Markaracter Tables and Q-Conjugacy Character Tables for Cyclic Groups. An Application to Combinatorial Enumeration

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Q-Conjugacy character tables for cyclic groups are obtained by starting from character tables. Thus, irreducible representations for a cyclic group are classified into primitive and non-primitive ones. They are collected to form a matrix corresponding to each subgroup. Such a matrix is shown to be a representation (called **Q**-conjugacy representation) for characterizing **Q**-conjugacy and dominant classes. The traces of the **Q**-conjugacy representation are collected to form a **Q**-conjugacy character table, which is shown to be a square matrix. The elements of such a **Q**-conjugacy character table for a cyclic group are shown to be integers, which are related to the values of the corresponding character tables. They are also correlated to the markaracter tables for the cyclic group. Characteristic monomial tables for cyclic groups are obtained by starting from the **Q**-conjugacy character tables and dominant unit-subduced-cycle-index tables. They are applied to combinatorial enumeration of isomers derived from a skeleton belonging to a cyclic group.

Character tables containing characters for irreducible representations[1—8] and mark tables containing marks for coset representations[9—21] have found their own applications in the respective fields in chemistry and in mathematics. Although they have been developed on the basis of different disciplines, their close relationship has been implied by the construction of symmetry adapted functions[22] and the alternative formulation of Pólya's theorem, both of which have come from the USCI (unit-subduced-cycle-index) approach we developed.[23] We have recently revealed that the key linking them is dominant representations and proposed the concept of markaracter (mark-character) to discuss characters and marks on a common basis.[24,25] However, the previous discussion[24] has limited scope, since it has dealt with special cases in which each dominant class contains only one conjugacy class. In order to have a comprehensive perspective, we shall treat general cases in which a dominant class contains one ore more conjugacy classes. Before we start the investigation of the final target, we shall deal with cyclic groups as another extreme case in which each member of a dominant class belongs to a one-membered conjugacy class. This paper shows the importance of **Q**-conjugacy character tables and characteristic monomial tables for cyclic groups, which are applied to the combinatorial enumeration of isomers.

1 Theoretical Foundations

1.1 Q-Conjugacy for Defining Dominant Classes. In Ref. 24, we have defined a dominant class as a disjoint union of conjugacy classes that correspond to the same cyclic subgroup, which is selected as a representative from conjugate cyclic subgroups. The definition is based on the fact that each element (h) of a finite group $\boldsymbol{G}$ corresponds to the cyclic group $\langle h \rangle$ generated by h. In this section, we aim at characterizing the relationship between dominant classes and conjugacy classes more clearly. First, we define **Q**-*conjugacy* as follows.

Definition 1 (Q-Conjugacy). *Let h_1 and h_2 be elements of a finite group $\boldsymbol{G}$. Suppose that $\langle h_1 \rangle$and $\langle h_2 \rangle$are cyclic groups generated respectively from h_1 and h_2. If $t \in \boldsymbol{G}$ exists satisfying $t^{-1}\langle h_1 \rangle t = \langle h_2 \rangle$, then the elements h_1 and h_2 are defined to be **Q**-conjugate to each other.*

The letter '**Q**' of the word '**Q**-conjugacy' stems from the field **Q** of rational numbers, since Def. 1 is equivalent to the condition for $\Gamma_{\mathbf{Q}}$-conjugacy described in Section 13.1 (Corollary) of Ref. 26. The **Q**-conjugacy is an equivalence relation and generates equivalence classes (**Q**-conjugacy classes), which we can redefine as dominant classes. Suppose that the group $\boldsymbol{G}$ is partitioned into dominant classes as follows:

$$\boldsymbol{G} = \boldsymbol{K}_1 + \boldsymbol{K}_2 + \cdots + \boldsymbol{K}_s, \tag{1}$$

in which $\boldsymbol{K}_i$ corresponds to the cyclic (dominant) subgroup $\boldsymbol{G}_i$ selected from a non-redundant set of cyclic subgroups (SCSG):[24]

$$\mathrm{SCSG}_{\boldsymbol{G}} = \{\boldsymbol{G}_1, \boldsymbol{G}_2, \cdots, \boldsymbol{G}_s\}, \quad (|\boldsymbol{G}_1| \leq |\boldsymbol{G}_2| \leq \cdots \leq |\boldsymbol{G}_s|) \tag{2}$$

where the group $\boldsymbol{G}_1$ is an identity group and each subgroup is a representative selected from a respective set of conjugate cyclic subgroups.

1.2 Q-Conjugacy Representations of Cyclic Groups. Let $\boldsymbol{G}$ be a cyclic group of order n; $\boldsymbol{G} = \{h, h^2, \cdots, h^r, \cdots, h^n (= I)\}$. The SCSG (Eq. 2) for $\boldsymbol{G}$ contains all of the cyclic subgroups the orders of which are the divisors of n. Let n_i denote the order of the cyclic subgroup of $\boldsymbol{G}_i$, i.e. $n_i = |\boldsymbol{G}_i|$. As shown in Eq. 1, each subgroup $\boldsymbol{G}_i$ corresponds to a dominant class $\boldsymbol{K}_i$.

Each conjugacy class of the cyclic group $\boldsymbol{G}$ consists of one element. In other words, each element in the dominant class $\boldsymbol{K}_i$ for the cyclic group $\boldsymbol{G}$ constructs a one-membered conjugacy class. The dominant class $\boldsymbol{K}_i$ contains all of the elements that generate the cyclic subgroup $\boldsymbol{G}_i$. Hence the size of $\boldsymbol{K}_i$ is equal to $\varphi(|\boldsymbol{G}_i|)$ $(=\varphi(n_i))$, where $\varphi(n_i)$ denotes the Euler function of the integer n_i. This value is also derived by starting from Theorem 11 of Ref. 24. Thus, the size for this case is represented by $|\boldsymbol{K}_i| = \varphi(n_i) = \varphi(|\boldsymbol{G}_i|)$, because the normalizer $\boldsymbol{N}_{\boldsymbol{G}}(\boldsymbol{G}_i)$ is identical with $\boldsymbol{G}$ for any cyclic subgroup $\boldsymbol{G}_i$, i.e., $|\boldsymbol{N}_{\boldsymbol{G}}(\boldsymbol{G}_i)| = |\boldsymbol{G}|$.

Let h be a generator of $\boldsymbol{G}$, i.e. $\boldsymbol{G} = \langle h\rangle$. Then h^r's $(r = 1,2,\cdots,n)$ are the elements of $\boldsymbol{G}$. Let us consider the character for $\boldsymbol{G}$, which is identical with the list of all irreducible representations. An irreducible represention (IR) is obtained by placing $\Gamma_h(h^r) = \varepsilon^r$, where ε is a primitive n-th root of 1 $(n = |\boldsymbol{G}|)$. The resulting IR Γ_h is considered to correspond to the element h. From this IR, we can construct another IR by placing $\Gamma_{h^s}((h^r)^s) = (\varepsilon^r)^s$. The resulting IR Γ_{h^s} is again considered to correspond to the element h^s where $s = 1,2,\cdots,n$.

If s and n are coprime (i.e., $(s,n) = 1$), the element h^s generates the group $\boldsymbol{G}$. Hence the resulting IRs are alternatively considered to correspond to the group $\boldsymbol{G}$. On the other hand, suppose that the element h^s generates a subgroup $\boldsymbol{G}_j$ i.e., $\boldsymbol{G}_j = \langle h^s\rangle$, because of $(s,n) > 1$. Then, the resulting IRs are alternatively considered to correspond to the subgroup $\boldsymbol{G}_j$. The discussion here allows us to classify irreducible representations (IRs) of a cyclic group into primitive and non-primitive ones as follows.

Definition 2 (Primitive and Non-primitive IRs). *1. Let* $\boldsymbol{G}$ *be a cyclic group of order n. An IR corresponding to* $h^s \in \boldsymbol{G}$ *is called a primitive irreducible representation (PIR), when s is an integer comprime to n. The resulting PIRs are considered to correspond to the group* $\boldsymbol{G}$ $(=\langle h^s\rangle)$.

2. Otherwise, they are called non-primitive irreducible representations (NPIR). The resulting NPIRs are considered to correspond to the respective subgroup $\boldsymbol{G}_j$ $(=\langle h^s\rangle)$.

Let ε be a primitive n-th root of 1 represented by exp $(2\pi i/n)$. Then, we have all of the primitive n-th roots of 1, denoting them by ε^s, where $(s,n) = 1$. Thereby, we obtain the PIRs: $\Gamma_{h^s}(g) = (\varepsilon^s)^r$ for $g = (h^s)^r$ $(r = 1,2,\cdots,n)$.

Let us consider a reducible representation $(\hat{\Gamma}_{n/n})$ that consists of all of the primitive irreducible representations (PIRs). From Definition 1, the number of such PIRs is equal to $\varphi(n)$ for the cyclic group $\boldsymbol{G}$. We number all of the primitive n-th roots of 1 to denote $\omega_1, \omega_2, \cdots$, and $\omega_{\varphi(n)}$, which are equal to ε^s $((s,n) = 1)$ in the ascending order of s. Then, the representation is a diagonal matrix represented by

$$\hat{\Gamma}_{n/n}(g) = \sum_{(s,n)=1} \Gamma_{h^s}(g) = \begin{pmatrix} \omega_1^r & & & 0 \\ & \omega_2^r & & \\ & & \ddots & \\ 0 & & & \omega_{\varphi(n)}^r \end{pmatrix}, \quad (3)$$

for $g = h^r$ $(r = 1,2,\cdots,n)$. the character $(\hat{\gamma}_{n/n})$ of the representation is calculated to be

$$\hat{\gamma}_{n/n}(g) = \omega_1^r + \omega_2^r + \cdots + \omega_{\varphi(n)}^r, \quad (4)$$

for an element of g of the cyclic group $\boldsymbol{G}$, where $g = h^r$ $(r = 1,2,\cdots,n)$. These values construct a **Q**-conjugacy character table for the cyclic group $\boldsymbol{G}$.

Let us first focus our attention on the column that corresponds to an element $g = h^r$ satisfying $(r,n) = 1$ in the character table; in other words, we take into consideration the element g in the dominant class $\boldsymbol{K}_s$ corresponding to the cyclic group $\boldsymbol{G}$ $(=\boldsymbol{G}_s)$. Then we have the following results:

$$\hat{\gamma}_{n/n}(g) = \omega_1^r + \omega_2^r + \cdots + \omega_{\varphi(n)}^r = \mu(n), \quad (5)$$

for $g = h^r$ $((r,n) = 1)$. The symbol $\mu(n)$ denotes the Möbius function. The equation $\omega_1 + \omega_2 + \cdots + \omega_{\varphi(n)} = \mu(n)$ is used without proof, since this summation represents the sum of primitive n-th roots of 1.[27] Note that the set $\{\omega_1, \omega_2, \cdots, \omega_{\varphi(n)}\}$ is identical with the set $\{\omega_1^r, \omega_2^r, \cdots, \omega_{\varphi(n)}^r\}$ without considering the order of elements, if r and n are coprime to each other (i.e., $(r,n) = 1$). It follows that Eq. 4 has the same value for all of the $g = h^r$ $((r,n) = 1)$.

Let us next consider $g \in \boldsymbol{K}_i$, where $|\boldsymbol{G}_i| = n_i$. When we write $d = n/n_i$ and $r = dr'$, we have Eq. 4 for this case:

$$\begin{aligned}\hat{\gamma}_{n/n}(g) &= (\omega_1)^{dr'} + (\omega_2)^{dr'} + \cdots + (\omega_{\varphi(n)})^{dr'} \\ &= (\omega_1^d)^{r'} + (\omega_2^d)^{r'} + \cdots + (\omega_{\varphi(n)}^d)^{r'} \\ &= \frac{\varphi(n)}{\varphi(n_i)} \times \left((\omega_1^d)^{r'} + (\omega_2^d)^{r'} + \cdots + (\omega_{\varphi(n_i)}^d)^{r'}\right) \\ &= \frac{\varphi(n)}{\varphi(n_i)} \times \mu(n_i).\end{aligned}$$

Note that each ω_k^d (for $k = 1,2,\cdots,\varphi(n_i)$) is equal to a primitive n_i-th root of 1 and that the total number of such primitive n_i-th roots is equal to $\varphi(n_i)$. Since $\varphi(n)/\varphi(n_i)$ is an integer, we obtain the following theorem.

Theorem 1. *Let* $\boldsymbol{G}$ *be a cyclic group of order n. For the dominant class* $\boldsymbol{K}_i$ *corresponding to the cyclic subgroup* $\boldsymbol{G}_i$ of $\boldsymbol{G}$, *the character of the reducible representation* $\hat{\gamma}_{n/n}$ *corresponding to the PIRs is calculated to be an integer represented by*

$$\hat{\gamma}_{n/n}(g) = \frac{\varphi(n)}{\varphi(n_i)} \times \mu(n_i), \quad (6)$$

for $g \in \boldsymbol{K}_i$, *where* $n = |\boldsymbol{G}|$ *and* $n_i = |\boldsymbol{G}_i|$.

Theorem 1 can be extended to be applied to non-irreducible representations of a cyclic subgroup. Thus we have Theorem 2, the proof of which will be given in Appendix A.

Theorem 2. *For the dominant class* $\boldsymbol{K}_i$ *corresponding to the cyclic subgroup* $\boldsymbol{G}_i$ *of order* n_i, *the character of the reducible representation* $\hat{\gamma}_{n/n_j}$ *is calculated to be an integer represented by*

$$\hat{\gamma}_{n/n_j}(g) = \frac{\varphi(n_j)\mu\left(\frac{n_i}{(d_j,\, n_i)}\right)}{\varphi\left(\frac{n_i}{(d_j,\, n_i)}\right)}. \quad (7)$$

for $g \in \boldsymbol{K}_i$ *and for* $j = 1,2,\cdots,s$, *where the symbol* $(d_j,\ n_i)$ *denotes the GCD of* d_j *and* n_i. The character $\hat{\gamma}_{n/n_j}$ is an integer as shown in the proof appearing in Appendix A.

Theorem 2 shows that the character of the reducible representation $\hat{\gamma}_{n/n_j}(g)$ has the same value for all g of the dominant class $\boldsymbol{K}_i$ corresponding to the cyclic subgroup $\boldsymbol{G}_i$. Hence Eq. 7 is rewritten to be $\hat{\gamma}_{n/n_j}(\boldsymbol{K}_i) = \hat{\gamma}_{n/n_j}(g)$ (for $g \in \boldsymbol{K}_i$).

Theorem 1 is a special cases of Theorem 2; thus, suppose that $n_j = n$ in Eq. 7 for Theorem 1. Hence the representation $\hat{\Gamma}_{n/n_j}$ corresponding to the character $\hat{\gamma}_{n/n_j}$ is called a **Q**-conjugacy representation. If the reader is interested in mathematical details, see Appendix A.

2 Q-Conjugacy Character Tables for Cyclic Groups

By means of Theorem 2, the character table of a cyclic group can be transformed to a **Q**-*conjugacy character table* in which the columns and the rows of the former are summed up respectively according to dominant classes. When we pay attention to the j-th row of the **Q**-conjugacy character table, the element at the intersection of the j-th row and l-th column represents $\tilde{\gamma}_{n/n_j}(g)$, which has the same value for all $g \in \boldsymbol{K}_l$ as calculated by Theorem 2. Hence the terms $\tilde{\gamma}_{n/n_j}(\boldsymbol{K}_l)$ ($= \hat{\gamma}_{n/n_j}(g)$ for $g \in \boldsymbol{K}_l$ as shown in Eq. 7) are capable of constructing a row vector,

$$\tilde{\gamma}_{n/n_j} = (\tilde{\gamma}_{n/n_j}(\boldsymbol{K}_1) \quad \tilde{\gamma}_{n/n_j}(\boldsymbol{K}_2) \quad \cdots \quad \tilde{\gamma}_{n/n_j}(\boldsymbol{K}_s)), \tag{8}$$

where the use of the symbol $\tilde{\gamma}_{n/n_j}$ designates the dependence upon $\boldsymbol{K}_l$ while the symbol $\hat{\gamma}_{n/n_j}$ indicates the dependence upon $g(\in \boldsymbol{K}_l \subset \boldsymbol{G})$. Thereby, the **Q**-conjugacy character table (D) for the group $\boldsymbol{G}$ is represented by

$$D^T = (\tilde{\gamma}_{n/n_1} \quad \tilde{\gamma}_{n/n_2} \quad \cdots \quad \tilde{\gamma}_{n/n_s}), \tag{9}$$

where the rows are aligned in the descending order of n/n_j.

We here show an illustrative example of making a **Q**-conjugacy character table from a character table of a cyclic group.

Example 1. Table 1 shows a character table for the point group C_6. The notations Γ_{C_6} and $\Gamma_{C_6^5}$ used here correspond to Mulliken's notation E_1; $\Gamma_{C_6^2}$ and $\Gamma_{C_6^4}$ correspond to E_2.[28] Although we use $\varepsilon = \exp(2\pi i/6)$ in this table to relate it to Theorems 1 and 2, we are able to obtain the usual form of the character table by placing $\varepsilon^2 = -\overline{\varepsilon}$, $\varepsilon^3 = -1$, $\varepsilon^4 = -\varepsilon$, $\varepsilon^5 = \overline{\varepsilon}$, and $\varepsilon^6 = 1$, where $\overline{\varepsilon} = \exp(-2\pi i/6)$.

Table 1. Character Table for the Point Group $\mathbf{C}_6$

Notations		Dominant classes and cyclic groups					
		$\boldsymbol{K}_1$,C$_1$	$\boldsymbol{K}_2$,C$_2$	$\boldsymbol{K}_3$,C$_3$		$\boldsymbol{K}_4$,C$_6$	
Mulliken	This work	C_1	C_2	C_3	C_3^2	C_6	C_6^5
A	$\Gamma_{C_6^6}$	$(\varepsilon^6)^6$	$(\varepsilon^6)^3$	$(\varepsilon^6)^2$	$(\varepsilon^6)^4$	$(\varepsilon^6)^1$	$(\varepsilon^6)^5$
B	$\Gamma_{C_6^3}(=\Gamma_{C_2})$	$(\varepsilon^3)^6$	$(\varepsilon^3)^3$	$(\varepsilon^3)^2$	$(\varepsilon^3)^4$	$(\varepsilon^3)^1$	$(\varepsilon^3)^5$
E_2	$\Gamma_{C_6^2}(=\Gamma_{C_3})$	$(\varepsilon^2)^6$	$(\varepsilon^2)^3$	$(\varepsilon^2)^2$	$(\varepsilon^2)^4$	$(\varepsilon^2)^1$	$(\varepsilon^2)^5$
E_2'	$\Gamma_{C_6^4}(=\Gamma_{C_3^2})$	$(\varepsilon^4)^6$	$(\varepsilon^4)^3$	$(\varepsilon^4)^2$	$(\varepsilon^4)^4$	$(\varepsilon^4)^1$	$(\varepsilon^4)^5$
E_1	Γ_{C_6}	$(\varepsilon^1)^6$	$(\varepsilon^1)^3$	$(\varepsilon^1)^2$	$(\varepsilon^1)^4$	$(\varepsilon^1)^1$	$(\varepsilon^1)^5$
E_1'	$\Gamma_{C_6^5}$	$(\varepsilon^5)^6$	$(\varepsilon^5)^3$	$(\varepsilon^5)^2$	$(\varepsilon^5)^4$	$(\varepsilon^5)^1$	$(\varepsilon^5)^5$

Note that $\varepsilon = \exp(2\pi i/6)$.

In the light of Theorem 1, the summation of the rows Γ_{C_6} and $\Gamma_{C_6^5}$ of the character table of C_6 (Table 1) gives the $\tilde{\gamma}_{6/6}$ row of the corresponding **Q**-conjugacy character table (Table 2). Note that $\varepsilon + \overline{\varepsilon} = -1$.

On the other hand, the summation of the rows $\Gamma_{C_6^2}$ and $\Gamma_{C_6^4}$ (corresponding to Mulliken's notation E_2) of Table 1 gives the $\tilde{\gamma}_{6/3}$ row of the corresponding Table 2 in accord with Theorem 2.

When we pay attention to the i-th column of the **Q**-conjugacy character table, the element at the intersection of the i-th column and the l-th row represents Δ_{li} calculated by Theorem 8; however the Δ_{li} value has originally corresponded to the values concerning the IR that corresponds to $\boldsymbol{G}_l$. Let $\tilde{\Delta}_i$ be a column vector represented by

$$\tilde{\Delta}_i^T = (\Delta_{1i} \quad \Delta_{2i} \quad \cdots \quad \Delta_{si}). \tag{10}$$

By using the $\tilde{\Delta}_i$ as the i-th column, the **Q**-conjugacy character table (D) for the group $\boldsymbol{G}$ is represented by

$$D = (\tilde{\Delta}_1 \quad \tilde{\Delta}_2 \quad \cdots \quad \tilde{\Delta}_s), \tag{11}$$

where the columns are aligned in the ascending order of $|\boldsymbol{G}_i|$.

The orthogonality relationship between irreducible representations (Γ_{h^s} and Γ_{h^r}) is represented by

$$|\boldsymbol{G}|\,\delta_{sr} = \sum_{g\in\boldsymbol{G}} \Gamma_{h^s}(g)\Gamma_{h^r}(g), \tag{12}$$

where δ_{sr} is Kronecker's delta. When we sum up the equations over s satisfying $(s/d_j, n_j)=1$, the summation remains non-zero with respect to only one IR if such an IR exists. Hence we have

$$\begin{aligned}|\boldsymbol{G}|\,\delta_{jr} &= \sum_{(s/d_j,n_j)=1}\sum_{g\in\boldsymbol{G}} \Gamma_{h^s}(g)\Gamma_{h^r}(g) = \sum_{g\in\boldsymbol{G}}\sum_{(s/d_j,n_j)=1} \Gamma_{h^s}(g)\Gamma_{h^r}(g)\\ &= \sum_{y\in\boldsymbol{G}} \hat{\gamma}_{n/n_j}(g)\Gamma_{h^r}(g).\end{aligned}$$

Theorem 2 shows that $\hat{\gamma}_{n/n_j}(g)$ in the last side can be replaced by $\tilde{\gamma}_{n/n_j}(\boldsymbol{K}_l)$. According to this replacement, we rewrite the suffixes of Kronecker's delta.

$$\begin{aligned}|\boldsymbol{G}|\,\delta_{ji} &= \sum_{l=1}^{s} \tilde{\gamma}_{n/n_j}(\boldsymbol{K}_l)\left(\sum_{g\in\boldsymbol{K}_l} \Gamma_{h^r}(g)\right) = \sum_{l=1}^{s} \tilde{\gamma}_{n/n_j}(\boldsymbol{K}_l)\Delta_{li}.\\ &= \langle \tilde{\gamma}_{n/n_j}, \Delta_i \rangle\end{aligned}$$

Since the last side of the transformation represents the ji-element of D^2, we have $D^2/|\boldsymbol{G}| = I$, where I represents an

Table 2. **Q**-Conjugacy Character Table for the Point Group $\mathbf{C}_6$

	$\boldsymbol{K}_1$ C$_1$	$\boldsymbol{K}_2$ C$_2$	$\boldsymbol{K}_3$ C$_3$	$\boldsymbol{K}_4$ C$_6$
$\Gamma_{C_6^6} \to \tilde{\gamma}_{6/1}$	1	1	1	1
$\Gamma_{C_2} \to \tilde{\gamma}_{6/2}$	1	-1	1	-1
$\Gamma_{C_3} + \Gamma_{C_3^2} \to \tilde{\gamma}_{6/3}$	2	2	-1	-1
$\Gamma_{C_6} + \Gamma_{C_6^5} \to \tilde{\gamma}_{6/6}$	2	-2	-1	1

$s \times s$ identity matirix. The discussion is summarized as a theorem.

Theorem 3. *Let D be the Q-conjugacy character table of a cyclic group G. Then, we have*

$$\frac{D^2}{|\mathbf{G}|} = I. \tag{13}$$

This theorem for a **Q**-conjugacy character table is the counterpart of the orthogonality theorem for a character table of a cyclic group. The following example illustrates this transformation by using the point group $\mathbf{C}_6$.

Example 2. Let us examine the point group $\mathbf{C}_6$, which is a cyclic subgroup of order 6. The character table of the group $\mathbf{C}_6$ is shown in Table 1, where $\varepsilon = \exp(2\pi i/6)$. Theorem 1 indicates $\tilde{\gamma}_{6/6}(\mathbf{K}_4) = \Gamma_{C_6}(C_6) + \Gamma_{C_6^5}(C_6) = \varepsilon + \varepsilon^5 = \mu(6) = 1$ for the **Q**-conjugacy class corresponding to $\mathbf{C}_6$. The results obtained from Table 1 are summarized to give Table 2. It should be noted that Table 2 is based on dominant classes and not on conjugacy class. Thus the columns of Table 1 are summed up with respect to the dominant classes and the rows of Table 1 are summed up with respect to PIRs for $\mathbf{C}_6$ and its subgroups. Hence the resulting Table 2 is a square matrix.

By regarding Table 2 as D, we have

$$\frac{D^2}{6} = \frac{1}{6}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 2 & 2 & -1 & -1 \\ 2 & -2 & -1 & 1 \end{pmatrix}^2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{14}$$

This is an example of Theorem 3.

3 Markaracter Tables for Cyclic Groups

Let us consider a coset representation (CR) $\mathbf{G}(/\mathbf{G}_k)$, the mark of which is the number of fixed points when the CR is restricted to a subgroup of $\mathbf{G}$. The CR can be considered to be of the permutational type as well as the matrix type.[29] Since the mark (the number of fixed points) in the CR of the permutation type is equal to the trace of the CR of the matrix type, we call the number *markaracter*. We have defined markaracter tables in our preceding papers.[24,25] For cyclic groups, markaracter tables are identical with mark tables. Thus the elements in the k-th row of the markaracter table $\mathbf{G}(/\mathbf{G}_k) = (\lambda_{kl})$ for a cyclic group are given as follows by Lemma 1 of Ref. 25.

$$\lambda_{kl} \begin{cases} = \dfrac{|\mathbf{G}|}{|\mathbf{G}_k|} & \text{for } \mathbf{G}_l\ (\leq \mathbf{G}_k) \quad (15a) \\ = 0 & \text{for } \mathbf{G}_l\ (\nleq \mathbf{G}_k) \quad (15b) \end{cases}$$

for $l = 1, 2, \cdots, k$ and $\lambda_{kl} = 0$ for $l > k$. Note that the markaracter table is a lower triangular matrix. For $\mathbf{G}_l$ (or $\mathbf{K}_l$), define the dominant class function f_{kl} on $\mathbf{G}$ by

$$f_{kl} \begin{cases} = 1 & \text{for } \mathbf{G}_l\ (\leq \mathbf{G}_k) \quad (16b) \\ = 0 & \text{for } \mathbf{G}_l\ (\nleq \mathbf{G}_k) \text{ or } \quad \text{for } l > k. \quad (16c) \end{cases}$$

Then, Eqs. 15a and 15b are transformed into

$$\lambda_{kl} = \frac{f_{kl}|\mathbf{G}|}{|\mathbf{G}_k|}. \tag{17}$$

If two or more elements of the cyclic group $\mathbf{G}$ belong to the same dominant class, their cycle structures are identical.[23] Hence the number of one-cycles in one element is equal to the number of one-cycles in another element belonging to the same dominant class. This means that the number of fixed points (the number of one-cycles) for each of the elements is equal to the markaracter for the subgroup $\mathbf{G}_i$ that corresponds to the dominant class $\mathbf{K}_i$.

In the light of Theorem 8 and Eq. 17, the multiplicity (ν_{kj}) of the IR Γ_{h^s} in the CR $\mathbf{G}(/\mathbf{G}_k)$ is calculated to be

$$\begin{aligned} \nu_{kj} = \langle \mathbf{G}(/\mathbf{G}_k), \Gamma_{h^s} \rangle &= \frac{1}{|\mathbf{G}|}\sum_{l=1}^{s} \lambda_{kl}\Delta_{jl} = \frac{1}{|\mathbf{G}|} \times \frac{|\mathbf{G}|}{|\mathbf{G}_k|} \times \sum_{l=1}^{s} f_{kl}\Delta_{jl} \\ &= \frac{1}{|\mathbf{G}_k|}\sum_{l=1}^{s} f_{kl}\Delta_{jl} \\ &= \frac{1}{|\mathbf{G}_k|}\sum_{l=1}^{s} \frac{f_{kl}\varphi(n_l)\mu\left(\frac{n_j}{(d_l, n_j)}\right)}{\varphi\left(\frac{n_j}{(d_l, n_j)}\right)}, \end{aligned} \tag{18}$$

where the mark for $\mathbf{G}_l$ in the row vector $\mathbf{G}(/\mathbf{G}_k)$ is multiplied in accord with the length of $|\mathbf{K}_l|$ and the IR Γ_{h^s} corresponds to the same $\mathbf{G}_j$. The ν_{kj} has the same value for the IRs Γ_{h^s} that correspond to the same $\mathbf{G}_j$. By using the column vector $\tilde{\Delta}_j^T$ (Eq. 10), we rewrite Eq. 18 as follows.

$$\nu_{kj} = \langle \mathbf{G}(/\mathbf{G}_k), \Gamma_{h^s} \rangle = \frac{1}{|\mathbf{G}|}\mathbf{G}(/\mathbf{G}_k)\tilde{\Delta}_j. \tag{19}$$

This discussion is summarized as a theorem.

Theorem 4. *The multiplicity (ν_{kj}) of the IR Γ_{h^s} (corresponding to the subgroup $\mathbf{G}_j$) in the CR $\mathbf{G}(/\mathbf{G}_k)$ is calculated to be*

$$\nu_{kj} = \frac{1}{|\mathbf{G}|}\mathbf{G}(/\mathbf{G}_k)\tilde{\Delta}_j, \tag{20}$$

where $\mathbf{G}(/\mathbf{G}_k)$ represents the k-th row of the markaracter table for a cyclic group $\mathbf{G}$ while $\tilde{\Delta}_j$ represents the j-th column of the Q-conjugacy character table for $\mathbf{G}$.

It should be noted here that the multiplicity (ν_{kj}) obtained by Theorem 4 was originally concerned with the IR Γ_{h^s}. However, the values ν_{kj} are equal to each other if the IRs Γ_{h^s} correspond to $\mathbf{G}_j$. In other words, the multiplicity (ν_{kj}) can be regarded as being concerned with the representation $\tilde{\Gamma}_{n/n_j}$. This point of view will be illustrated in Example 3.

Theorem 4 is converted into a more convenient corollary by using the markaracter table and the **Q**-conjugacy character table (D defined by Eq. 9) directly. Let M be the markaracter table for $\mathbf{G}$, in which each $\mathbf{G}(/\mathbf{G}_k)$ is the k-th row. We define the multiplicity matrix N by the following equation.

$$N = (\nu_{kj}) = \begin{pmatrix} \nu_{11} & \nu_{12} & \cdots & \nu_{1s} \\ \nu_{21} & \nu_{22} & \cdots & \nu_{2s} \\ \vdots & \vdots & & \vdots \\ \nu_{s1} & \nu_{s2} & \cdots & \nu_{ss} \end{pmatrix} \tag{21}$$

Then, we have

$$N = \frac{1}{|\mathbf{G}|}MD = \frac{1}{|\mathbf{G}|}\begin{pmatrix} \mathbf{G}(/\mathbf{G}_1) \\ \mathbf{G}(/\mathbf{G}_2) \\ \vdots \\ \mathbf{G}(/\mathbf{G}_s) \end{pmatrix}(\tilde{\Delta}_1 \quad \tilde{\Delta}_2 \quad \cdots \quad \tilde{\Delta}_s) \tag{22}$$

Hence we arrive at a corollary.

Corollary 1. *Let D be the **Q**-conjugacy character table for **G**, a cyclic group, and let M be the markaracter table for **G**. Suppose that N denotes a matrix collecting multiplicities (ν_{kj}) of the IRs Γ_{h^s} (corresponding to the subgroup G_j) in the CR $G(/G_k)$. Then*

$$N = MD^{-1} = \frac{1}{|G|}MD \tag{23}$$

For illustrating Theorem 4 and Corollary 1, we continue to study the point group $\mathbf{C}_6$.

Example 3. The regular representation $\mathbf{C}_6(/\mathbf{C}_1)$ contains IRs with the following multiplicities calculated by means of Theorem 4.

$$\hat{\Gamma}_{6/1} : (1/6)(6,0,0,0)(1,1,2,2)^T = 1$$
$$\hat{\Gamma}_{6/2} : (1/6)(6,0,0,0)(1,-1,2,-2)^T = 1$$
$$\hat{\Gamma}_{6/3} : (1/6)(6,0,0,0)(1,1,-1,-1)^T = 1$$
$$\hat{\Gamma}_{6/6} : (1/6)(6,0,0,0)(1,-1,-1,1)^T = 1$$

In this calculation, we use the $\mathbf{C}_6(/\mathbf{C}_1)$-row of Table 3 and the $\boldsymbol{K}_i$-column ($i = 1,2,3,4$) of Table 2. This means that

$$C_6(/C_1) = \tilde{\gamma}_{6/1} + \tilde{\gamma}_{6/2} + \tilde{\gamma}_{6/3} + \tilde{\gamma}_{6/6} \tag{24}$$

Note that the resulting multiplicities can be considered to be concerned with the IRs as well as with the representations $\hat{\Gamma}_{6/n_j}$.

Corollary 1 gives the multiplicities of IRs as a matrix form. By using Table 3 as M and Table 2 as D, we have

$$N = \frac{1}{6}\begin{pmatrix} 6 & 0 & 0 & 0 \\ 3 & 3 & 0 & 0 \\ 2 & 0 & 2 & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 2 & 2 & -1 & -1 \\ 2 & -2 & -1 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{25}$$

The first row of the matrix on the right-hand side gives the same result as that represented by Eq. 24. On the other hand, the 2nd to 4th rows of the matrix give the following results of the reductions.

$$C_6(/C_2) = \tilde{\gamma}_{6/1} + \tilde{\gamma}_{6/3} \tag{26}$$

$$C_6(/C_3) = \tilde{\gamma}_{6/1} + \tilde{\gamma}_{6/2} \tag{27}$$

$$C_6(/C_6) = \tilde{\gamma}_{6/1} \tag{28}$$

The results show that each CR (here a dominant representation) contains the **Q**-conjugacy representation $\hat{\Gamma}_{6/6}$ one time.

Table 3. Mark(aracter) Table for the Point Group $\mathbf{C}_6$

	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_3$	$\mathbf{C}_6$
$C_6(/C_1)$	6	0	0	0
$C_6(/C_2)$	3	3	0	0
$C_6(/C_3)$	2	0	2	0
$C_6(/C_6)$	1	1	1	1

The inverse of the markaracter table for a cyclic group, which has been given as Lemma 2 of Ref. 25, can be written by using the **Q**-conjugacy class function (Eqs. 16a and 16b) as follows.

$$\bar{\lambda}_{lk} = \frac{f_{lk}n_k}{n}\mu\left(\frac{n_l}{n_k}\right). \tag{29}$$

The multiplicity (χ_{jk}) of the CR $G(/G_k)$ in the IR Γ_{h^s} (corresponding to the subgroup G_j) is calculated to be

$$\chi_{jk} = \sum_{l=k}^{s} \tilde{\gamma}_{n/n_j}\bar{\lambda}_{lk} = \sum_{l=k}^{s} \frac{\varphi(n_j)\mu\left(\frac{n_l}{(d_j,\, n_l)}\right)}{\varphi\left(\frac{n_l}{(d_j,\, n_l)}\right)} \times \frac{f_{lk}n_k}{n}\mu\left(\frac{n_l}{n_k}\right). \tag{30}$$

Let X be the matrix (χ_{jk}). Then this equation is equivalent to the following matrix form, $DM^{-1} = X$. Hence we have $X^{-1} = MD^{-1} = MD/|G|$ because of Theorem 3. By using Eq. 23, we have $NX = I$. The discussion is summarized as a theorem.

Theorem 5. *Let D be the **Q**-conjugacy character table for a cyclic group **G** and let M be the markaracter table for **G**. The multiplicity matrix ($X = (\chi_{jk})$) of the CR $G(/G_k)$ in the IR Γ_{h^s} (corresponding to the subgroup G_j) is calculated to be*

$$DM^{-1} = X \tag{31}$$

The resulting X and the matrix N in Corollary 1 satisfy

$$NX = I. \tag{32}$$

Example 4. Theorem 5 gives the multiplicities of CRs as a matrix form. By using M^{-1} (calculated from Table 3) and D (Table 2) for $\mathbf{C}_6$, we have

$$X = DM^{-1}$$
$$= \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 2 & 2 & -1 & -1 \\ 2 & -2 & -1 & 1 \end{pmatrix}\begin{pmatrix} \frac{1}{6} & 0 & 0 & 0 \\ -\frac{1}{6} & \frac{1}{3} & 0 & 0 \\ -\frac{1}{6} & 0 & \frac{1}{2} & 0 \\ \frac{1}{6} & -\frac{1}{3} & -\frac{1}{2} & 1 \end{pmatrix}$$
$$= \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \tag{33}$$

The last side indicates that the respective representations are shown to be

$$\tilde{\gamma}_{6/1} = C_6(/C_6) \tag{34}$$

$$\tilde{\gamma}_{6/2} = C_6(/C_3) - C_6(/C_6) \tag{35}$$

$$\tilde{\gamma}_{6/3} = C_6(/C_2) - C_6(/C_6) \tag{36}$$

$$\tilde{\gamma}_{6/6} = C_6(/C_1) - C_6(/C_2) - C_6(/C_3) + C_6(/C_6). \tag{37}$$

Equation 33 combined with Eq. 25 gives

$$NX = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{38}$$

which is consistent with Theorem 5.

Theorem 30 of Ref. 26 has implied that a representation of a finite group $\boldsymbol{G}$ in the field $\mathbf{Q}$ of rational numbers is a linear combination of characters $1_{\mathbf{H}}^{\mathbf{G}}$ with coefficients in $\mathbf{Q}$, where $1_{\mathbf{H}}^{\mathbf{G}}$ represents the character of $\boldsymbol{G}$ induced by $1_{\mathbf{H}}$, and $\mathbf{H}$ runs over the set of cyclic subgroups of $\boldsymbol{G}$. This is formulated in a more concrete form by the concept of mararakter tables discussed in this paper. Moreover $\mathbf{Q}$-conjugacy character tables directly link character tables with mark tables via markaracter tables.

4 Combinatorial Enumeration

4.1 Characteristic Monomial Tables for Cyclic Groups. The $\mathbf{Q}$-conjugacy characters discussed above correspond to $\mathbf{Q}$-conjugacy representations. Hence we are able to consider the subduction of the $\mathbf{Q}$-conjugacy representations. The purpose of this section is to obtain such $\mathbf{Q}$-conjugacy representations for cyclic groups.

In Ref. 25, we have reported subduction of dominant representations and dominant USCI (unit-subduced-cycle-index) tables for combinatorial enumeration. We will pursue a method of transforming such dominant USCI tables to characteristic monomial tables, which are related to subduction of $\mathbf{Q}$-conjugacy representations.

In the light of Theorem 5, we have the following equation:

$$\hat{\Gamma}_{n/n_j} = \sum_{k=1}^{s} \chi_{jk} C_n(/C_k) \qquad (39)$$

for a cyclic subgroup. Note that the symbol $\hat{\Gamma}_{n/n_j}$ is used for designating a $\mathbf{Q}$-conjugacy representation, while the symbol $\hat{\Gamma}_{n/n_j}$ is used for designating the corresponding $\mathbf{Q}$-conjugacy character. An example of this equation has appeared for the group $\mathbf{C}_6$ in Eq. 34 to 37 (Example 4). The $\mathbf{Q}$-conjugacy representation appearing in the left-hand side of Eq. 39 is subduced into a subgroup $\mathbf{C}_l$. This subduction ($\hat{\Gamma}_{n/n_j}\downarrow C_l$) results in the subduction of each coset representation appearing in the right-hand side of Eq. 39. Thereby we have the following equation.

$$\hat{\Gamma}_{n/n_j} \downarrow \mathbf{C}_l = \sum_{k=1}^{s} \chi_{jk} \mathbf{C}_n(/\mathbf{C}_k) \downarrow \mathbf{C}_l. \qquad (40)$$

Suppose that each term of the right-hand side gives the corresponding USCI represented by $Z(\mathbf{C}_n(/\mathbf{C}_k)\downarrow\mathbf{C}_l;\, s_d)$.[25] Then, we have a monomial,

$$Z(\hat{\Gamma}_{n/n_j} \downarrow \mathbf{C}_l;\, s_d) = \prod_{k=1}^{s} (Z(\mathbf{C}_n(/\mathbf{C}_k) \downarrow \mathbf{C}_l;\, s_d))^{\chi_{jk}} \qquad (41)$$

where the power χ_{jk} appears in Eq. 39. The monomial represented by Eq. 41 is called a characteristic monomial for the subduction $\hat{\Gamma}_{n/n_j}\downarrow C_l$. When j and l run over all of the subgroups, Eq. 41 gives an $s \times s$ table (or matrix). The resulting table is called a *characteristic monomial table* for the cyclic group $\mathbf{C}_n$, which is applicable to combinatorial enumeration.

Example 5. Since the point group $\mathbf{C}_6$ is isomorphic to $\mathbf{C}_{3h}$, the USCI table for the latter[18] is rewritten for the former as shown in Table 4, where the original USCI

Table 4. USCI Table for the Point Group $\mathbf{C}_6$

$\mathbf{C}_6$			$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_3$	$\mathbf{C}_6$
	$\mathbf{C}_{3h}$		$\mathbf{C}_1$	$\mathbf{C}_s$	$\mathbf{C}_3$	$\mathbf{C}_{3h}$
		$\mathbf{S}_6$	$\mathbf{C}_1$	$\mathbf{C}_i$	$\mathbf{C}_3$	$\mathbf{S}_6$
$C_6(/C_1)$	$C_{3h}(/C_1)$	$S_6(/C_1)$	s_1^6	s_2^3	s_3^2	s_6
$C_6(/C_2)$	$C_{3h}(/C_s)$	$S_6(/C_i)$	s_1^3	s_1^3	s_3	s_3
$C_6(/C_3)$	$C_{3h}(/C_3)$	$S_6(/C_3)$	s_1^2	s_2	s_1^2	s_2
$C_6(/C_6)$	$C_{3h}(/C_{3h})$	$S_6(/S_6)$	s_1	s_1	s_1	s_1
	N_l		$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$

for $\mathbf{C}_{3h}(/\mathbf{C}_s)\downarrow\mathbf{C}_3$ is replaced by the correct USCI (s_3 for $\mathbf{C}_6(/\mathbf{C}_2)\downarrow\mathbf{C}_3$).

In the light of Eq. 41, the characteristic monomial for the subduction $\Gamma_{C_6^6}\downarrow\mathbf{C}_6$ is obtained by using the coefficient appearing in each term of the right-hand side in Eq. 37 (Example 4) as follows:

$$s_6^1 \times s_3^{-1} \times s_2^{-1} \times s_6^1 = s_1 s_2^{-1} s_3^{-1} s_6, \qquad (42)$$

where the respective dummy variables (USCIs) in the left-hand side are taken from the $\mathbf{C}_6$ column of Table 4. Similarly, Table 4 is converted into the characteristic monomial table for the point group $\mathbf{C}_6$ (Table 5).

4.2 Enumeration Based on Characteristic Monomial Tables. Suppose that a skeleton of symmetry $\mathbf{C}_n$ ($=\boldsymbol{G}$) has a set of positions, which are associated with a permutation representation $\boldsymbol{P}$, which is regarded as as a matrix representation. The number of points fixed under every subgroup action is collected to give a fixed-point vector (FPV), which is regarded as a $\mathbf{Q}$-conjugacy character. The FPV is multiplied by the inverse of the $\mathbf{Q}$-conjugacy character table of $\mathbf{C}_n$ (i.e., $D_{\mathbf{C}_n}^{-1}$) to give the multiplicies of $\mathbf{Q}$-conjugacy characters. By using these multiplicities (α_i), we have

$$\boldsymbol{P} = \sum_i \alpha_i \hat{\Gamma}_{n/n_i} \qquad (43)$$

for $i = 1, 2, \cdots$, where the symbol $\hat{\Gamma}_{n/n_i}$ represents a $\mathbf{Q}$-conjugacy representation. Equation 43 represents a subdivision of the positions under the action of the group $\mathbf{C}_n$.

Since the subductions of every representations $\hat{\Gamma}_{n/n_i}$ are assigned to the characteristic monomials represented by Eq. 41, we can define a subduced cycle index (SCI):

$$\mathrm{SCI}(\mathbf{C}_n \downarrow \mathbf{C}_l;\, s_d) = \prod_i (Z(\hat{\Gamma}_{n/n_i} \downarrow \mathbf{C}_l;\, s_d))^{\alpha_i}. \qquad (44)$$

Table 5. Characteristic Monomial Table for the Point Group $\mathbf{C}_6$

$\mathbf{C}_6$			$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{C}_6$
	$\mathbf{C}_{3h}$		$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{C}_{3h}$
		$\mathbf{S}_6$	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_i$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{S}_6$
$\hat{\Gamma}_{6/1}(A)$	A'	A_g	s_1	s_1	s_1	s_1
$\hat{\Gamma}_{6/2}(B)$	A''	A_u	s_1	$s_1^{-1}s_2$	s_1	$s_1^{-1}s_2$
$\hat{\Gamma}_{6/3}(E_2)$	E'	E_g	s_1^2	s_1^2	$s_1^{-1}s_3$	$s_1^{-1}s_3$
$\hat{\Gamma}_{6/6}(E_1)$	E''	E_u	s_1^2	$s_1^{-2}s_2^2$	$s_1^{-1}s_3$	$s_1 s_2^{-1} s_3^{-1} s_6$
	N_l		$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$

By starting from Eq. 44, we have the definition of a cycle index (CI)

$$\mathrm{CI}(\boldsymbol{G};\, s_d) = \sum_{l} N_l \prod_{i} (Z(\hat{\Gamma}_i \downarrow \mathbf{C}_l;\, s_d))^{\alpha_i} \tag{45}$$

in a similar way to Def. 4 of Ref. 23. In the light of Eq. 54 of Ref. 24, The coefficient N_l appearing in the right-hand side of Eq. 45 is represented by

$$N_l = \frac{\varphi(|\mathbf{C}_l|)}{|\mathbf{N}_{\mathbf{C}_n}(\mathbf{C}_l)|}, \tag{46}$$

where the symbol $\mathbf{N}_{\mathbf{C}_n}(\mathbf{C}_l)$ denotes the normalizer of $\mathbf{C}_l$ within $\mathbf{C}_n$. The CI based on Eq. 45 is applicable to combinatorial enumeration according to the following theorem:

Theorem 6. *Consider a skeleton of symmetry $\mathbf{C}_n$ having p of positions, which are occupied by p of ligands selected from a ligand set,*

$$\boldsymbol{Y} = \{Y_1, Y_2, \cdots, Y_{|Y|}\}, \tag{47}$$

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

$$[\nu] : \nu_1 + \nu_2 + \cdots + \nu_{|Y|} = p. \tag{48}$$

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

$$W_\nu = \prod_{\iota=1}^{|Y|} Y_\iota^{\nu_\iota} \tag{49}$$

A generating function for the total number A_ι of such isomers as have the weight W_ι is represented by

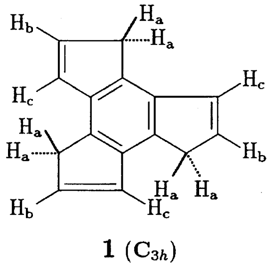
$$\sum_{[\nu]} A_\nu W_\nu = \mathrm{CI}(\mathbf{C}_l;\, s_d), \tag{50}$$

where

$$s_d = \sum_{\iota=1}^{\nu} Y_\iota^d. \tag{51}$$

This theorem gives enumeration results equivalent to those of Pólya's theorem or to those of the USCI approach, though the definitions of the cycle index (CI) are different among them.

Example 6. Let us consider isomer enumeration on the basis of skeleton **1**, which belongs to the point group $\mathbf{C}_{3h}$ (Chart 1). Since the point group $\mathbf{C}_{3h}$ is isomorphic to the cyclic group $\mathbf{C}_6$, Table 2 can be used as the **Q**-conjugacy character table of $\mathbf{C}_{3h}$. When Table 2 is regarded as a matrix ($D_{\mathbf{C}_{3h}}$), the inverse of $D_{\mathbf{C}_{3h}}$ is calculated to be



1 ($\mathbf{C}_{3h}$)

Chart 1.

$$D_{\mathbf{C}_{3h}}^{-1} = \begin{pmatrix} \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} \\ \frac{1}{6} & -\frac{1}{6} & \frac{1}{6} & -\frac{1}{6} \\ \frac{1}{3} & \frac{1}{3} & -\frac{1}{6} & -\frac{1}{6} \\ \frac{1}{3} & -\frac{1}{3} & -\frac{1}{6} & \frac{1}{6} \end{pmatrix}. \tag{52}$$

The skeleton (**1**) has 12 positions (6 positions designated by H_a, 3 positions by H_b, and 3 positions by H_c) to be taken into consideration. The FPV of the skeleton **1** is obtained to be FPV=(12,6,0,0), which is multiplied by the inverse matrix to give

$$(12, 6, 0, 0) D_{\mathbf{C}_{3h}}^{-1} = (3, 1, 3, 1). \tag{53}$$

The row vector appearing on the right-hand side shows the multiplicities of the **Q**-conjugacy representations of $\mathbf{C}_{3h}$. Hence we have the following expression.

$$\boldsymbol{P} = 3A' + A'' + 3E' + E''. \tag{54}$$

According to the multiplicities, the CI for the skeleton **1** is obtained by means of Eq. 45:

$$\begin{aligned} f &= \mathrm{CI}(\mathbf{C}_{3h};\, s_d) \\ &= \frac{1}{6}(s_1)^3(s_1)(s_1^2)^3(s_1^2) + \frac{1}{6}(s_1)^3(s_1^{-1}s_2)(s_1^2)^3(s_1^{-2}s_2^2) \\ &\quad + \frac{1}{3}(s_1)^3(s_1)(s_1^{-1}s_3)^3(s_1^{-1}s_3) \\ &\quad + \frac{1}{3}(s_1)^3(s_1^{-1}s_2)(s_1^{-1}s_3)^3(s_1 s_2^{-1} s_3^{-1} s_6) \\ &= \frac{1}{6}s_1^{12} + \frac{1}{6}s_1^6 s_2^3 + \frac{1}{3}s_3^4 + \frac{1}{3}s_3^2 s_6, \end{aligned} \tag{55}$$

where the data collected in the characteristic monomial table for the point group $\mathbf{C}_{3h}$ (Table 5) are used. When we take account of one kind of ligands (Y), the corresponding ligand inventory is represented by

$$s_d = 1 + Y^d. \tag{56}$$

Introduction of Eq. 56 into Eq. 55 gives the corresponding generating function,

$$\begin{aligned} f &= \frac{1}{6}(1+Y)^{12} + \frac{1}{6}(1+Y)^6(1+Y^2)^3 + \frac{1}{3}(1+Y^3)^4 + \frac{1}{3}(1+Y^3)^2(1+Y^6) \\ &= Y^{12} + 3Y^{11} + 14Y^{10} + 45Y^9 + 93Y^8 + 146Y^7 + 172Y^6 \\ &\quad + 146Y^5 + 93Y^4 + 45Y^3 + 14Y^2 + 3Y + 1, \end{aligned} \tag{57}$$

where the coefficient of the term Y^y indicates the number of isomers with y of ligands Y. For an illustration of the results shown by the term $14Y^2$, Fig. 1 depicts fourteen disubstituted isomers.

5 Conclusion

A dominant class is defined by the concept of **Q**-conjugacy, which is based on conjugate subgroups. Then a dominant class for a cyclic group $\boldsymbol{G}$ is examined as an extreme case in which each element in the dominant class constructs a one-membered conjugacy class. Each irreducible representation (IR) for a cyclic group $\boldsymbol{G}$ is considered to correspond to a $|\boldsymbol{G}|$-th root of 1 as well as to a cyclic subgroup of $\boldsymbol{G}$. Thereby the IRs are classified into primitive and non-primitive ones which are related to respective dominant classes. The IRs are

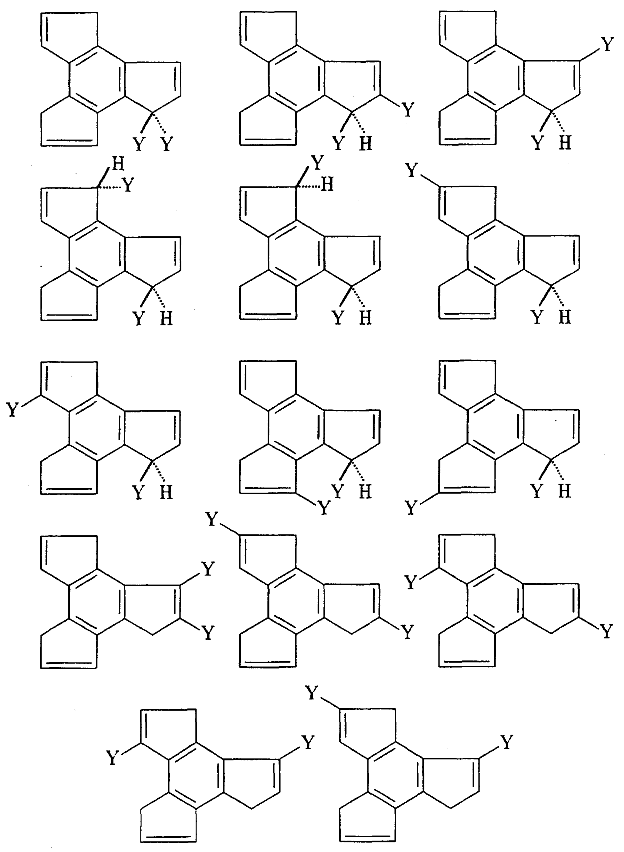


Fig. 1. Fourteen di-substituted derivatives of **1**.

collected to form a matrix corresponding to each subgroup. The matrix is called a **Q**-conjugacy representation, which characterizes **Q**-conjugacy and dominant classes. The corresponding **Q**-conjugacy character table, which is shown to be a square matrix, is constructed by collecting the traces of the representation. The elements of the **Q**-conjugacy character table for a cyclic group are obtained by using Euler's and Möbius' functions and shown to be integers. They are related to the markaracter tables for $\boldsymbol{G}$. Characteristic monomial tables, which are obtained on the basis of the **Q**-conjugacy character tables and dominant unit-subduced-cycle-index tables, are applied to combinatorial enumeration.

Appendix A. The Proof of Theorem 2.

Let us consider a reducible representation ($\hat{\Gamma}_{n/n_j}$) that consists of all of the irreducible representations Γ_{h^s} corresponding to $(s/d_j, n_j) = 1$, where $d_j = n/n_j$. Since the number of such irreducible representations is equal to $\varphi(n_j)$, we have

$$\hat{\Gamma}_{n/n_j}(g) = \sum_{(s/d_j,\, n_j)=1} \Gamma_{h^s}(g) = \begin{pmatrix} (\omega_1^{d_j})^r & & & 0 \\ & (\omega_2^{d_j})^r & & \\ & & \ddots & \\ 0 & & & (\omega_{\varphi(n_j)}^{d_j})^r \end{pmatrix} \tag{58}$$

for $g = h^r$ $(r = 1,2,\cdots,n)$, where each $\omega_k^{d_j}$ is equal to a primitive n_j-th root of 1. The character ($\hat{\gamma}_{n/n_j}$) of the representation is calculated to be

$$\hat{\gamma}_{n/n_j}(g) = (\omega_1^{d_j})^r + (\omega_2^{d_j})^r + \cdots + (\omega_{\varphi(n_j)}^{d_j})^r \tag{59}$$

for $g = h^r$ $(r = 1,2,\cdots,n)$.

Let us first focus our attention on the column that corresponds to an element $g = h^r$ satisfying $(r,n)=1$ in the character table; in other words, we take into consideration the element g in the dominant class $\boldsymbol{K}_s$ corresponding to the cyclic subgroup $\boldsymbol{G}_s = \boldsymbol{G}$, Then we have the following results:

$$\hat{\gamma}_{n/n_j}(g) = (\omega_1^{d_j})^r + (\omega_2^{d_j})^r + \cdots + (\omega_{\varphi(n_j)}^{d_j})^r = \mu(n_j) \tag{60}$$

for $g=h^r$ $((r,n)=1)$. Note that each $\omega_k^{d_j}$ is equal to a primitive n_j-th root of 1 and that, if r (mod n) belongs to a reduced system of residues, r (mod n_j) belongs to a reduced system of residues.#

Theorem 7. *For the dominant class $\boldsymbol{K}_s$ corresponding to the cyclic subgroup $\boldsymbol{G}_s = \boldsymbol{G}$, the character of the reducible representation $\hat{\gamma}_{n/n_j}$ is calculated to be:*

$$\hat{\gamma}_{n/n_j}(g) = \mu(n_j), \tag{61}$$

for $g \in \boldsymbol{K}_s$.

This theorem is exemplified in the case of $\mathbf{C}_6$. Thus the summation of Γ_{C_3}- and $\Gamma_{C_3^2}$-rows for the C_6-column of Table 1 gives the value $(\varepsilon^2)^1+(\varepsilon^4)^1 = -1$, which is equal to the value $(\varepsilon^2)^5+(\varepsilon^4)^5 = -1$ for the C_6^5-column of Table 1. Hence these columns are collected to give the single $\mathbf{C}_6$-column of Table 2.

Finally we shall take account of general cases to give the proof of Theorem 2. Consider $g \in \boldsymbol{K}_i$, where $|\boldsymbol{G}_i| = n_i$. Suppose that the symbol d denotes the greatest common divisor (GCD) of d_j and n_i, i.e.,

$$d = (d_j,\, n_i). \tag{62}$$

Then we have integers d_j/d and n_i/d satisfying

$$\left(\frac{d_j}{d}, \frac{n_i}{d}\right) = 1. \tag{63}$$

We write $d_i = n/n_i$ and $r = d_i r'$, where r' and n_i are coprime, i.e.,

$$(r', n_i) = 1 \tag{64}$$

Then, we have Eq. 4 for this case:

$$\begin{aligned}\hat{\gamma}_{n/n_j}(g) &= (\omega_1^{d_j})^{d_i r'} + (\omega_2^{d_j})^{d_i r'} + \cdots + (\omega_{\varphi(n_j)}^{d_j})^{d_i r'} \\ &= (\omega_1^{d_i d})^{r' d_j/d} + (\omega_2^{d_i d})^{r' d_j/d} + \cdots + (\omega_{\varphi(n_j)}^{d_i d})^{r' d_j/d}\end{aligned} \tag{65}$$

From the inner power $d_i d$ appearing in Eq. 65, we obtain the following value:

$$\frac{n}{d_i d} = \frac{n_i d_i}{d_i d} = \frac{n_i}{d}, \tag{66}$$

which is an integer. This means that $\Omega'' = \{\omega_1^{d_i d}, \omega_2^{d_i d}, \cdots, \omega_{\varphi(n_j)}^{d_i d}\}$, all elements of which appear in Eq. 65, are the set of all the primitive n_i/d-th roots of 1, since $\Omega = \{\omega_1, \omega_2, \cdots, \omega_{\varphi(n)}\}$ represents the set of all the primitive n-th roots of 1, from which the set $\Omega' = \{\omega_1^{d_i}, \omega_2^{d_i}, \cdots, \omega_{\varphi(n_j)}^{d_i}\}$ is selected as the primitive n_j-th roots of 1 $(n/d_j = n_j)$.

For $na+r$, we have $(n,r) = 1$. Let n be equal to $n'b$. Then we have $na+r = n'ba+r$. If n' and r are not coprime, we can write $n' = dn''$ and $r = dr'$. Then, $na+r = n'ba+r = (n''ba+r')d$. This contradicts the assumption $(n,r) = 1$.

Moreover, the outer power $r'd_j/d$ is an integer, because d_j/d is an integer. Note that d_j/d and n_i/d are coprime (Eq. 63) and that r' and n_i/d are coprime because of Eq. 64. Hence the power $r'd_j/d$ is coprime to the integer n_i/d, i.e.,

$$\left(\frac{r'd_j}{d}, \frac{n_i}{d}\right) = 1. \tag{67}$$

As a result, the last side of Eq. 65 is concluded to be a duplicated sum of the primitive n_i/d-th roots of 1. The number of the terms in Eq. 65 is originally equal to $\varphi(n_j)$, while the number of all the primitive n_i/d-th roots of 1 is equal to $\varphi(n_i/d)$. We shall clarify the relationship between these Euler functions. For this purpose, we have

$$n_j = \frac{n}{d_j} = \frac{n_i d_i}{d_j} = \frac{(n_i/d)d_i}{d_j/d}. \tag{68}$$

By means of Eq. 63, Eq. 68 shows that d_i is a multiple of d_j/d. It follows that the number represented by

$$\frac{n_j}{n_i/d} = \frac{n/d_j}{n/d_i d} = \frac{d_i}{d_j/d} \tag{69}$$

is an integer. Thereby, we conclude that $\varphi(n_j)/\varphi(n_i/d)$ is also an integer. By combining this result and Eq. 67, we are able to continue the transformation of Eq. 65 as follows:

$$\begin{aligned}\tilde{\gamma}_{n/n_j}(g) &= \frac{\varphi(n_j)}{\varphi(n_i/d)} \times \{(\omega_1^{d_i d})^{r'd_j/d} + (\omega_2^{d_i d})^{r'd_j/d} + \cdots + (\omega_{\varphi(n_i/d)}^{d_i d})^{r'd_j/d}\} \\ &= \frac{\varphi(n_j)\mu(n_i/d)}{\varphi(n_i/d)}.\end{aligned} \tag{70}$$

Hence we arrive at Theorem 2.

Theorems 1 and 7 are special cases of Theorem 2; thus, suppose that $n_j = n$ in Eq. 7 for Theorem 1 and that $n_i = n$ in Eq. 7 for Theorem 7.

When we remember the character table of the group $\boldsymbol{G}$, Theorem 2 is considered to fix a column tentatively to the element $g \in \boldsymbol{K}_i$ and to indicate that the character $\tilde{\gamma}_{n/n_j}$ represents the sum running over the part corresponding to the primitive n_j-th roots of 1.

Let us next consider the Γ_{h^s} row in the character table of the group $\boldsymbol{G}$. Thus we sum up $\Gamma_{h^s}(g)$ over all $g \in \boldsymbol{K}_i$. Obviously, we are able to obtain the sum by exchanging the d_j and the d_i in Eq. 65. The same discussion resulting in Eq. 70 can be applied to this case to give

$$\begin{aligned}\Delta_{ji} = \sum_{g \in \boldsymbol{K}_i} \Gamma_{h^s}(g) &= (\omega_1^{d_i})^{d_j r'} + (\omega_2^{d_i})^{d_j r'} + \cdots + (\omega_{\varphi(n_i)}^{d_i})^{d_j r'} \\ &= \frac{\varphi(n_i)\mu(n_j/d)}{\varphi(n_j/d)},\end{aligned} \tag{71}$$

where $d = (d_i, n_j)$. Although the sum is calculated for Γ_{h^s}, the symbol Δ_{ji} is used because the Δ_{ji} has the same value for the IRs Γ_{h^s} that give $\langle h^s \rangle = \boldsymbol{G}_j$. Hence we arrive at a theorem:

Theorem 8. *Let the dominant class* $\boldsymbol{K}_i$ *correspond to the cyclic subgroup* $\boldsymbol{G}_i$ *of the order* n_i. *For the IR* Γ_{h^s} *corresponding to the subgroup* $\boldsymbol{G}_j$ $(= \langle h^s \rangle)$, *the sum running over* $\boldsymbol{K}_i$ *is calculated to be:*

$$\Delta_{ji} = \sum_{g \in \boldsymbol{K}_i} \Gamma_{h^s}(g) = \frac{\varphi(n_i)\mu\left(\frac{n_j}{(d_i, n_j)}\right)}{\varphi\left(\frac{n_j}{(d_i, n_j)}\right)}. \tag{72}$$

for $j = 1, 2, \cdots, s$, *where* (d_i, n_j) *denotes the GCD of* d_i *and* n_j.

The sum Δ_{ji} is an integer as shown above. Theorem 8 shows that the sum Δ_{ji} has the same value for all of the IRs corresponding to the cyclic subgroup $\boldsymbol{G}_j$.

Appendix B. Q-Conjugacy Character Tables and Markaracter Tables for Several Cyclic Point Groups.

We here collect **Q**-conjugacy character tables (left) and markaracter tables (right) for several cyclic point groups. It should be noted that markaracter tables are identical with the corresponding mark tables in case of cyclic groups.[18]

Order p (p represents a prime number)—$\mathbf{C}_p$:

Q-Conjugacy character table

	$\mathbf{C}_1$	$\mathbf{C}_p$
A	1	1
E	$p-1$	-1

Markaracter table

	$\mathbf{C}_1$	$\mathbf{C}_p$
$\boldsymbol{C}_p(/\boldsymbol{C}_1)$	p	0
$\boldsymbol{C}_p(/\boldsymbol{C}_p)$	1	1

Order 2—$\mathbf{C}_2$, $\mathbf{C}_s$, and $\mathbf{C}_i$:

Q-Conjugacy character table

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

Markaracter table

	$\mathbf{C}_1$	$\mathbf{C}_a$
$\boldsymbol{C}_a(/\boldsymbol{C}_1)$	2	0
$\boldsymbol{C}_a(/\boldsymbol{C}_a)$	1	1

$a = 2, s, i.$

Order 3—$\mathbf{C}_3$:

Q-Conjugacy character table

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

Markaracter table

	$\mathbf{C}_1$	$\mathbf{C}_3$
$\boldsymbol{C}_3(/\boldsymbol{C}_1)$	3	0
$\boldsymbol{C}_3(/\boldsymbol{C}_3)$	1	1

Order 4—$\mathbf{C}_4$, $\mathbf{S}_4$:

Q-Conjugacy character table

$\mathbf{C}_4$		$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_4$
	$\mathbf{S}_4$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{S}_4$
A	A	1	1	1
B	B	1	1	-1
E	E	2	-2	0

Markaracter table

$\mathbf{C}_4$		$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_4$
	$\mathbf{S}_4$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{S}_4$
$\boldsymbol{C}_4(/\boldsymbol{C}_1)$	$\boldsymbol{S}_4(/\boldsymbol{C}_1)$	4	0	0
$\boldsymbol{C}_4(/\boldsymbol{C}_2)$	$\boldsymbol{S}_4(/\boldsymbol{C}_2)$	2	2	0
$\boldsymbol{C}_4(/\boldsymbol{C}_4)$	$\boldsymbol{S}_4(/\boldsymbol{S}_4)$	1	1	1

Order 5—$\mathbf{C}_5$:

Q-Conjugacy character table

	$\mathbf{C}_1$	$\mathbf{C}_5$
A	1	1
E	4	-1

Markaracter table

	$\mathbf{C}_1$	$\mathbf{C}_5$
$\boldsymbol{C}_5(/\boldsymbol{C}_1)$	5	0
$\boldsymbol{C}_5(/\boldsymbol{C}_5)$	1	1

Order 6—$\mathbf{C}_6$, $\mathbf{C}_{3h}$, $\mathbf{S}_6$:

Q-Conjugacy character table

$\mathbf{C}_6$			$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_3$	$\mathbf{C}_6$
	$\mathbf{C}_{3h}$		$\mathbf{C}_1$	$\mathbf{C}_s$	$\mathbf{C}_3$	$\mathbf{C}_{3h}$
		$\mathbf{S}_6$	$\mathbf{C}_1$	$\mathbf{C}_i$	$\mathbf{C}_3$	$\mathbf{S}_6$
A	A'	A_g	1	1	1	1
B	A''	A_u	1	−1	1	−1
E_2	E'	E_g	2	2	−1	−1
E_1	E''	E_u	2	−2	−1	1

Markaracter table

$\mathbf{C}_6$			$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_3$	$\mathbf{C}_6$
	$\mathbf{C}_{3h}$		$\mathbf{C}_1$	$\mathbf{C}_s$	$\mathbf{C}_3$	$\mathbf{C}_{3h}$
		$\mathbf{S}_6$	$\mathbf{C}_1$	$\mathbf{C}_i$	$\mathbf{C}_3$	$\mathbf{S}_6$
$C_6(/C_1)$	$C_{3h}(/C_1)$	$S_6(/C_1)$	6	0	0	0
$C_6(/C_2)$	$C_{3h}(/C_s)$	$S_6(/C_i)$	3	3	0	0
$C_6(/C_3)$	$C_{3h}(/C_3)$	$S_6(/C_3)$	2	0	2	0
$C_6(/C_6)$	$C_{3h}(/C_{3h})$	$S_6(/S_6)$	1	1	1	1

Order 7—$\mathbf{C}_7$:

Q-Conjugacy character table

	$\mathbf{C}_1$	$\mathbf{C}_7$
A	1	1
E	6	−1

Markaracter table

	$\mathbf{C}_1$	$\mathbf{C}_7$
$C_7(/C_1)$	7	0
$C_7(/C_7)$	1	1

Order 8—$\mathbf{C}_8$, $\mathbf{S}_8$:

Q-Conjugacy character table

$\mathbf{C}_8$		$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_4$	$\mathbf{C}_8$
	$\mathbf{S}_8$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_4$	$\mathbf{S}_8$
A	A	1	1	1	1
B	B	1	1	1	−1
E_2	E_2	2	2	−2	0
E_1+E_3	E_1+E_3	4	−4	0	0

Markaracter table

$\mathbf{C}_8$		$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_4$	$\mathbf{C}_8$
	$\mathbf{S}_8$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_4$	$\mathbf{C}_8$
$C_8(/C_1)$	$S_8(/C_1)$	8	0	0	0
$C_8(/C_2)$	$S_8(/C_2)$	4	4	0	0
$C_8(/C_4)$	$S_8(/C_4)$	2	2	2	0
$C_8(/C_8)$	$S_6(/S_8)$	1	1	1	1

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