$

for $r=1,2,\cdots,n$ and $n=|\langle h_1\rangle|=|\langle h_2\rangle|$. It follows that conjugate elements h_1 and h_2 are $\mathbf{Q}$-conjugate with each other; however, note that the contrary is not always true. As a result, we obtain the following theorem.

Theorem 1. *A dominant class* $\mathbf{K}_i$ $(i=1,2,\cdots,s)$ *is partitioned into one or more conjugacy classes as follows.*

$$\mathbf{K}_i=\mathbf{K}_{i1}+\mathbf{K}_{i2}+\cdots+\mathbf{K}_{it}\ \ (t\geq 1). \tag{3}$$

Since it is important to discuss whether or not each dominant class consists of only one conjugacy class, we define matured and unmatured dominant classes as follows.

Definition 1. (Matured and unmatured dominant classes) *Let* $\mathbf{G}$ *be a finite group. Suppose that its cyclic subgroup* $\mathbf{G}_i$ *corresponds to a dominant class* $\mathbf{K}_i$.

1. When the dominant class $\mathbf{K}_i$ *contains only one conjugacy class* (i.e., *t is equal to 1 in Eq. 3*), *it is defined to be* matured. *The group* $\mathbf{G}$ *is referred to as being* matured *with respect to the cyclic subgroup* $\mathbf{G}_i$.

2. Otherwise (i.e., *t is larger than 1 in Eq. 3*), *the dominant class* $\mathbf{K}_i$ *and the group* $\mathbf{G}$ *is* unmatured *concerning the cyclic subgroup* $\mathbf{G}_i$.

The number ($|\mathbf{K}_i|$) of the elements contained in the dominant class $\mathbf{K}_i$ represented by

$$|\mathbf{K}_i|=\frac{|\mathbf{G}|\varphi(|\mathbf{G}_i|)}{|\mathbf{N}_\mathbf{G}(\mathbf{G}_i)|}, \tag{4}$$

wherein $\mathbf{N}_\mathbf{G}(\mathbf{G}_i)$ is the normalizer of $\mathbf{G}_i$ within the group $\mathbf{G}$ (Theorem 11 of Ref. 21). The symbol $\varphi(n)$ denotes the Euler function for an integer n. On the other hand, the number ($|\mathbf{K}_{ij}|$) of the elements in the conjugacy class $\mathbf{K}_{ij}$ is represented by

$$c = |\mathbf{K}_{ij}| = \frac{|\mathbf{G}|}{|\mathbf{C_G}(h)|}, \tag{5}$$

wherein $\mathbf{C_G}(h)$ is the centralizer of h ($\in\mathbf{K}_{ij}$) within the group $\mathbf{G}$. In the present situation, c (Eq. 5) depends upon the conjugacy classes $\mathbf{K}_{ij}$; however it will be proved to be constant for the dominant class $\mathbf{K}_i$ (see Lemma 1).

Example 1. (An unmatured dominant class in a finite group: $\mathbf{T}_h$)

Let us examine the point group $\mathbf{T}_h$ of order 24. Since $\mathbf{T}_h$ contains an SCSG:

$$\mathrm{SCSG} = \{\mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_s, \mathbf{C}_i, \mathbf{C}_3, \mathbf{S}_6\},$$

we have six dominant classes:

$$\mathbf{K}_1 = \{I\} \tag{6}$$

$$\mathbf{K}_2 = \{C_{2(1)}, C_{2(2)}, C_{2(3)}\} \tag{7}$$

$$\mathbf{K}_3 = \{\sigma_{h(1)}, \sigma_{h(2)}, \sigma_{h(3)}\} \tag{8}$$

$$\mathbf{K}_4 = \{i\} \tag{9}$$

$$\begin{aligned}\mathbf{K}_5 &= \mathbf{K}_{51} + \mathbf{K}_{52} \\ &= \{C_{3(1)}, C_{3(2)}, C_{3(3)}, C_{3(4)}\} + \{C_{3(1)}^2, C_{3(2)}^2, C_{3(3)}^2, C_{3(4)}^2\}\end{aligned} \tag{10}$$

$$\begin{aligned}\mathbf{K}_6 &= \mathbf{K}_{61} + \mathbf{K}_{62} \\ &= \{S_{6(1)}, S_{6(2)}, S_{6(3)}, S_{6(4)}\} + \{S_{6(1)}^5, S_{6(2)}^5, S_{6(3)}^5, S_{6(4)}^5\}\end{aligned} \tag{11}$$

The dominant class $\mathbf{K}_5$, which corresponds to $\mathbf{C}_3$, is unmatured because it is subdivided into two conjugacy classes, $\mathbf{K}_{51}$ and $\mathbf{K}_{52}$. The dominant class $\mathbf{K}_6$, which corresponds to $\mathbf{S}_6$ (=$\mathbf{C}_{3i}$), is also unmatured because it is subdivided into two conjugacy classes, $\mathbf{K}_{61}$ and $\mathbf{K}_{62}$. Since the group $\mathbf{C}_3$ is a subgroup of the group $\mathbf{S}_6$, the group $\mathbf{T}_h$ is unmatured with respect to the $\mathbf{S}_6$-group.

1.2 Cyclic Subgroups and Their Normalizers. 1.2.1 Conservation of Maturity. Let us select a cyclic subgroup $\mathbf{H}$ (=$\mathbf{G}_i$) from the SCSG of $\mathbf{G}$. Suppose that $\mathbf{N}$ it the normalizer of $\mathbf{H}$ within the group $\mathbf{G}$, i.e., $\mathbf{N}=\mathbf{N_G}(\mathbf{H})$. Then, we have coset decompositions:

$$\mathbf{G} = \mathbf{N}g_1 + \mathbf{N}g_2 + \cdots + \mathbf{N}g_a \tag{12}$$

$$\mathbf{N} = \mathbf{H}t_1 + \mathbf{H}t_2 + \cdots + \mathbf{H}t_b \tag{13}$$

where $a = |\mathbf{G}|/|\mathbf{N}|$ and $b = |\mathbf{N}|/|\mathbf{H}|$. The transversals appearing in these equations are denoted as follows:

$$\mathbf{A} = \{g_1, g_2, \cdots, g_a\} \tag{14}$$

$$\mathbf{B} = \{t_1, t_2, \cdots, t_b\} \tag{15}$$

As shown in Corollary 2 (Appendix A), the number of the conjugate subgroups of the cyclic subgroups is equal to $|\mathbf{G}|/|\mathbf{N}|$.

Example 2. (Conjugate cyclic subgroups for $\mathbf{T}_h$ and their normalizer)

Let us examine the cyclic subgroup $\mathbf{S}_6$ (=$\mathbf{S}_{6(1)}$) of the point group $\mathbf{T}_h$ described in Example 1. The normalizer of the group $\mathbf{S}_6$ is the $\mathbf{S}_6$ itself, i.e., $\mathbf{N}_{\mathbf{T}_h}(\mathbf{S}_6)=\mathbf{S}_6$. Equation 12 for the present case is expressed by

$$\mathbf{T}_h = \mathbf{S}_6 + \mathbf{S}_6 C_{2(1)} + \mathbf{S}_6 C_{2(2)} + \mathbf{S}_6 C_{2(3)}. \tag{16}$$

Transversals (Eqs. 14 and 15) are expressed as follows:

$$\mathbf{A} = \{I, C_{2(1)}, C_{2(2)}, C_{2(3)}\} \tag{17}$$

$$\mathbf{B} = \{I\} \tag{18}$$

Corollary 2 (Appendix A) is exemplified by the following equations:

$$C_{2(1)}^{-1}\mathbf{S}_6 C_{2(1)} = \mathbf{S}_{6(2)}, \quad C_{2(2)}^{-1}\mathbf{S}_6 C_{2(2)} = \mathbf{S}_{6(3)}, \quad C_{2(3)}^{-1}\mathbf{S}_6 C_{2(3)} = \mathbf{S}_{6(4)}, \tag{19}$$

where the number of the cyclic subgroups is 4. This value is equal to $a=|\mathbf{T}_h|/|\mathbf{S}_6|=24/6=4$.

The normalizer of the group $\mathbf{C}_3$ is the $\mathbf{S}_6$, i.e., $\mathbf{N}_{\mathbf{T}_h}(\mathbf{C}_3)=\mathbf{S}_6$. This is an example of Lemma 8 (Appendix A).

As shown in Appendix A, the dominant class corresponding to $\mathbf{H}$ within the normalizer $\mathbf{N}$ is correlated to the one within $\mathbf{G}$. Thus, we have a theorem:

Theorem 2. (Conservation of Maturity)

Let $\mathbf{H}$ *be a cyclic subgroup of* $\mathbf{G}$ *and* $\mathbf{N}$ *represent* $\mathbf{N_G}(\mathbf{H})$.

1. If the dominant class corresponding to $\mathbf{H}$ *is matured in* $\mathbf{N}$, *it is also matured in* $\mathbf{G}$.

2. If the dominant class corresponding to $\mathbf{H}$ *is matured in* $\mathbf{G}$, *it is also matured in* $\mathbf{N}$.

The following example shows an unmatured case which represents a case of the contraposition of Theorem 2.

Example 3. Let us consider the unmatured dominant class $\mathbf{K}_6$ of $\mathbf{T}_h$ described in Example 1. It corresponds to the cyclic group $\mathbf{S}_6$, the normalizer of which is determined to be $\mathbf{S}_6$ itself, as shown in Example 2. When the normalizer $\mathbf{S}_6$ is taken into consideration, the unmatured dominant $\mathbf{K}_6$ is restricted into $\mathbf{K}_6'=\{S_{6(1)}\}+\{S_{6(1)}^5\}$, which is also unmatured in the normalizer $\mathbf{S}_6$.

On the other hand, the unmatured dominant class $\mathbf{K}_5$ of $\mathbf{T}_h$ (Example 1) corresponds to the cyclic group $\mathbf{C}_3$, the normalizer of which is determined to be $\mathbf{S}_6$, as shown in Example 2. When the normalizer $\mathbf{S}_6$ is taken into consideration, the unmatured dominant $\mathbf{K}_5$ is restricted into $\mathbf{K}_5'=\{C_{3(1)}\}+\{C_{3(1)}^2\}$, which is also unmatured in the normalizer $\mathbf{S}_6$.

1.2.2 Dominant Classes in the Normalizer of a Cyclic Subgroup. Let us focus our attention on the elements of the cyclic group $\mathbf{H}$. Theorem 2 (along with Theorem 9 in Appendix A) implies that two conjugacy classes concerning the cyclic $\mathbf{H}$ (note that they are produced by the first proposition of Theorem 9) are not changed if we take either $\mathbf{N}$ or $\mathbf{G}$ into consideration. The purpose of this subsection is to clarify how such conjugacy classes behave within $\mathbf{N}$ and $\mathbf{G}$.

Let us consider the conjugacy class $\mathbf{K}_{ij}$ belonging to the dominant class $\mathbf{K}_i$ (Eq. 3). Since the dominant class $\mathbf{K}_i$ corresponds to the cyclic group $\mathbf{H}$ (=$\mathbf{G}_i$), there are a (=$|\mathbf{G}|/|\mathbf{N}|$) subgroups, $g_k^{-1}\mathbf{H}g_k$ ($k=1,2,\cdots,a$), which are conjugate to $\mathbf{H}$ within $\mathbf{G}$. For each $h \in\mathbf{H}$, there exists a conjugate element $g_k^{-1}hg_k$ involved in the respective $g_k^{-1}\mathbf{H}g_k$ ($k=1,2,\cdots,a$). When the group $\mathbf{G}$ is restricted to $\mathbf{N}$, each $\mathbf{K}_{ij}$ is restricted to

$\mathbf{K}_{ij}\cap\mathbf{H}$, as indicated by Theorem 9 (Appendix A). A similar discussion shows that each $\mathbf{K}_{ij}$ is restricted to $\mathbf{K}_{ij}\cap g_k^{-1}\mathbf{H}g_k$, when the group $\mathbf{G}$ is restricted to $g_k^{-1}\mathbf{N}g_k$. It follows that each element $g_k^{-1}hg_k$ distinctly belongs to $\mathbf{K}_{ij}\cap g_k^{-1}\mathbf{H}g_k$ (k=1, 2,$\cdots$,a). By considering the third proposition of Theorem 8 (Appendix A), we have the following theorem:

Theorem 3. *Let the conjugacy classes $\mathbf{K}_{ij}$ belong to the dominant class $\mathbf{K}_i$ (Eq. 3). Then, we have*

$$\mathbf{K}_{ij} = \sum_{k=1}^{a}(\mathbf{K}_{ij}\cap g_k^{-1}\mathbf{H}g_k), \tag{20}$$

where the summation represents a disjoint union and the element g_k runs over the transversal $\mathbf{A}$ (Eq. 14).

Example 4. This is a continuation of Example 2. Let us examine the conjugacy classes $\mathbf{K}_{51}$ and $\mathbf{K}_{52}$ contained in the dominant class $\mathbf{K}_5$ (Example 1). The dominant class corresponds to the four cyclic subgroups, $\mathbf{C}_{3(1)}$ (=$\mathbf{C}_3$), $\mathbf{C}_{3(2)}$, $\mathbf{C}_{3(3)}$, and $\mathbf{C}_{3(4)}$, which are conjugate to each other. The conjugation relationship is in the same situation as $\mathbf{S}_6$, which has been examplified in Example 2. The corresponding transversal is represented as follows:

$$\mathbf{A} = \{I, C_{2(1)}, C_{2(2)}, C_{2(3)}\} \tag{21}$$

Then, we have

$$\mathbf{K}_{31}\cap\mathbf{C}_{3(k)} = \{C_{3(k)}\} \quad \text{for } k = 1,2,3,4 \tag{22}$$

$$\mathbf{K}_{32}\cap\mathbf{C}_{3(k)} = \{C_{3(k)}^2\} \quad \text{for } k = 1,2,3,4 \tag{23}$$

each summation of which exemplifies Theorem 3.

Since the dominant class $\mathbf{K}_i$ contains all of the elements of order $|\mathbf{H}|$ concerning the cyclic subgroup $\mathbf{H}$ (=$\mathbf{G}_i$), we have the following result:

$$\bigcup_{j=1}^{t}(\mathbf{K}_{ij}\cap\mathbf{H}) = \left(\bigcup_{j=1}^{t}\mathbf{K}_{ij}\right)\cap\mathbf{H} = \mathbf{K}_i\cap\mathbf{H}. \tag{24}$$

$$\bigcup_{j=1}^{t}(\mathbf{K}_{ij}\cap g_k^{-1}\mathbf{H}g_k) = \left(\bigcup_{j=1}^{t}\mathbf{K}_{ij}\right)\cap g_k^{-1}\mathbf{H}g_k = \mathbf{K}_i\cap g_k^{-1}\mathbf{H}g_k. \tag{25}$$

Hence, we can discuss conjugacy classes in a dominant class even when we restrict our consideration within $\mathbf{N}$. Thus, by taking the normalizer $\mathbf{N}$ into consideration, we are able to regard $\mathbf{K}_i\cap\mathbf{H}$ as a dominant class in $\mathbf{N}$. In addition, the restricted sets, $\mathbf{K}_{ij}\cap\mathbf{H}$ (j=1,2,$\cdots$$t$), are conjugacy classes within $\mathbf{N}$.

	in **G**	in **N**
dominant class	$\mathbf{K}_i$	$\mathbf{K}_i\cap\mathbf{H}$
conjugacy classes	$\mathbf{K}_{ij}$	$\mathbf{K}_{ij}\cap\mathbf{H}$

Let h ($\in\mathbf{G}$) generate the cyclic subgroup $\langle h\rangle$ of order n (n=$|\langle h\rangle|$). Then, $\langle h^r\rangle$ is identical with $\langle h\rangle$ if r and n are coprime, i.e., (r, n)=1. Hence, the elements h and h^r are **Q**-conjugate to each other. Moreover, an element h^r ($\in\mathbf{G}$) and its inverse h^{-r} are **Q**-congugate in any cases, because $\langle h^r\rangle$ is identical with $\langle h^{-r}\rangle$; on the contrary, the two elements (h^r and h^{-r}) are not always conjugate.

Thus, any conjugacy class $\mathbf{K}_{ij}$ of the dominant class $\mathbf{K}_i$ (Eq. 3) contains elements corresponding to such integers r that satisfy (r, n)=1. Suppose that the conjugacy class $\mathbf{K}_{ij}$ contains c elements as follows:

$$\mathbf{K}_{ij} = \{h_1, h_2, \cdots, h_c\}, \tag{26}$$

where c is given in Eq. 5. For simplicity's sake, we write h=h_1. Let us then consider the following set:

$$\mathbf{K}'_{ij} = \{h_1^r, h_2^r, \cdots, h_c^r\}. \tag{27}$$

When r runs over integers coprime to n (n=$|\langle h\rangle|$), there emerge two cases:

Case 1. The integer r generates h^r that is identical with h_k ($\exists k$=1,2,$\cdots$,c) contained in the conjugacy class $\mathbf{K}_{ij}$.

Case 2. The integer r generates h^r that is not involved in the conjugacy class $\mathbf{K}_{ij}$.

In the first case, the set $\mathbf{K}'_{ij}$ (Eq. 27) is identical with the original $\mathbf{K}_{ij}$ (Eq. 26). In order words, the set $\mathbf{K}'_{ij}$ (Eq. 27) is obtained by permuting the elements of the $\mathbf{K}_{ij}$.

On the other hand, if h^r is not involved in $\mathbf{K}_{ij}$ (the second case), the set represented by Eq. 27 is different from the original $\mathbf{K}_{ij}$ (Eq. 26). Since $\mathbf{K}_{ij}$ (Eq. 26) is a conjugacy class, we have $\exists g\in\mathbf{G}$, $g^{-1}hg$=h_k ($\in\mathbf{K}_{ij}$). It follows that we have $g^{-1}h^rg$=h_k^r($\in\mathbf{K}'_{ij}$). This means that the set $\mathbf{K}'_{ij}$ is also a conjugacy class. Hence, the $\mathbf{K}'_{ij}$ is identical with either one of the conjugacy classes in the dominant class $\mathbf{K}_i$. Note that $|\mathbf{K}_{ij}|$=$|\mathbf{K}'_{ij}|$=c. As a result, we have arrived at a lemma.

Lemma 1. *Let $\mathbf{K}_i$ be a dominant class represented by Eq. 3. The conjugacy classes in $\mathbf{K}_i$ have the same number of elements*, i.e.,

$$c = |\mathbf{K}_{i1}| = |\mathbf{K}_{i2}| = \cdots = |\mathbf{K}_{it}|, \tag{28}$$

where we take $\mathbf{G}$ into consideration.

Example 5. Let us examine the point group $\mathbf{D}_5$. Since the group $\mathbf{D}_5$ contains an SCSG=$\{\mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_5\}$, we have three dominant classes:

$$\mathbf{K}_1 = \{I\} \tag{29}$$

$$\mathbf{K}_2 = \{C_{2(1)}, C_{2(2)}, C_{2(3)}, C_{2(4)}, C_{2(5)}\} \tag{30}$$

$$\mathbf{K}_3 = \mathbf{K}_{31} + \mathbf{K}_{32}. \tag{31}$$

It should be noted that the dominant class $\mathbf{K}_3$, which corresponds to the cyclic subgroup $\mathbf{C}_5$, is subdivided into two conjugacy classes,

$$\mathbf{K}_{31} = \{C_5, C_5^4\} \tag{32}$$

$$\mathbf{K}_{32} = \{C_5^2, C_5^3\}. \tag{33}$$

Hence, the group $\mathbf{D}_5$ is unmatured with respect to the subgroup $\mathbf{C}_5$.

Let us consider the interger 4 that is coprime to 5. By starting from the conjugacy class $\mathbf{K}_{31}$, the transformation of Eq. 26 into Eq. 27 is calculated to be

$$\mathbf{K}'_{31} = \{C_5^4, (C_5^4)^4\} = \{C_5^4, C_5\}, \tag{34}$$

which is identical with the original conjugacy class $\mathbf{K}_{31}$. Hence, this is an example of Case 1 described above.

On the other hand, the actions of the intergers 2 and 3 (that are also coprime to 5) on $\mathbf{K}_{31}$ create the following sets:

$$\mathbf{K}_{31}'' = \{C_5^2, (C_5^4)^2\} = \{C_5^2, C_5^3\} \quad (35)$$

$$\mathbf{K}_{31}''' = \{C_5^3, (C_5^4)^3\} = \{C_5^3, C_5^2\}. \quad (36)$$

These sets are identical with the other conjugacy class $\mathbf{K}_{32}$. Hence, they are examples of Case 2 described above.

1.3 Maturity Discriminant. This section is devoted to the derivation of the maturity discriminant that determines whether a group is matured or not. Lemma 1 shows that c given by Eq. 5 is constant. This result implies that the centralizers appearing Eq. 5 are conjugate to each other when $\mathbf{K}_{ij}$ runs over $\mathbf{K}_i$. This can be proved directly as follows. Let h be an element of $\mathbf{K}_{ij}$ and $\mathbf{C_G}(h)$ be the centralizer of the element h. Consider an element $g^{-1}hg$ belonging to $\mathbf{K}_{ij}$. From the fact that $\forall u \in \mathbf{C_G}(h)$, $u^{-1}hu=h$, we have

$$(g^{-1}ug)g^{-1}hg(g^{-1}ug) = g^{-1}(u^{-1}hu)g = g^{-1}hg, \quad (37)$$

which means that the group repsented by

$$g^{-1}\mathbf{C_G}(h)g = \{g^{-1}ug \mid u \in \mathbf{C_G}(h)\} \quad (38)$$

is the centralizer of $g^{-1}hg$ ($\in \mathbf{K}_{ij}$). Next, we consider $h' = h^r (\in \mathbf{H})$ belonging to $\mathbf{K}'_{ij} (\neq \mathbf{K}_{ij})$. Then, we have

$$u^{-1}h'u = u^{-1}h^r u = \underbrace{(u^{-1}hu)(u^{-1}hu)\cdots(u^{-1}hu)}_{r} = h^r = h' \quad (39)$$

which shows that the centralizer $\mathbf{C_G}(h)$ is also the centralizer of the element h', i.e., $\mathbf{C_G}(h)=\mathbf{C_G}(h')$ for $h' \in \mathbf{K}'_{ij}$. Similarly, we can prove that $\mathbf{C_G}(g^{-1}hg)$ is identical with $\mathbf{C_G}(g^{-1}h'g)$. The discussion is summarized as a lemma:

Lemma 2. *The set of centralizers for the elements of the conjugacy class $\mathbf{K}_{ij}$ is invariant when $\mathbf{K}_{ij}$ runs over the dominant class $\mathbf{K}_i$. In other words, we have the following propositions.*

1. Let $\mathbf{C_G}(h)$ be the centralizer of $h \in \mathbf{K}_{ij}$. Then, $g^{-1}\mathbf{C_G}(h)g$ is the centralizer of $g^{-1}hg$ if the $g^{-1}hg$ belongs to $\mathbf{K}_{ij}$.

2. Let $\mathbf{C_G}(h)$ be the centralizer of $h \in \mathbf{K}_{ij}$. Then, we have $\exists h' \in \mathbf{K}'_{ij}$, $\mathbf{C_G}(h)=\mathbf{C_G}(h')$.

This lemma is transfomed to describe the generated cyclic subgroup $\mathbf{H}(=\langle h \rangle)$ and its conjugate subgroups $g^{-1}\mathbf{H}g$. For any $u \in \mathbf{C_G}(h)$, we have $u^{-1}hu=h$. Then, we have

$$u^{-1}h^r u = \underbrace{(u^{-1}hu)(u^{-1}hu)\cdots(u^{-1}hu)}_{r} = h^r \quad (40)$$

for $r=1,2,\cdots,n$. Note that the element h^r does not always belong to $\mathbf{K}'_{ij}$ (cf. Eq. 40). This equation shows that the centralizer $\mathbf{C_G}(h)$ is also the centralizer of the element h^r, i.e., $u \in \mathbf{C_G}(h^r)$ for $r=1,2,\cdots,n$. Thereby, the centralizer $\mathbf{C_G}(h)$ can be regarded as the centralizer of the generated cyclic group $\langle h \rangle$ (=$\mathbf{H}$=$\mathbf{G}_i$). Accordingly, we obtain a lemma.

Lemma 3. *Let $\mathbf{H}$ ($=\langle h \rangle$) be a cyclic subgroup of $\mathbf{G}$. Then, we have $\mathbf{C_G}(\mathbf{H})=\mathbf{C_G}(h)$.*

Note that the element h is a generator of $\mathbf{H}$. If h is not a generator of $\mathbf{H}$, Lemma 3 does not hold true. Hereafter, we use the symbol $\mathbf{C_G}(\mathbf{H})$ is used in terms of Lemma 3.

In the same line that $u^{-1}hu=h$ gives Eq. 40, the relationship shown by Eq. 37 indicates that $\mathbf{C_G}(g^{-1}hg)$ is identical with $\mathbf{C_G}(g^{-1}h^r g)$ for $r=1,2,\cdots,n$; hence, they are represented by the symbol $\mathbf{C_G}(g^{-1}\mathbf{H}g)$. It follows that, when $\mathbf{C_G}(\mathbf{H})$ is the centralizer of the cyclic subgroup $\mathbf{H}$, the conjugate subgroup $g^{-1}\mathbf{C_G}(\mathbf{H})g$ is the centralizer of $g^{-1}\mathbf{H}g$. In other words, Eq. 38 is transformed into the following expression:

$$g^{-1}\mathbf{C_G}(\mathbf{H})g = \mathbf{C_G}(g^{-1}\mathbf{H}g) \quad (41)$$

The discussion here is summarized as follows:

$\mathbf{K}_i (\leftrightarrow \mathbf{G}_i = \mathbf{H})$	$\mathbf{H}$	$g^{-1}\mathbf{H}g$
$\mathbf{K}_{ij}$	h	$g^{-1}hg$
$\mathbf{K}'_{ij}$	h'	$g^{-1}h'g$
Centralizer	$\mathbf{C_G}(\mathbf{H})$	$g^{-1}\mathbf{C_G}(\mathbf{H})g$

Hence Lemma 2 is transformed into the following lemma.

Lemma 4. *Let $\mathbf{H}$ ($=\mathbf{G}_i$) correspond to the dominant class $\mathbf{K}_i$. The set of centralizers for the elements of each conjugacy class $\mathbf{K}_{ij}$ in $\mathbf{K}_i$ is represented by $g^{-1}\mathbf{C_G}(\mathbf{H})g$ ($\forall g \in \mathbf{A}$), which is invariant when the j of $\mathbf{K}_{ij}$ runs to cover the dominant class $\mathbf{K}_i$.*

The sets $\mathbf{K}_{ij} \cap g^{-1}\mathbf{H}g$ ($\forall g \in \mathbf{A}$) are disjoint to each other (Theorem 3). Select the element h as a representative of $\mathbf{K}_{ij} \cap \mathbf{H}$; then, the element $g^{-1}hg$ belongs to $\mathbf{K}_{ij} \cap g^{-1}\mathbf{H}g$, where g runs over the transvasal $\mathbf{A}$ (Eq. 14). When we replace the $\mathbf{K}_{ij}$ of Eq. 26 by $\mathbf{K}_{ij} \cap g^{-1}\mathbf{H}g$ and the $\mathbf{K}'_{ij}$ of Eq. 27 by $\mathbf{K}'_{ij} \cap g^{-1}\mathbf{H}g$, the discussion for Lemma 1 turns out to hold true, giving the following proposition.

Lemma 5. *For the $\mathbf{K}_i \cap g^{-1}\mathbf{H}g$ that is a dominant class in $g^{-1}\mathbf{N}g$, we have*

$$|\mathbf{K}_{i1} \cap g^{-1}\mathbf{H}g| = |\mathbf{K}_{i2} \cap g^{-1}\mathbf{H}g| = \cdots = |\mathbf{K}_{it} \cap g^{-1}\mathbf{H}g|, \quad (42)$$

where g runs over the transvasal $\mathbf{A}$ (Eq. 14). In particular, putting $g=I$ gives the following proposition. For the $\mathbf{K}_i \cap \mathbf{H}$ (Eq. 24) that is a dominant class in $\mathbf{N}$, we have

$$|\mathbf{K}_{i1} \cap \mathbf{H}| = |\mathbf{K}_{i2} \cap \mathbf{H}| = \cdots = |\mathbf{K}_{it} \cap \mathbf{H}|. \quad (43)$$

The restriction of $\mathbf{G}$ into $\mathbf{N}$ is realized when the $\mathbf{K}_{ij}$ is replaced by $\mathbf{K}_{ij} \cap \mathbf{H}$. For any element t of the normalizer $\mathbf{N}$ ($=\mathbf{N_G}(\mathbf{H})$), we have $t^{-1}ht=\tilde{h}$ ($\in \mathbf{H}$). Since $\tilde{h}$ is an element of $\mathbf{H}$, Lemma 3 indicates that $\mathbf{C_N}(t^{-1}ht)=\mathbf{C_N}(\tilde{h})=\mathbf{C_G}(\mathbf{H})$. This is summarized as a lemma.

Lemma 6. *Let $\mathbf{H}$ ($=\langle h \rangle$) be a cyclic subgroup of $\mathbf{G}$. For any element t of the normalizer $\mathbf{N}$ ($=\mathbf{N_G}(\mathbf{H})$), we have $\mathbf{C_N}(h)=\mathbf{C_N}(t^{-1}ht)=\mathbf{C_G}(\mathbf{H})$.*

Hence, Lemma 2 is modified into the following lemma in the light of Theorem 3.

Lemma 7. *The centralizer in the elements contained in the conjugacy class $\mathbf{K}_{ij} \cap \mathbf{H}$ is $\mathbf{C_N}(\mathbf{H})$, being invariant when $\mathbf{K}_{ij} \cap \mathbf{H}$ runs over the dominant class $\mathbf{K}_i \cap \mathbf{N}$.*

In other words, we have the following propositions:

1. Let $\mathbf{C_N}(h)$ (=$\mathbf{C_N}(\mathbf{H})$) be the centralizer of $h \in \mathbf{K}_{ij} \cap \mathbf{H}$. Then, $\mathbf{C_N}(\mathbf{H})$ (=$t^{-1}\mathbf{C_N}(h)t$) is also the centralizer of $t^{-1}ht$ if the $t^{-1}ht$ belongs to $\mathbf{K}_{ij} \cap \mathbf{H}$ for $t \in \mathbf{N}$.

2. For $h' \in \mathbf{K}'_{ij}$, we have $\mathbf{C_N}(h) = \mathbf{C_N}(h') = \mathbf{C_N}(\mathbf{H})$.

Since the set $\mathbf{K}_{ij} \cap \mathbf{H}$ is a conjugacy class in $\mathbf{H}$, we have

$$q = |\mathbf{K}_{ij} \cap \mathbf{H}| = \frac{|\mathbf{N}|}{|\mathbf{C_N}(\mathbf{H})|} \tag{44}$$

Note that h in Eq. 44 can be any element of $\mathbf{K}_i \cap \mathbf{H}$ in the present situation. The dominant class $\mathbf{K}_i \cap \mathbf{H}$ contains all the generators of $\mathbf{H}$. Hence, the number of the generators is equal to the number of primitive $|\mathbf{H}|$-th root, i.e.,

$$|\mathbf{K}_i \cap \mathbf{H}| = \varphi(|\mathbf{H}|). \tag{45}$$

The second proposition of Theorem 1 shows that $t|\mathbf{K}_{ij} \cap \mathbf{H}| = |\mathbf{K}_i \cap \mathbf{H}|$. This result is combined with Eq. 45 giving the following theorem:

Theorem 4. *The number of the conjugacy classes involved in each dominant class* $\mathbf{K}_i \cap \mathbf{H}$ *within* $\mathbf{N}$ *is represented by*

$$t = \frac{\varphi(|\mathbf{H}|)|\mathbf{C_N}(\mathbf{H})|}{|\mathbf{N_G}(\mathbf{H})|}. \tag{46}$$

The number t is alternatively calculated from $t|\mathbf{K}_{ij}| = |\mathbf{K}_i|$ (derived from Eq. 28) by introducing Eqs. 4 and 5 ($\mathbf{G}_i = \mathbf{H}$):

$$t = \frac{|\mathbf{K}_i|}{|\mathbf{K}_{ij}|} = \frac{\varphi(|\mathbf{H}|)|\mathbf{C_G}(\mathbf{H})|}{|\mathbf{N_G}(\mathbf{H})|}. \tag{47}$$

Since $\mathbf{N}$ is the normalizer of $\mathbf{H}$, we have $\mathbf{C_G}(h) \subset \mathbf{N_G}(\mathbf{H}) = \mathbf{N}$. Hence, $\mathbf{C_G}(h)$ is identical with $\mathbf{C_N}(h)$, and $\mathbf{C_G}(\mathbf{H})$ is identical with $\mathbf{C_N}(\mathbf{H})$. It follows that Eq. 46 is equal to Eq. 47. By applying $t=1$ or $t>1$ to Theorem 4, we have the following corollary.

Corollary 1. *Let* $\mathbf{H}$ (=$\mathbf{G}_i$) *be a cyclic subgroup of the group* $\mathbf{G}$ *of a finite order. Suppose that* $\mathbf{N_G}(\mathbf{H})$ *is the normalizer of* $\mathbf{H}$ *in* $\mathbf{G}$, *that a dominant class* $\mathbf{K}_i \cap \mathbf{H}$ *corresponds to the subgroup* $\mathbf{H}$ (=$\mathbf{G}_i$), *and that* $\mathbf{C_N}(\mathbf{H})$ (=$\mathbf{C_N}(h)$) *is the centralizer of h belonging to* $\mathbf{K}_i \cap \mathbf{H}$. *The dominant class* $\mathbf{K}_i \cap \mathbf{H}$ *is characterized to be either of two cases:*

$$q = \frac{|\mathbf{N_G}(\mathbf{H})|}{|\mathbf{C_N}(\mathbf{H})|} \begin{cases} = \varphi(|\mathbf{H}|) & \text{if } \mathbf{K}_i \cap \mathbf{H} \text{ is matured,} \quad (48a) \\ < \varphi(|\mathbf{H}|) & \text{if } \mathbf{K}_i \cap \mathbf{H} \text{ is unmatured.} \quad (48b) \end{cases}$$

The constant q described in Corollary 1 is here called the *maturity discriminant*. The following theorem derived from Eq. 47 is essentially equivalent to Corollary 1. Theorem 5 deals with a dominant class $\mathbf{K}_i$ in $\mathbf{G}$, while Corollary 1 takes account of a dominant class $\mathbf{K}_i \cap \mathbf{H}$ in $\mathbf{N}$ (=$\mathbf{N_G}(\mathbf{H})$).

Theorem 5. *Let* $\mathbf{H}$ (=$\mathbf{G}_i$) *be a cyclic subgroup of the group* $\mathbf{G}$ *of a finite order. Suppose that* $\mathbf{N_G}(\mathbf{H})$ *is the normalizer of* $\mathbf{H}$ *in* $\mathbf{G}$, *that a dominant class* $\mathbf{K}_i$ *corresponds to the subgroup* $\mathbf{G}_i$, *and that* $\mathbf{C_G}(\mathbf{H})$ (=$\mathbf{C_G}(h)$) *is the centralizer of h belonging to* $\mathbf{K}_i \cap \mathbf{H}$. *The dominant class* $\mathbf{K}_i$ *is characterized to be either of two cases:*

$$q = \frac{|\mathbf{N_G}(\mathbf{H})|}{|\mathbf{C_G}(\mathbf{H})|} \begin{cases} = \varphi(|\mathbf{H}|) & \text{if } \mathbf{K}_i \text{ is matured,} \quad (49a) \\ < \varphi(|\mathbf{H}|) & \text{if } \mathbf{K}_i \text{ is unmatured.} \quad (49b) \end{cases}$$

Note that q represents the number of elements conjugate to the generator h of $\mathbf{H}$ within the normalizer $\mathbf{N_G}(\mathbf{H})$. Theorem 5 shows that the integer q is a discriminant for the maturaity of a finite group. In case that $\mathbf{G}$ is a cyclic group, we have $\mathbf{N_G}(\mathbf{H}) = \mathbf{C_G}(\mathbf{H}) = \mathbf{G}$; hence, we have $q = |\mathbf{N_G}(\mathbf{H})|/|\mathbf{C_G}(\mathbf{H})| = 1$. This indicates an extremely unmatured case. Example 6 shows another type of an extremely unmatured case.

Example 6. Let us reexamine the point group $\mathbf{T}_h$ of order 24. The dominant class $\mathbf{K}_6$ corresponds to the cyclic group $\mathbf{S}_6$, as shown in Example 1. Note that the normalizer of the group $\mathbf{S}_6$ is $\mathbf{S}_6$ itself, i.e., $\mathbf{N}_{\mathbf{T}_h}(\mathbf{S}_6) = \mathbf{S}_6$ (see Examples 2). The dominant class is converted into the counterpart of the normalizer as follows:

$$\mathbf{K}_6 \cap \mathbf{S}_6 = \mathbf{K}_{61} \cap \mathbf{S}_6 + \mathbf{K}_{62} \cap \mathbf{S}_6, \tag{50}$$

the right-hand side of which is represented by $\mathbf{K}_{61} \cap \mathbf{S}_6 = \{S_{6(1)}\}$ and $\mathbf{K}_{62} \cap \mathbf{S}_6 = \{S_{6(1)}^5\}$, where we place $\mathbf{S}_6 = \langle S_{6(1)} \rangle$. Hence, the dominant class $\mathbf{K}_6$ is unmatured even when the group $\mathbf{T}_h$ is restricted into $\mathbf{N_T}(\mathbf{S}_6)$ (=$\mathbf{S}_6$).

Since the centralizer ($\mathbf{C_T}(\mathbf{S}_6)$) is equal to the normalizer ($\mathbf{N_T}(\mathbf{S}_6)$), we have $q = |\mathbf{N}_{\mathbf{T}_h}(\mathbf{S}_6)|/|\mathbf{C}_{\mathbf{T}_h}(\mathbf{S}_6)| = 1$.

2 Combinatorial Enumeration

2.1 Dominant and Non-Dominant Representations as Matured Representations. We have reported **Q**-conjugacy character tables and characteristic monomial tables for cyclic groups.[23] In the present section, we shall pursue a method of combinatorial enumeration by utilizing these tables, where the scope of enumeration is extended so as to treat cases in which a starting skeleton belongs to a finite group. Note that **Q**-conjugacy character tables and characteristic monomial tables for finite groups are not required.

In general, a character is a class function, each value of which is given to each conjugacy class. On the other hand, a markaracter is given to each dominant class (**Q**-conjugacy class). Hence, there exists some characters that cannot be regarded as markaracters in an unmatured group. For example, one of the irreducible characters E_g for $\mathbf{T}_h$ (an unmatured group),

	$\mathbf{K}_1$	$\mathbf{K}_2$	$\mathbf{K}_3$	$\mathbf{K}_4$	$\mathbf{K}_{51}$	$\mathbf{K}_{52}$	$\mathbf{K}_{61}$	$\mathbf{K}_{62}$
	I	$3C_2$	$3\sigma_h$	i	$4C_3$	$4C_3^2$	$4S_6$	$4S_6^5$
$E_{g(1)}$	2	1	1	1	ε	$\overline{\varepsilon}$	ε	$\overline{\varepsilon}$

(51)

shows that the values of $\mathbf{K}_{51}$ and $\mathbf{K}_{52}$ (as well as those of $\mathbf{K}_{61}$ and $\mathbf{K}_{62}$) are not equal to each other, where $\varepsilon = \exp(2\pi i/3)$ and $\overline{\varepsilon} = \exp(-2\pi i/3)$. In contrast, $\mathbf{T}_h(/\mathbf{C}_s)$ gives the number of fixed points to each conjugacy class,

	$\mathbf{K}_1$	$\mathbf{K}_2$	$\mathbf{K}_3$	$\mathbf{K}_4$	$\mathbf{K}_5$		$\mathbf{K}_6$	
	$\mathbf{K}_1$	$\mathbf{K}_2$	$\mathbf{K}_3$	$\mathbf{K}_4$	$\mathbf{K}_{51}$	$\mathbf{K}_{52}$	$\mathbf{K}_{61}$	$\mathbf{K}_{62}$
	I	$3C_2$	$3\sigma_h$	i	$4C_3$	$4C_3^2$	$4S_6$	$4S_6^5$
$\mathbf{T}_h(/\mathbf{C}_s)$	12	0	4	0	0	0	0	0

(52)

This can be regarded as a character of $\mathbf{T}_h$, where the values of $\mathbf{K}_{51}$ and $\mathbf{K}_{52}$ (as well as those of $\mathbf{K}_{61}$ and $\mathbf{K}_{62}$) are equal to each other. Hence, the character is alternatively regarded as a markaracter of $\mathbf{T}_h$, when we take acount of dominant classes (**Q**-conjugacy classes).

	$\mathbf{K}_1$	$\mathbf{K}_2$	$\mathbf{K}_3$	$\mathbf{K}_4$	$\mathbf{K}_5$	$\mathbf{K}_6$
$\mathbf{T}_h(/\mathbf{C}_s)$	12	0	4	0	0	0

(53)

When this example is extended to general cases, we are able to define a *matured representation* as a representation whose character has the equal values for the elements involved in each dominant class. The character of such a matured representation is called a *matured character*, which is equalized to a markaracter as shown above. It follows that *a matured group gives matured representations only*, *while an unmatured group gives both matured and unmatured representations*. Obviously, for dominant and non-dominant representations defined in Refs. 21 and 22, we have the following theorem:

Theorem 6. *Dominant and non-dominant representations are matured representations in terms of the present definiton.*

This theorem holds true for both matured and unmatured groups. The details of matured representations other than dominant and non-dominant representations will be discussed elsewhere. Note that, although the group $\mathbf{T}_h$ is an unmatured group, it is possible to obtain such matured characters (markaracters) in cases of combinatorial enumeration.

2.2 A New Method of Calculating Cycle Indices. Consider a skeleton belonging to the **G** group, in which a set of p positions is governed by a permutation representation **P**. The representation **P** is subduced into a cyclic subgroup $\mathbf{G}_j$ (corresponding to a **Q**-conjugacy class $\mathbf{K}_j$) to give

$$\mathbf{P} \downarrow \mathbf{G}_j = \sum_{k=1}^{\nu_j} \beta_{jk} \Gamma_k^{(j)}, \tag{54}$$

where the symbol $\Gamma_k^{(j)}$ designates a **Q**-conjugacy representation of $\mathbf{G}_j$. The multiplicities (β_{jk}) appearing in the right-hand side of Eq. 54 is obtained from

$$FPV_{\mathbf{P}} \downarrow \mathbf{G}_j \times D_{\mathbf{G}_j}^{-1} = (\beta_{j1}, \beta_{j2}, \cdots, \beta_{j\nu_j}), \tag{55}$$

where the $FPV_{\mathbf{P}}{\downarrow}\mathbf{G}_j$ denotes the fixed-point vector ($FPV_{\mathbf{P}}$) on the action of **P** that is subduced into the cyclic subgroup $\mathbf{G}_j$; and $D_{\mathbf{G}_j}$ is the **Q**-conjugacy character table of $\mathbf{G}_j$.

Let a characteristic monomial for the representation $\Gamma_k^{(j)}$ be $Z(\Gamma_k^{(j)}, s_d)$, which has been already discussed for the cyclic group ($\mathbf{G}_j$).[23] By using the multiplicities appearing in Eq. 54, we can define a subduced cycle index (*SCI*):

$$SCI(\mathbf{P} \downarrow \mathbf{G}_j; s_d) = \prod_{k=1}^{\nu_j} (Z(\Gamma_k^{(j)}; s_d))^{\beta_{jk}}. \tag{56}$$

By starting from Eq. 56, we have the definition of a cycle index (*CI*):

$$CI(\mathbf{P}; s_d) = \sum_{j=1}^{s} N_j SCI(\mathbf{P} \downarrow \mathbf{G}_j; s_d)$$

$$= \sum_{j=1}^{s} N_j \prod_{k=1}^{\nu_j} (Z(\Gamma_k^{(j)}; s_d))^{\beta_{jk}}, \tag{57}$$

where the coefficient N_j is equal to $\varphi(|\mathbf{G}_j|)/|\mathbf{N}_\mathbf{G}(\mathbf{G}_j)|$ ($=|\mathbf{K}_j|/|\mathbf{G}|$ in the light of Eq. 4). It should be noted that the *CI* (Eq. 57) is composed of characteristic monomials for the representation $\Gamma_k^{(j)}$ of a cyclic group $\mathbf{G}_j$.

Although the definition of the cycle index (*CI*) is different from that of Pólya's theorem[25,26] or from that of the USCI approach,[27] it gives enumeration results equivalent to Pólya's theorem or the USCI approach. Thus, the *CI* (Eq. 57) is applied to combinatorial enumeration, as shown in the following theorem.

Theorem 7. *Consider a skeleton of symmetry* **G** *having p positions, which is governed by a permutation representation* **P**. *Suppose that the positions are occupied by p ligands selected from a ligand set,*

$$\mathbf{Y} = \{Y_1, Y_2, \cdots, Y_{|\mathbf{Y}|}\}, \tag{58}$$

to give an isomer, where the selected set contains ν_ι *of ligands* Y_ι ($\iota = 1, 2, \cdots, |\mathbf{Y}|$) *satisfies a partition:*

$$[\nu]: \ \nu_1 + \nu_2 + \cdots + \nu_{|\mathbf{Y}|} = p. \tag{59}$$

Since the weight (molecular formula) of the isomer is represented by

$$W_\nu = \prod_{\iota=1}^{|\mathbf{Y}|} Y_\iota^{\nu_\iota}, \tag{60}$$

a generating function for the total number A_ι *of isomers with the weight* W_ι *is represented by*

$$\sum_{[\nu]} A_\nu W_\nu = CI(\mathbf{P}; s_d), \tag{61}$$

where

$$s_d = \sum_{\iota=1}^{\nu} Y_\iota^d. \tag{62}$$

Example 7. Let us consider the enumeration of isomers by starting from a $\mathbf{T}_h$ skeleton (**1**), which is a [60]fullerene derivative with six methano groups, where each small circle denotes a hydrogen atom. For the sake of simplicity, we depict the skeleton in the form of a simpler one shown as **1′**, where each small circle on a thick-lined cross denotes a hydrogen atom of a methano group. Suppose that an appropriate set of hydrogens on the methano groups are replaced by halogen atoms (Y) to give an isomer. The target of this example is to obtain the number of such isomers with a respective molecular formula.

Table 1. **Q**-Conjugacy Character Tables (Left) and Characteristic Monomial Tables (Right) for $\mathbf{C}_2$, $\mathbf{C}_s$, $\mathbf{C}_i$

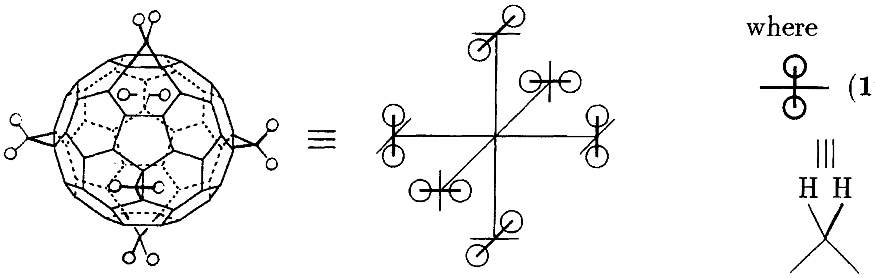
$\mathbf{C}_2$			$\mathbf{C}_1$	$\mathbf{C}_2$
	$\mathbf{C}_s$		$\mathbf{C}_1$	$\mathbf{C}_s$
		$\mathbf{C}_i$	$\mathbf{C}_1$	$\mathbf{C}_i$
A	A'	A_g	1	1
B	A''	A_u	1	-1

$\mathbf{C}_2$			$\mathbf{C}_1$	$\mathbf{C}_2$
	$\mathbf{C}_s$		$\mathbf{C}_1$	$\mathbf{C}_s$
		$\mathbf{C}_i$	$\mathbf{C}_1$	$\mathbf{C}_i$
A	A'	A_g	s_1	s_1
B	A''	A_u	s_1	$s_1^{-1}s_2$
	N_l		$\frac{1}{2}$	$\frac{1}{2}$

Table 2. **Q**-Conjugacy Character Table (Left) and Characteristic Monomial Table (Right) for $\mathbf{C}_3$

	$\mathbf{C}_1$	$\mathbf{C}_3$
A	1	1
E	2	-1

	$\mathbf{C}_1$	$\mathbf{C}_3$
A	s_1	s_1
E	s_1^2	$s_1^{-1}s_3$
N_l	$\frac{1}{3}$	$\frac{2}{3}$



1 **1′**

Table 3. **Q**-Conjugacy Character Table (Left) and Characteristic Monomial Table (Right) for the Point Group $\mathbf{S}_6$

	$\mathbf{K}_1$ $\mathbf{C}_1$	$\mathbf{K}_2$ $\mathbf{C}_i$	$\mathbf{K}_3$ $\mathbf{C}_3$	$\mathbf{K}_4$ $\mathbf{S}_6$
A_g	1	1	1	1
B_u	1	-1	1	-1
E_g	2	2	-1	-1
E_u	2	-2	-1	1

$\mathbf{S}_6$	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_i$	$\downarrow \mathbf{C}_3$	$\downarrow \mathbf{S}_6$
A_g	s_1	s_1	s_1	s_1
A_u	s_1	$s_1^{-1}s_2$	s_1	$s_1^{-1}s_2$
E_g	s_1^2	s_1^2	$s_1^{-1}s_3$	$s_1^{-1}s_3$
E_u	s_1^2	$s_1^{-2}s_2^2$	$s_1^{-1}s_3$	$s_1s_2^{-1}s_3^{-1}s_6$
N_l	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$

Since the point group $\mathbf{T}_h$ has the SCSG shown in Eq. 1 (Example 1), the enumeration on such a $\mathbf{T}_h$ skeleton requires the **Q**-conjugacy character tables and characteristic monomial tables for the SCSG (Tables 1, 2, and 3).

The twelve positions of the skeleton **1** are governed by a permutation representation (**P**), which has an FPV on the action of $\mathbf{T}_h$:

$$FPV = (12,0,4,0,0,0), \tag{63}$$

the elements of which are aligned in the order of the SCSG (Eq. 1). The subduction of **P** into the subgroup $\mathbf{C}_2$ gives a row vector (12, 0), which is multiplied by the inverse of the **Q**-conjugacy character table of $\mathbf{C}_2$ (Table 3, left):

$$(12,0)\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix} = (6,6). \tag{64}$$

The resulting matrix means that

$$\mathbf{P} \downarrow \mathbf{C}_2 = 6A + 6B, \tag{65}$$

which in turn corresponds to the following monomial (SCI):

$$SCI(\mathbf{P} \downarrow \mathbf{C}_2; s_d) = (s_1)^6(s_1^{-1}s_2)^6 = s_2^6, \tag{66}$$

where we use the characteristic monomials of $\mathbf{C}_2$ collected in the rightmost column of Table 1 (right). Since the subduction of **P** into the subgroup $\mathbf{C}_i$ gives the row vector (12,0), we have the same *SCI* s_2^6 corresponding to $\mathbf{P} \downarrow \mathbf{C}_i = 6A_g + 6A_u$.

The subduction $\mathbf{P}\downarrow\mathbf{C}_s$ gives a row vector (12,4), which is multiplied by the inverse of the **Q**-conjugacy character table of $\mathbf{C}_s$ (Table 1, left):

$$(12,4)\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix} = (8,4). \tag{67}$$

Hence, we have

$$\mathbf{P} \downarrow \mathbf{C}_s = 8A' + 4A'', \tag{68}$$

which in turn corresponds to the following *SCI*:

$$SCI(\mathbf{P} \downarrow \mathbf{C}_s; s_d) = (s_1)^8(s_1^{-1}s_2)^4 = s_1^4s_2^4. \tag{69}$$

For the subduction $\mathbf{P}\downarrow\mathbf{C}_3$, the corresponding row vector (12,0) is multiplied by the inverse of the **Q**-conjugacy character table of $\mathbf{C}_3$ (Table 2, left):

$$(12,4)\begin{pmatrix} \frac{1}{3} & \frac{1}{3} \\ \frac{2}{3} & -\frac{1}{3} \end{pmatrix} = (4,4). \tag{70}$$

Hence, we have

$$\mathbf{P} \downarrow \mathbf{C}_3 = 4A + 4E, \tag{71}$$

which in turn corresponds to the following monomial (*SCI*):

$$SCI(\mathbf{P} \downarrow \mathbf{C}_3; s_d) = (s_1)^4(s_1^{-1}s_3)^4 = s_3^4, \tag{72}$$

where we use the characteristic monomials of $\mathbf{C}_3$ collected in the rightmost column of Table 2 (right).

The subduction $\mathbf{P}\downarrow\mathbf{S}_6$ characterized by a row vector (12, 0, 0, 0) gives the multiplicities,

$$(12,0,0,0)\begin{pmatrix} \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} \\ \frac{1}{6} & -\frac{1}{6} & \frac{1}{6} & -\frac{1}{6} \\ \frac{1}{3} & \frac{1}{3} & -\frac{1}{6} & -\frac{1}{6} \\ \frac{1}{3} & -\frac{1}{3} & -\frac{1}{6} & \frac{1}{6} \end{pmatrix} = (2,2,2,2), \tag{73}$$

where the second 4×4 matrix in the left-hand side is the inverse of the **Q**-conjugacy character table of $\mathbf{S}_6$ (Table 3, left). Hence, we have

$$\mathbf{P} \downarrow \mathbf{S}_6 = 2A_g + 2A_u + 2E_g + 2E_u \tag{74}$$

which in turn corresponds to the following *SCI*:

$$SCI(\mathbf{P} \downarrow \mathbf{S}_6; s_d) = (s_1)^2(s_1^{-1}s_2)^2(s_1^{-1}s_3)^2(s_1s_2^{-1}s_3^{-1}s_6)^2 = s_6^2, \tag{75}$$

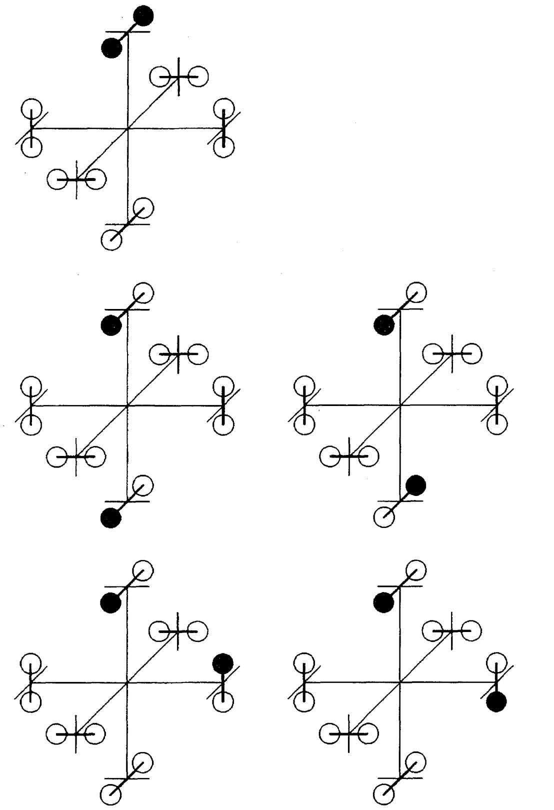


Fig. 1. Five di-substituted isomers from the skeleton **1**.

where we use the characteristic monomials of $\mathbf{S}_6$ collected in the rightmost column of Table 3 (right). These *SCIs* are collected in terms of Eq. 57 to give

$$f = CI(\mathbf{P}; s_d) = \frac{1}{24}s_1^{12} + \frac{1}{8}s_2^{6} + \frac{1}{8}s_1^4 s_2^4 + \frac{1}{24}s_2^{6} + \frac{1}{3}s_3^{4} + \frac{1}{3}s_6^{2}, \tag{76}$$

where the coefficients (i.e., N_j in Eq. 57) are obtained by $\varphi(|\mathbf{G}_j|)/|\mathbf{N}_{\mathbf{T}_h}(\mathbf{G}_j)|$ (each cyclic subgroup $\mathbf{G}_j$ is selected from the SCSG). Into the *CI* (Eq. 76), a figure-inventory,

$$s_d = 1 + y^d, \tag{77}$$

is introduced according to Theorem 7. Thereby, we obtain the following generating function:

$$\begin{aligned} f &= \frac{1}{24}(1+y)^{12} + \frac{1}{8}(1+y^2)^6 + \frac{1}{8}(1+y)^4(1+y^2)^4 + \frac{1}{24}(1+y^2)^6 \\ &\quad + \frac{1}{3}(1+y^3)^4 + \frac{1}{3}(1+y^6)^2 \\ &= y^{12} + y^{11} + 5y^{10} + 13y^9 + 27y^8 + 38y^7 + 50y^6 + 38y^5 + 27y^4 \\ &\quad + 13y^3 + 5y^2 + y + 1 \end{aligned} \tag{78}$$

For the illustration of the results (Eq. 78), Fig. 1 shows five di-substituted isomers (corresponding to the term $5y^2$), where each solid circle denotes a halogen atom (Y).

3 Conclusion

A finite group **G** is classified into a matured or unmatured group by examining how a dominant class (**Q**-conjugacy class) corresponding to a cyclic subgroup **H** contains conjugacy classes. For the determination of such maturity, the maturity discriminant is proposed:

1. If the ingeter $q=|\mathbf{N_G}(\mathbf{H})|/|\mathbf{C_G}(\mathbf{H})|$ is less than an Euler function $\varphi(|\mathbf{H}|)$, the group $|\mathbf{G}|$ is concluded to be unmatured concerning **H**.
2. Otherwise, the group $|\mathbf{G}|$ is matured concerning **H**.

Here, $\mathbf{N_G}(\mathbf{H})$ and $\mathbf{C_G}(\mathbf{H})$ respectively denote the normalizer and the centralizer of **H** within **G**. A matured representation is defined in terms of the maturity concept. It is subduced into cyclic subgroups to give the corresponding monomials, which are applied to the combinatorial enumeration of isomers.

Appendix A. Conservation of Maturity

This Appendix is devoted to the proof of Theorem 2 and several related comments. For the simplicity of discussion, the cyclic subgroup **H** is selected to have the largest order, if other cyclic subgroups are present so as to satisfy a group-subgroup relationship. The following lemma is the basis of such a convention.

Lemma 8. *If* $\mathbf{H}'$ *is a subgroup of the cyclic group* **H**, *the cyclic subgroup* $\mathbf{H}'$ *has the same normalizer as that of* **H**.

Proof. Let $\mathbf{H}'$ be a subgroup of the cyclic group **H**. When we take an element h that is a generator of **H**, for any element t ($\in\mathbf{N}$), we have $t^{-1}ht=h^s$ for an appropriate integer s. It follows that $t^{-1}h^rt=(h^s)^r=(h^r)^s$. If the resulting h^r be a generator of $\mathbf{H}'$, the element $(h^r)^s$ appearing in the equation is involved in $\mathbf{H}'$. Hence, we have $t^{-1}\mathbf{H}'t=\mathbf{H}'$. This means that **N** is also the normalizer of $\mathbf{H}'$.

Since the **N** is the normalizer of **H**, we have $\mathbf{H}=t^{-1}\mathbf{H}t$ for any $t\in\mathbf{N}$ and $\mathbf{H}\neq g^{-1}\mathbf{H}g$ for any $g\in\mathbf{G}-\mathbf{N}$. Moreover, we have $\mathbf{H}\cap g^{-1}\mathbf{H}g=\{I\}$ for $g\in\mathbf{G}-\mathbf{N}$, because **H** is cyclic. These results are summarized to give a theorem.

Theorem 8. *Let* **H** (=$\mathbf{G}_i$) *be a cyclic subgroup selected from the SCSG of* **G** *and* **N** *the normalizer of* **H** *within* **G**. *Then any* $g(\in\mathbf{G})$ *acts on* **H** *in three ways:*

1. $\mathbf{H}=g^{-1}\mathbf{H}g$ for $g\in\mathbf{H}$
2. $\mathbf{H}=g^{-1}\mathbf{H}g$ for $g\in\mathbf{N}-\mathbf{H}$

and

3. $\mathbf{H}\cap g^{-1}\mathbf{H}g=\{I\}$ for $g\in\mathbf{G}-\mathbf{N}$.

When g is an element of the coset $\mathbf{N}g_i$, we have $g=tg_i$ for an appropriate t in **N**. Since we have $g^{-1}\mathbf{H}g=g_i^{-1}t^{-1}\mathbf{H}tg_i=g_i^{-1}\mathbf{H}g_i$ (for $i=1,2,\cdots,a$), any element of the coset $\mathbf{N}g_i$ gives the same conjugate subgroup $g_i^{-1}\mathbf{H}g_i$. This means that the coset $\mathbf{N}g_i$ corresponds to the group $g_i^{-1}\mathbf{H}g_i$ in one-to-one fashion; hence, the number of such conjugate subgroups as $g_i^{-1}\mathbf{H}g_i$ is concluded to be equal to the number of the cosets, $a=|\mathbf{G}|/|\mathbf{N}|$. This result is summarized as a corollary.

Corollary 2. *Let* g_i ($i=1,2,\cdots,a$) *be selected from the transversal* **A** (*Eq. 14*). *All the conjugate subgroups of the cyclic subgroup* **H** *involved in* **G** *are represented by* $g_i^{-1}\mathbf{H}g_i$, *the number of which is equal to* $a=|\mathbf{G}|/|\mathbf{N}|$.

A conjugate subgroup of the normalizer **N**, i.e., $g^{-1}\mathbf{N}g$, may or may not be equal to **N**. If the normalizer $\mathbf{N_G}(\mathbf{N})$ is taken into consideration, a discussion similar to the one for Corollary 2 can be applied to this case. As a result, we have the following corollary.

Corollary 3. *Let* **H** (=$\mathbf{G}_i$) *be a cyclic subgroup selected from the SCSG of* **G** *and* **N** *the normalizer of* **H** *within* **G**. *All the subgroups conjugate to the normalizer* **N** *are represented by* $g^{-1}{}_i\mathbf{N}g_i$ ($i=1,2,\cdots,a$), *which may contain duplicity when each* g_i *is selected from the transversal* **A**.

Let us consider an element h ($\in\mathbf{H}$). The following theorem is obvious because of the definitions of **G**, **H**, and **N**.

Theorem 9. *Let h be an element of the cyclic subgroup* **H**, *the normalizer of which is denoted to be* $\mathbf{N} \equiv \mathbf{N_G}(\mathbf{H})$. *Any element that is conjugate to h within* **G** *belongs to either of the following cases:*

1. The element $t^{-1}ht$ ($\in \mathbf{H}$ *for any* $t \in \mathbf{N}$) *is conjugate to h within* **G** *as well as within* **N**. *It is involved in* **N**.

2. The element $g^{-1}hg$ ($\in g^{-1}\mathbf{H}g$ *for any* $g \in \mathbf{G}-\mathbf{N}$) *is conjugate to h within* **G** *but not within* **N**, *whether it is involved in* **N** *or not.*

It should be noted that there are two subsidiary cases for the second proposition of Theorem 9 in the light of Theorem 11:

(*a*) *If we have* $g^{-1}\mathbf{N}g \neq \mathbf{N}$ *for* $g \in \mathbf{G}-\mathbf{N}$, *the element* $g^{-1}hg$ *is involved in* $g^{-1}\mathbf{N}g$ *but not in* **N** ($\neq g^{-1}\mathbf{N}g$). *Hence, it is not conjugate to h within* **N**.

(*b*) *If we have* $g^{-1}\mathbf{N}g = \mathbf{N}$ *for* $g \in \mathbf{G}-\mathbf{N}$, *the element* $g^{-1}hg$ *is an element of* **N**, *as shown in Theorem 11. Note that we have the third proposition of Theorem 8; hence, we have* $g^{-1}hg \in g^{-1}\mathbf{H}g \subset \mathbf{N}$ *and* $g^{-1}hg \notin \mathbf{H} \subset \mathbf{N}$. *In other words, the element* $g^{-1}hg$ *belongs to either one of the isomorphic but non-conjugate subgroups described above* ($\mathbf{H}_\rho$). *As a result, the element* $g^{-1}hg$ ($\in g^{-1}\mathbf{N}g = \mathbf{N}$) *is not conjugate to h within* **N**.

In both of the two subsidiary cases, the element $g^{-1}hg$ *is not conjugate to h within* **N**.

Theorem 9 can be rewritten as follows so as to describe the behaviors of dominant classes, giving Theorem 2. The proof of Theorem 2 is given here.

Proof of Theorem 2. Let h be a generator of **H**. Then, h^r is another generator of **H**, where $(r, n)=1$.

If the dominant class corresponding to **H** is matured in **N**, we have $t^{-1}ht = h^r$ for an appropriate t ($\in \mathbf{N} \subset \mathbf{G}$). Hence, we have the first proposition.

If the dominant class corresponding to **H** is matured in **G**, we have $t^{-1}ht = h^r$ for an appropriate t ($\in \mathbf{G}$). Hence, we obtain $t^{-1}\langle h \rangle t = \langle h^r \rangle$, which is equal to $t^{-1}\mathbf{H}t = \mathbf{H}$. This means that $t \in \mathbf{N}$ because of the definition of the normalizer **N**. Hence, h and h^r is also conjugate to each other within **N**. Thereby, we have the second proposition.

Although Theorem 9 shows that the element h ($\in \mathbf{H}$) is not conjugate to the element $g^{-1}hg$ within **N**, we are able to obtain the following corollary for comparing these elements.

Corollary 4. *Suppose that two elements h and* $t^{-1}ht$ *of the cyclic group* **H** *are conjugate to each other within* **N** (*i.e.,* $t \in \mathbf{N}$). *Then,* $g^{-1}hg$ *and* $g^{-1}(t^{-1}ht)g$ *of the group* $g^{-1}\mathbf{H}g$ *are conjugate to each other within* $g^{-1}\mathbf{N}g$ *for* $g \in \mathbf{G}$.

Proof. Since t is an element of **N**, the element $g^{-1}tg$ is an element of $g^{-1}\mathbf{N}g$. Hence, the element

$$(g^{-1}tg)^{-1}(g^{-1}hg)(g^{-1}tg) = g^{-1}(t^{-1}hg)g$$

is conjugate to $g^{-1}hg$.

Let **N/H** be a set of cosets produced by Eq. 13 as follows:

$$\mathbf{N}/\mathbf{H} = \{\mathbf{H}t_1, \mathbf{H}t_2, \cdots, \mathbf{H}t_\alpha, \cdots, \mathbf{H}t_b\} \quad (79)$$

where **N** is the normalizer of the cyclic subgroup **H**, i.e., $\mathbf{N} = \mathbf{N_G}(\mathbf{H})$. Let us now consider the group $g^{-1}\mathbf{N}g$ that is conjugate to **N** as well as the cyclic group $g^{-1}\mathbf{H}g$ that is conjugate to **H** within **G**, where the element g is presumed to be selected from **A** without losing generality. Obviously, we have $g^{-1}\mathbf{H}g \subset g^{-1}\mathbf{N}g$. Any element $t_\alpha \in \mathbf{B}$ satisfies $t_\alpha^{-1}\mathbf{H}t_\alpha = \mathbf{H}$. Consider the element $g^{-1}t_\alpha g$ conjugate to t_α, where $g^{-1}t_\alpha g \in g^{-1}\mathbf{N}g$ ($\forall t_\alpha \in \mathbf{N}$). Then we have

$$\begin{aligned}(g^{-1}t_\alpha g)^{-1}(g^{-1}\mathbf{H}g)(g^{-1}t_\alpha g) &= g^{-1}t_\alpha^{-1}gg^{-1}\mathbf{H}gg^{-1}t_\alpha g \\ &= g^{-1}t_\alpha^{-1}\mathbf{H}t_\alpha g = g^{-1}\mathbf{H}g. \quad (80)\end{aligned}$$

It follows that the element $g^{-1}t_\alpha g$ is contained in the normalizer of $g^{-1}\mathbf{H}g$, i.e., $g^{-1}t_\alpha g \in \mathbf{N_G}(g^{-1}\mathbf{H}g)$. As the t_α runs over the normalizer **N**, the element $g^{-1}t_\alpha g$ runs to generate the normalizer $\mathbf{N_G}(g^{-1}\mathbf{H}g)$. Hence, we obtain the following theorem.

Theorem 10. *Within the group* **G**, *the normalizer of the cyclic group* **H** *and that of* $g^{-1}\mathbf{H}g$ ($\forall g \in \mathbf{A}$) *are conjugate to each other,* i.e., $g^{-1}\mathbf{N_G}(\mathbf{H})g = \mathbf{N_G}(g^{-1}\mathbf{H}g)$.

Since we have $(g^{-1}\mathbf{H}g)(g^{-1}t_\alpha g) = g^{-1}\mathbf{H}t_\alpha g$, a coset decomposition of $g^{-1}\mathbf{N}g$ by $g^{-1}\mathbf{H}g$ is represented by

$$\begin{aligned}g^{-1}\mathbf{N}g &= (g^{-1}\mathbf{H}g)(g^{-1}t_1 g) + (g^{-1}\mathbf{H}g)(g^{-1}t_2 g) + \cdots \\ &\quad + (g^{-1}\mathbf{H}g)(g^{-1}t_b g) \\ &= g^{-1}\mathbf{H}t_1 g + g^{-1}\mathbf{H}t_2 g + \cdots + g^{-1}\mathbf{H}t_b g, \quad (81)\end{aligned}$$

which produces cosets as follows.

$$\begin{aligned}&g^{-1}\mathbf{N}g/g^{-1}\mathbf{H}g \\ &= \{g^{-1}\mathbf{H}t_1 g, g^{-1}\mathbf{H}t_2 g, \cdots, g^{-1}\mathbf{H}t_\alpha g, \cdots, g^{-1}\mathbf{H}t_b g\}. \quad (82)\end{aligned}$$

In a special case that g belongs to $\mathbf{N_G}(\mathbf{N})$, i.e., $g^{-1}\mathbf{N}g = \mathbf{N}$, Theorem 10 shows that $\mathbf{N_G}(\mathbf{H}) = \mathbf{N_G}(g^{-1}\mathbf{H}g)$. In other words, **N** is also the normalizer of the cyclic group $g^{-1}\mathbf{H}g$. This is summarized as follows:

Theorem 11. *For* $g \in \mathbf{N_G}(\mathbf{N})$, *the group* $g^{-1}\mathbf{H}g$, *which is not conjugate to* **H** *within* **N**, *is a normal subgroup of* **N**.

Proof. For any $t \in \mathbf{N}$, we have $gtg^{-1} \in \mathbf{N}$, since g is an element of the normalizer $\mathbf{N_G}(\mathbf{N})$. Because **N** is the normalizer of **H**, we obtain $(gtg^{-1})^{-1}\mathbf{H}(gtg^{-1}) = \mathbf{H}$. This is transformed into $t^{-1}(g^{-1}\mathbf{H}g)t = g^{-1}\mathbf{H}g$. It follows that the normalizer of $g^{-1}\mathbf{H}g$ is also **N**.

Moreover, the condition $g^{-1}\mathbf{N}g = \mathbf{N}$ converts Eq. 81 into

$$\begin{aligned}\mathbf{N} &= (g^{-1}\mathbf{H}g)(g^{-1}t_1 g) + (g^{-1}\mathbf{H}g)(g^{-1}t_2 g) + \cdots + (g^{-1}\mathbf{H}g)(g^{-1}t_b g) \\ &= g^{-1}\mathbf{H}t_1 g + g^{-1}\mathbf{H}t_2 g + \cdots + g^{-1}\mathbf{H}t_b g, \quad (83)\end{aligned}$$

Let us consider the commutator subgroup $[\mathbf{H}, g^{-1}\mathbf{H}g]$ derived from **H** and $g^{-1}\mathbf{H}g$ of Theorem 11. Theorem 11 and Theorem 3.2 of Chapter 5 in Ref. 28 indicate that the group $[\mathbf{H}, g^{-1}\mathbf{H}g]$ is a normal subgroup satisfying $[\mathbf{H}, g^{-1}\mathbf{H}g] \subset \mathbf{H} \cap g^{-1}\mathbf{H}g$. This result combined with Case 3 of Theorem 8 shows that $[\mathbf{H}, g^{-1}\mathbf{H}g] = \{I\}$. This gives the following corollary.

Corollary 5. *For* **H** *and* $g^{-1}\mathbf{H}g$ *described in Theorem 11, any element of* **H** *is commutative with any element of* $g^{-1}\mathbf{H}g$.

The group $g^{-1}\mathbf{H}g$ described in Corollary 5 is a normal subgroup of the centralizer $\mathbf{C_G}(\mathbf{H})$. However, the centralizer $\mathbf{C_G}(\mathbf{H})$ is not always the centralizer of the group $g^{-1}\mathbf{H}g$. In other words, the $\mathbf{C_G}(\mathbf{H})$ is not always identical with $\mathbf{C_G}(g^{-1}\mathbf{H}g)$.

If the $\mathbf{C_G}(\mathbf{H})$ is identical with $\mathbf{C_G}(g^{-1}\mathbf{H}g)$, the groups **H** and $g^{-1}\mathbf{H}g$ are contained in the center of the centralizer $\mathbf{C_G}(\mathbf{H})$.

Appendix B. Notes on Theorem 5

It should be noted here how Theorem 5 is related to automorphism. An automorphism of a group **G** is an isomorphism from **G** to **G**. All the automorphisms concerning **G** form a group called the automorphism group, designated as Aut **G**.[29,30] A fixed element g of **G** gives an inner automorphism $x \rightarrow g^{-1}xg$ by conjugation. All the inner automorphisms form the inner automorphism group designated as Inn **G**.

When a group **H** is a subgroup of **G**, the automorphism group of the subgroup (**H**) within **G** is represented by the factor group $\mathbf{N_G}(\mathbf{H})/\mathbf{C_G}(\mathbf{H})$, which is a subgroup of Aut **H** (Theorem 3.5 of Ref. 30). If the subgroup **H** is a cyclic group, the order $|\mathbf{H_G}(\mathbf{H})|/|\mathbf{C_G}(\mathbf{H})|$ represents the number of elements involved in a conjugacy class (Eq. 26). Hence, the number $|\mathbf{H_G}(\mathbf{H})|/|\mathbf{C_G}(\mathbf{H})|$ runs from 1 to $\varphi(|\mathbf{H}|)$ in accord with Theorem 5.

We now consider the case where the cyclic subgroup **H** (=$\mathbf{G}_i$) corresponds to the dominant class $\mathbf{K}_i$, which in turn consists of two or more conjugacy classes (Eq. 26). Suppose that the conjugacy class ($\mathbf{K}_{ij}$) in **G** (Eq. 26) is restricted to the conjugacy class $\mathbf{K}_{ij}\cap\mathbf{H}$ in the normalizer **N**. The elements of the conjugacy class $\mathbf{K}_{ij}\cap\mathbf{H}$ is represented as follows by using h ($\in\mathbf{H}$) and the transversal **B** (Eq. 15):

$$\mathbf{K}_{ij}\cap\mathbf{H}=\{t_1^{-1}ht_1\ (=h),\ t_2^{-1}ht_2,\cdots,t_\alpha^{-1}ht_\alpha,\cdots,t_b^{-1}ht_b\} \quad (84)$$

The right-hand side of Eq. 84 contains all of the elements conjugate to h ($\in\mathbf{H}$). Thus, select any element t from a coset $\mathbf{H}t_\alpha$ appearing in Eq. 13, i.e., $t\in\mathbf{H}t_\alpha$. Then, we can denote $t=\tilde{h}t_\alpha$ where $\tilde{h}\in\mathbf{H}$. By using the fact that h ($\in\mathbf{H}$) and $\tilde{h}$ are commutative, we have

$$t^{-1}ht=t_\alpha^{-1}\tilde{h}^{-1}h\tilde{h}t_\alpha=t_\alpha^{-1}\tilde{h}^{-1}\tilde{h}ht_\alpha=t_\alpha^{-1}ht_\alpha\ (\in t_\alpha^{-1}\mathbf{H}t_\alpha=\mathbf{H}). \quad (85)$$

This means that any element in the coset $\mathbf{H}t_\alpha$ can be selected as a representative, giving the same element $t_\alpha^{-1}ht_\alpha$ conjugate to h. As a result, each element $t_\alpha^{-1}ht_\alpha$ appearing in Eq. 84 is concluded to correspond to the coset $\mathbf{H}t_\alpha$ in one-to-one fashion.

The right-hand side of Eq. 84 may contain some duplicity; that is to say, $|\mathbf{K}_{ij}\cap\mathbf{H}|\leq b$ (=$|\mathbf{N}|/|\mathbf{H}|$). The multiplicity is calculated as follows:

$$m=\frac{b}{q}=\frac{|\mathbf{N}|/|\mathbf{H}|}{|\mathbf{N}|/|\mathbf{C_N(H)}|}=\frac{|\mathbf{C_N(H)}|}{|\mathbf{H}|}. \quad (86)$$

Let us consider a double coset decomposition:

$$\mathbf{N}=\mathbf{C_N(H)}t_1\mathbf{H}+\mathbf{C_N(H)}t_2\mathbf{H}+\cdots+\mathbf{C_N(H)}t_q\mathbf{H}, \quad (87)$$

where q is given in Eq. 44 and the transversal is selected appropriately from **B**:

$$\mathbf{B}'=\{t_1,t_2,\cdots,t_q\}. \quad (88)$$

The multiplicity m can be alternatively calculated as the number of cosets in a double coset $\mathbf{C_N}(h)t_\alpha\mathbf{H}$:

$$m=\frac{|\mathbf{C_N}(h)|}{|\mathbf{C_N}(h)\cap t_\alpha^{-1}\mathbf{H}t_\alpha|}=\frac{|\mathbf{C_N}(h)|}{|\mathbf{C_N}(h)\cap\mathbf{H}|}=\frac{|\mathbf{C_N(H)}|}{|\mathbf{H}|}, \quad (89)$$

which is equal to the value given in Eq. 86. Since **H** is a normal subgroup of **N** and $\mathbf{N}\supset\mathbf{C_N(H)}\supset\mathbf{H}$, the cyclic group **H** is a normal subgroup of $\mathbf{C_N(H)}$. Hence, Eq. 87 is transformed as follows.

$$\mathbf{N}=\mathbf{C_N(H)H}t_1+\mathbf{C_N(H)H}t_2+\cdots+\mathbf{C_N(H)H}t_q \quad (90)$$

$$=\mathbf{C_N(H)}t_1+\mathbf{C_N(H)}t_2+\cdots+\mathbf{C_N(H)}t_q. \quad (91)$$

As a result, we arrive at a theorem:

Theorem 12. *By using the transversal* $\mathbf{B}'$, *the conjugacy class* $\mathbf{K}_{ij}\cap\mathbf{H}$ *in the normalizer* **N** *is represented with no duplicity as follows*:

$$\mathbf{K}_{ij}\cap\mathbf{H}=\{t_1^{-1}ht_1\ (=h),t_2^{-1}ht_2,\cdots,t_\alpha^{-1}ht_\alpha,\cdots,t_q^{-1}ht_q\}. \quad (92)$$

References

1) F. A. Cotton, "Chemical Applications of Group Theory," Wiley-International, New York (1971).
2) H. H. Jaffé and M. Orchin, "Symmetry in Chemistry," Wiley, Chichester (1965).
3) L. H. Hall, "Group Theory and Symmetry in Chemistry," McGraw-Hill, New York (1969).
4) D. M. Bishop, "Group Theory and Chemistry," Clarendon, Oxford (1973).
5) S. F. A. Kettle, "Symmetry and Structure," Wiley, Chichester (1985).
6) M. F. C. Ladd, "Symmetry in Molecules and Crystals," Ellis Horwood, Chichester (1989).
7) D. C. Harris and M. D. Bertolucci, "Symmetry and Spectroscopy," Dover, New York (1989).
8) I. Hargittai and H. Hargittai, "Symmetry through the Eyes of a Chemist," VCH, Weinheim (1986).
9) W. Burnside, "Theory of Groups of Finite Order," 2nd ed, Cambridge University Press, Cambridge (1911).
10) J. Sheehan, *Can. J. Math.*, **20**, 1068 (1968).
11) A. Kerber and K.-J. Thürlings, in "Combinatorial Theory," ed by D. Jngnickel and K. Vedder, Springer, Berlin (1982), pp. 191—211.
12) J. H. Redfield, *J. Graph Theory*, **8**, 205 (1984).
13) S. Fujita, *J. Math. Chem.*, **12**, 173 (1993).
14) S. Fujita, *J. Graph Theory*, **18**, 349 (1994).
15) W. Hässelbarth, *Theor. Chim, Acta*, **67**, 339 (1985).
16) C. A. Mead, *J. Am. Chem. Soc.*, **109**, 2130 (1987).
17) S. Fujita, *Theor. Chim. Acta*, **76**, 247 (1989).
18) S. Fujita, "Symmetry and Combinatorial Enumeration in Chemistry," Springer-Verlag, Berlin and Heidelberg (1991).
19) S. Fujita, *Theor. Chim. Acta*, **82**, 473 (1992).
20) E. K. Lloyd, *J. Math. Chem.*, **11**, 207 (1992).
21) S. Fujita, *Theor. Chim. Acta*, **91**, 291 (1995).
22) S. Fujita, *Theor. Chim. Acta*, **91**, 315 (1995).
23) S. Fujita, *Bull. Chem. Soc. Jpn.*, **71**, 1587 (1998).
24) S. Fujita, *Theor. Chem. Acc*, in press.
25) G. Pólya, *Acta Math.*, **68**, 145 (1937).
26) G. Pólya and R. C. Read, "Combinatorial Enumeration of Groups, Graphs, and Chemical Compounds," Springer-Verlag, New York (1987).
27) S. Fujita, *J. Math. Chem.*, **5**, 99 (1990).
28) K. Asano and H. Nagao, "Group Theory (Gunron)," Iwanami, Tokyo (1965).
29) M. Oshima, "Group Theory (Gunron)," Kyoritu, Tokyo (1954).
30) T. Oyama, "Finite Permutation Groups (Yugen-Chikan-Gun)," Shokabo, Tokyo (1981).