Characteristic Monomials with Chirality Fittingness for Combinatorial Enumeration of Isomers with Chiral and Achiral Ligands

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A new method of combinatorial enumeration based on characteristic monomials with chirality fittingness (CM-CFs) has been proposed in order to enumerate isomers with chiral ligands as well as with achiral ones. The CM-CFs have been defined as monomials that consist of three kinds of dummy variables in light of the subduction of the **Q**-conjugacy representations for chiral and achiral cyclic groups. A procedure of calculating CM-CFs for cyclic groups and finite groups has been discribed so as to tabulate them as CM-CF tables. Then the CM-CF method has been applied to the enumeration of isomers with achiral ligands as well as chiral ones.

1. INTRODUCTION

1.1. Backgrounds. Each approach for enumeration of isomers is characterized by two steps of evolution. The first step is the development of a method to treat achiral ligands only, and the second step is the extension that takes account of both achiral and chiral ligands. The difference between the two steps is conceptually large despite its appearance. Thus, the first step is based on a methodology that regards isomers as chemical graphs, where substituents (or ligands) to be placed on their vertexes are essentially structureless, not three-dimensional objects. In other words, the first step involves direct applications of mathematichal theorems to chemical problems. On the other hand, the second step postulates a more sophisticated methodology that regards isomers as three-dimensional objects. This methodology requires stereochemical examination of both isomers and substituents as three-dimensional objects.

Representative approaches to enumerate isomers with given molecular formulas are Pólya's theorem[1] and Redfield's group-reduced distribution.[2] They have continuously been used, as examined in excellent reviews[3,4] and books,[5,6] where they are considered to be at the first step of the evolution described above. An alternative approach for solving such enumeration problems as concerning molecular formulas is based on the Redfield−Read superposition theorem[2] and related formulations,[7−9] which have been discussed extensively from mathematical[10,11] and chemical points[12] of view. A further approach based on double coset decompositions[13,14] has been reported and correlated to the Pólya cycle−index method and de-Bruijin's extension.[15] These approaches that originally aim at mathematical applications are essetially concerned with structureless (or achiral) substituents.

For further chemical applications along these approaches, a methodology of the second step should be developed in order to treat achiral ligands as well as chiral ones. Thus, the double-coset method[13,14] has been extended to be applied to the enumeration of isomers with achiral and chiral ligands.[16]

The unit-subduced-cycle-index (USCI) approach has recently been reported in order to enumerate isomers with given molecular formulas and given symmetries.[17,18] The USCI approach at the first step of evolution is concerned with the enumeration of isomers with achiral ligands. Thus, four methods of the USCI approach developed from the concept of the subduction of coset representations aim at the enumeration of isomers with achiral ligands.[17,18] In particular, generating-function methods using subduced cycle indices (SCIs)[17] and partial cycle indices (PCIs)[19] have been correlated to Pólya's theorem.[20]

For further chemical applications, i.e., for the second step of evolution, the USCI approach has been extended after the proposal of the concept of chirality fittingness so that USCIs with chirality fittingness (USCI-CFs) are applied to the enumeration of isomers with chiral and achiral ligands.[21]

More recently, we have investigated another approach based on **Q**-conjugacy representation theory[22−24] and have recently developed the characteristic-monomial (CM) method for enumerating isomers.[25−27] However, the scope of the CM method has been restricted within isomer enumeration concerning achiral ligands, i.e., within the first step of evolution. Hence, isomer enumeration considering chiral ligands along with achiral ones should be examined at the second step of evolution of the CM method.

To do this task, we shall first clarify that the concept of chirality fittingness[28] can be extended to be applied to the CM method. Thus, the first target of the present paper is to study the subduction of cyclic groups, where achiral and chiral subductions of homospheric and enantiospheric orbits are examined with respect to the concept of chirality fittingness for respective subgroups. Thereby, we shall indicate that the concept is also effective to **Q**-conjugacy representations. The second target is to propose characteristic monomials with chirality fittingness (CM-CFs) as a new tool for combinatorial enumeration in order to treat chiral ligands as well as achiral ones.

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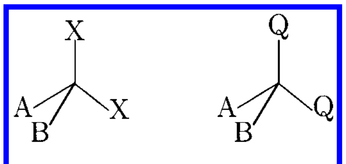
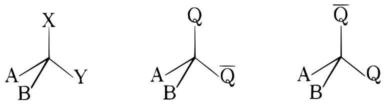


1 ($\mathbf{C}_s$) **2** ($\mathbf{C}_1$)

Figure 1. Methane derivatives with ABXX and ABQQ.



3 ($\mathbf{C}_1$) **4** ($\mathbf{C}_s$) **5** ($\mathbf{C}_s$)

Figure 2. Methane derivatives with ABXY and ABQ$\bar{\mathrm{Q}}$.

1.2. Problem Setting. As shown in the preceding paragraphs, one of the most remarkable differences between the first and second steps of evolution in each approach of combinatorial enumeration is whether the chirality/achirality of substituents (or ligands, or matters) is taken into consideration.

In the first step of evolution, substituents to be placed on a set of positions are regarded as being structureless or, in other words, as being always achiral. Thus, the structure of a substituent is ignored so that only the global symmetry of an isomer is taken into consideration. This means that the permutation-group theory is used as an analyzing tool.

In the second step of evolution on the other hand, such substituents have a three-dimensional structure exhibiting chirality/achirality. In other words, the global and the local symmetry of an isomer are both taken into account. Stress on both the global and the local symmetry of an isomer means that a permutation representation of a point group (coset representation, CR) plays an essential role in chemical combinatorics of the second step.

Let us, for example, compare methane derivatives **1** and **2**, where symbols A, B, and X represent achiral ligands and symbol Q represents a chiral ligand (Figure 1). They belong to the same symmetry under the permutation-group theory, where the chirality/achirality is ignored. In contrast, they belong to different symmetries ($\mathbf{C}_s$ and $\mathbf{C}_1$) under the point-group theory so that they are distinguished to be achiral and chiral. The difference becomes clearer when the local symmetries of **1** and **2** are considered. According to the permutation-group theory, the two achiral ligand Xs in **1** are equivalent and the two chiral ligand Qs in **2** are also equivalent. On the other hand, the point-group theory indicates that the two Xs in **1** are equivalent, while the two Qs in **2** are nonequivalent to each other. This situation becomes clearer by using coset representations (CRs). Thus, the two Xs in **1** are involved in a two-membered orbit governed by the CR $\mathbf{C}_s(/\mathbf{C}_1)$, while the two Qs in **2** construct two distinct one-membered orbits governed by the CR $\mathbf{C}_1(/\mathbf{C}_1)$.

Let us next compare methane derivatives **3** and **4** (or **5**), where symbols A, B, X, and Y represent achiral ligands and symbols Q and $\bar{\mathrm{Q}}$ represent chiral ligands of opposite chirality (Figure 2). They belong to the same symmetry under the permutation-group theory, where the chirality/achirality is ignored. Note that **4** and **5** are meso compounds that exhibit so-called pseudo-asymmetry and that they are diastereomeric to each other. In contrast, they belong to different symmetries under the point-group theory so that they are distinguished to be chiral ($\mathbf{C}_1$) and achiral ($\mathbf{C}_s$).

According to the permutation-group theory, the two achiral ligands X and Y in **3** are nonequivalent and the two chiral ligands Q and $\bar{\mathrm{Q}}$ in **4** (or in **5**) are nonequivalent. On the other hand, the point-group theory indicates that X and Y in **3** are nonequivalent, while Q and $\bar{\mathrm{Q}}$ in **4** (or in **5**) are equivalent to each other. The substituents X and Y in **3** construct distinct one-membered orbits governed by the CR $(\mathbf{C}_1(/\mathbf{C}_1)$. The enantiomeric substituents Q and $\bar{\mathrm{Q}}$ in **4** are involved in a two-membered orbit governed by the CR $\mathbf{C}_s(/\mathbf{C}_1)$.

The difference from the second step to the first step of evolution results in an advanced viewpoint of stereoisomerism, which comes from a new methodology based on the sphericity concept.[21] The sphericity concept is linked to the chirality fittingness of each position, which controls the acceptability of a substituent to be selected. Thereby, the enantiosphericity allows the $\mathbf{C}_s(/\mathbf{C}_1)$ orbit to accommodates a pair of two Xs or a pair of Q and $\bar{\mathrm{Q}}$, as found in Figures 1 and 2. To apply this concept to a characteristic-monomial method,[25−27] we shall first examine cyclic groups, the results of which are then extended to general cases of point groups.

Table 1. (Dominant) Subduction Table for $\mathbf{C}_6$

	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{C}_6$
$\mathbf{C}_6(/\mathbf{C}_1)$	$6\mathbf{C}_1(/\mathbf{C}_1)$	$3\mathbf{C}_2(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{C}_6(/\mathbf{C}_1)$
$\mathbf{C}_6(/\mathbf{C}_2)$	$3\mathbf{C}_1(/\mathbf{C}_1)$	$3\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{C}_6(/\mathbf{C}_2)$
$\mathbf{C}_6(/\mathbf{C}_3)$	$2\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_2(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{C}_6(/\mathbf{C}_3)$
$\mathbf{C}_6(/\mathbf{C}_6)$	$\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{C}_6(/\mathbf{C}_6)$

Table 2. (Dominant) USCI-CF Table for $\mathbf{C}_6$

	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{C}_6$
$\mathbf{C}_6(/\mathbf{C}_1)$	b_1^6	b_2^3	b_3^2	b_6
$\mathbf{C}_6(/\mathbf{C}_2)$	b_1^3	b_1^3	b_3	b_3
$\mathbf{C}_6(/\mathbf{C}_3)$	b_1^2	b_2	b_1^2	b_2
$\mathbf{C}_6(/\mathbf{C}_6)$	b_1	b_1	b_1	b_1

2. RESULTS

2.1. Achiral and Chiral Cyclic Groups. In general, a coset representation (CR) for a cyclic group is subduced into its subgroup so that the orbit governed by the CR is divided into a set of suborbits of the same kind. This is proved in Appendix A.1 for general cases (eq 49). Thereby, the corresponding unit subduced cycle index with chirality fittingness (USCI−CF) is represented in the form of $\$_\gamma^\alpha$, where γ is the size of each of the suborbits and α is the multiplicity of the suborbits (eq 53). The dummy variable \$ in the USCI-CF is selected according to the sphericity of the suborbit: *a* for a homospheric orbit, *b* for a hemispheric orbit, and *c* for a enantiospheric orbit.

For example, the point group $\mathbf{C}_6$ represents a chiral cyclic group of order 6. The subduction table for $\mathbf{C}_6$ is shown in Table 1. The subductions collected in Table 1 exemplify eq 49. Since the participant subgroups for $\mathbf{C}_6$ are all chiral, we select *b* as a dummy variable. The subduction data collected in Table 1 translated into the USCIs as shown in Table 2.

On the other hand, the point group $\mathbf{S}_6$ represents an achiral cyclic group of order 6, which is represented by $\mathbf{S}_6$. The group $\mathbf{S}_6$ is isomorphic to the group $\mathbf{C}_6$ described above.

Table 3. (Dominant) Subduction Table for $\mathbf{S}_6$

	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_i$	$\downarrow \mathbf{C}_3$	$\downarrow \mathbf{S}_6$
$\mathbf{S}_6(/\mathbf{C}_1)$	$6\mathbf{C}_1(/\mathbf{C}_1)$	$3\mathbf{C}_i(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{S}_6(/\mathbf{C}_1)$
$\mathbf{S}_6(/\mathbf{C}_i)$	$3\mathbf{C}_1(/\mathbf{C}_1)$	$3\mathbf{C}_i(/\mathbf{C}_i)$	$\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{S}_6(/\mathbf{C}_i)$
$\mathbf{S}_6(/\mathbf{C}_3)$	$2\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_i(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{S}_6(/\mathbf{C}_3)$
$\mathbf{S}_6(/\mathbf{C}_6)$	$\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_i(/\mathbf{C}_i)$	$\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{S}_6(/\mathbf{S}_6)$

Table 4. (Dominant) USCI-CF Table for $\mathbf{S}_6$

	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_i$	$\downarrow \mathbf{C}_3$	$\downarrow \mathbf{S}_6$
$\mathbf{S}_6(/\mathbf{C}_1)$	b_1^6	c_2^3	b_3^2	c_6
$\mathbf{S}_6(/\mathbf{C}_i)$	b_1^3	a_1^3	b_3	a_3
$\mathbf{S}_6(/\mathbf{C}_3)$	b_1^2	c_2	b_1^2	c_2
$\mathbf{S}_6(/\mathbf{C}_6)$	b_1	a_1	b_1	a_1

However, the chirality/achirality nature of $\mathbf{S}_6$ is different for that of $\mathbf{C}_6$. Accordingly, the subgroups of $\mathbf{S}_6$ are categorized into chiral or achiral subgroups as follows:

$$\mathbf{S}_6 = \{S_6, S_6^{\ 2}, S_6^{\ 3}, S_6^{\ 4}, S_6^{\ 5}, S_6^{\ 6}\} = \{S_6, C_3, i, C_3^{\ 2}, S_6^{\ 5}, I\} \quad \text{(achiral)} \quad (1)$$

$$\mathbf{C}_3 = \{C_3, S_3^{\ 2}, I\} \quad \text{(chiral)} \quad (2)$$

$$\mathbf{C}_i = \{i, I\} \quad \text{(achiral)} \quad (3)$$

The subduction table for $\mathbf{S}_6$ is shown in Table 3. The subductions collected in Table 1 also exemplify eq 49. Since the participant subgroups for $\mathbf{S}_6$ are achiral or chiral, we select a or c as dummy variables. From the data of Table 3, we obtain the USCI-CF table for $\mathbf{S}_6$ (Table 4).

2.2. Classification of Achiral Cyclic Groups. Achiral cyclic groups $\mathbf{S}_x$ generated by a rotoreflection S_x are classified into type I (x: even) and type II (x: odd).

An achiral cyclic group of Type I ($\mathbf{S}_x$ where x is even) has the oreder of x so that it contains a chiral subgroup $\mathbf{C}_x$ (eq 56), as shown in Appendix A.2. Hence, there exists a coset representation (CR) represented by $\mathbf{S}_x(/\mathbf{C}_{x/2})$. Since $\mathbf{S}_x$ is achiral and $\mathbf{C}_{x/2}$ is chiral, the coset representation $\mathbf{S}_n(/\mathbf{C}_{x/2})$ is concluded to be enantiospheric. Obviously, the degree of the CR is equal to $|\mathbf{S}_n|/|\mathbf{C}_{x/2}| = 2$. The $\mathbf{S}_6$ group is an example of type I, where its subduction table is found in Table 3 and its USCI-CF table is found in Table 4.

On the other hand, an achiral cyclic group of type II ($\mathbf{S}_x = \mathbf{C}_{xh}$, where x is odd) has the order of $2x$ so that it contains a chiral subgroup $\mathbf{C}_x$ (eq 59), as shown in Appendix A.3. Hence, we have the CR represented by $\mathbf{S}_x(/\mathbf{C}_x)$, which is concluded to be enantiospheric, since $\mathbf{S}_x$ is achiral and $\mathbf{C}_x$ is chiral. Obviously, the degree of the CR is equal to $|\mathbf{S}_n|/|\mathbf{C}_x| = 2$.

For an example of type II, we have the point group $\mathbf{C}_{3h}$ ($=\mathbf{S}_3 = \langle S_3 \rangle$), which is isomorphic to $\mathbf{S}_6$ (and to $\mathbf{C}_6$). The subgroups of $\mathbf{C}_{3h}$ correspond to those of $\mathbf{S}_6$ in one-to-one fashion as follows:

$$\mathbf{C}_{3h} = \{S_3, C_3^{\ 2}, S_3^{\ 3}, C_3^{\ 4}, S_3^{\ 5}, S_6^{\ 6}(=I)\} = \{S_3, C_3^{\ 2}, \sigma_h, C_3^{\ 4}, S_3^{\ 5}, I\} \quad \text{(achiral)} \quad (4)$$

$$\mathbf{C}_3 = \{C_3, S_3^2, I\} \quad \text{(chiral)} \quad (5)$$

$$\mathbf{C}_s = \{\sigma_h, I\} \quad \text{(achiral)} \quad (6)$$

Table 5. (Dominant) Subduction Table for $\mathbf{C}_{3h}$ ($=\mathbf{S}_3$)

	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_s$	$\downarrow \mathbf{C}_3$	$\downarrow \mathbf{C}_{3h}$
$\mathbf{C}_{3h}(/\mathbf{C}_1)$	$6\mathbf{C}_1(/\mathbf{C}_1)$	$3\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{C}_{3h}(/\mathbf{C}_1)$
$\mathbf{C}_{3h}(/\mathbf{C}_s)$	$3\mathbf{C}_1(/\mathbf{C}_1)$	$3\mathbf{C}_s(/\mathbf{C}_s)$	$\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{C}_{3h}(/\mathbf{C}_s)$
$\mathbf{C}_{3h}(/\mathbf{C}_3)$	$2\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{C}_{3h}(/\mathbf{C}_3)$
$\mathbf{C}_{3h}(/\mathbf{C}_{3h})$	$\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_s(/\mathbf{C}_s)$	$\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{C}_{3h}(/\mathbf{C}_{3h})$

Table 6. (Dominant) USCI−CF Table for $\mathbf{C}_{3h}$ ($=\mathbf{S}_3$)

	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_s$	$\downarrow \mathbf{C}_3$	$\downarrow \mathbf{C}_{3h}$
$\mathbf{C}_{3h}(/\mathbf{C}_1)$	b_1^6	c_2^3	b_3^2	c_6
$\mathbf{C}_{3h}(/\mathbf{C}_s)$	b_1^3	a_1^3	b_3	a_3
$\mathbf{C}_{3h}(/\mathbf{C}_3)$	b_1^2	c_2	b_1^2	c_2
$\mathbf{C}_{3h}(/\mathbf{C}_{3h})$	b_1	a_1	b_1	a_1

Table 7. Bisected (Dominant) Subduction Table for $\mathbf{S}_6$

	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_3$	$\downarrow \mathbf{C}_i$	$\downarrow \mathbf{S}_6$
$\mathbf{S}_6(/\mathbf{C}_1)$	$6\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_1)$	$3\mathbf{C}_i(/\mathbf{C}_1)$	$\mathbf{S}_6(/\mathbf{C}_1)$
$\mathbf{S}_6(/\mathbf{C}_3)$	$2\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{C}_i(/\mathbf{C}_1)$	$\mathbf{S}_6(/\mathbf{C}_3)$
$\mathbf{S}_6(/\mathbf{C}_i)$	$3\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_3(/\mathbf{C}_1)$	$3\mathbf{C}_i(/\mathbf{C}_i)$	$\mathbf{S}_6(/\mathbf{C}_i)$
$\mathbf{S}_6(/\mathbf{S}_6)$	$\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{C}_i(/\mathbf{C}_i)$	$\mathbf{S}_6(/\mathbf{S}_6)$

The subduction table for $\mathbf{C}_{3h}$ ($=\mathbf{S}_3$) shown in Table 5 is essentially equivalent to the one for $\mathbf{S}_6$ shown in Table 3. Thus, Table 5 also exemplifies eq 49. From the data of Table 5, we obtain the USCI-CF table for $\mathbf{C}_{3h}$ ($=\mathbf{S}_3$), as shown in Table 6, which is essentially equivalent to the one for $\mathbf{S}_6$ (Table 4).

2.3. Bisected Subduction Tables and Bisected USCI-CF Tables. The CR of degree 2 for an achiral cyclic group ($\mathbf{S}_x(/\mathbf{C}_{x/2})$ for type I and $\mathbf{S}_x(/\mathbf{C}_x)$ for Type II) is enantiospheric, as found in the preceding paragraphs. Since any chiral subgroup $\mathbf{C}_{x'}$ is a subgroup of $\mathbf{C}_{x/2}$ (type I) or $\mathbf{C}_x$ (type II), the corresponding CR $\mathbf{S}_x(/\mathbf{C}_{x'})$ has a degree of even number. Since only one subgroup of a given order exists in the case of a cyclic group, there is no achiral group whose order is equal to that of the chiral subgroup $\mathbf{C}_{x'}$. This intuitive explanation leads us to a theorem.

Theorem 1. *As for an achiral cyclic group, whether it is type I or type II, its coset representation of even degree is enantiospheric, while its coset representation of odd degree is homospheric.*

Theorem 1 is proved more rigorously in Appendices B and C.

Theorem 1 is effectively exemplified by a bisected subduction table, which is defined as a table bisected in terms of the chirality/achirality of subgroups.[29] For example, Table 7 is the bisected subduction table of $\mathbf{S}_6$, where the upper-right part contains enantiospheric coset representations of even degree, while the lower-right part contains homospheric coset representations of odd degree.

As for an achiral subduction of an enantiospheric coset representation (even degree), the discussions in Appendices B and C provide us with a theorem.

Theorem 2. *As for an achiral cyclic group, whether it is type I or type II, an achiral subduction of an enantiospheric coset representation (even degree) gives an odd number of enantiospheric coset representations.*

The upper-right part of Table 7 contains several examples of this theorem. The corresponding bisected USCI-CF Table (Table 8) has the upper-right part that consists of dummy

Table 8. Bisected (Dominant) USCI-CF Table for $\mathbf{S}_6$

	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_3$	$\downarrow \mathbf{C}_i$	$\downarrow \mathbf{S}_6$
$\mathbf{S}_6(/\mathbf{C}_1)$	b_1^6	b_3^2	c_2^3	c_6
$\mathbf{S}_6(/\mathbf{C}_3)$	b_1^2	b_1^2	c_2	c_2
$\mathbf{S}_6(/\mathbf{C}_i)$	b_1^3	b_3	a_1^3	a_3
$\mathbf{S}_6(/\mathbf{S}_6)$	b_1	b_1	a_1	a_1

variables of c_d-type, where the subscripts are even and the powers are odd.

By virtue of the discussion describe in Appendices B and C, we also arrive at a theorem concerning achiral subduction of homospheric coset representations (odd degree).

Theorem 3. *As for an achiral cyclic group, whether it is type I or type II, an achiral subduction of an homospheric coset representation (odd degree) gives an odd number of homospheric coset representations.*

The lower-right part of Table 7 involves several examples of this theorem. The lower-right part of Table 8 has dummy variables of a_d-type, where the subscripts are odd and the powers are odd.

2.4. Definition of Characteristic Monomials with Chirality Fittingness. 2.4.1. Characteristic Monomials with Chirality Fittingness For Cyclic Groups. The properties of USCI-CFs for cyclic groups have been clarified in the preceding subsections. Thereby, we propose here characteristic monomials with chirality fittingness (CM-CFs), which are an extension of characteristic monomials (without chirality fittingness) reported in ref 30. Theorem 3 of ref 30 shows that if we have

$$g(\tilde{x}) = \sum^{\delta|\tilde{x}} f(\delta) \tag{7}$$

then, we have

$$f(\tilde{x}) = \sum^{\delta|\tilde{x}} \mu(\delta, \tilde{x})\, g(\delta) \tag{8}$$

where the symbol $\mu(\delta, \tilde{x})$ represents Möbius function, and we place

$$g(\tilde{x}) = \mathbf{S}_x(/\mathbf{S}_d) \underset{=}{\text{amp}} \mathbf{S}_{\tilde{x}}(/\mathbf{C}_1) \tag{9}$$

$$f(\tilde{x}) = \Gamma_{x/\tilde{x}} \tag{10}$$

where $\tilde{x} = x/d$. The symbol $\Gamma_{x/\tilde{x}}$ represents a **Q**-cocjugacy character corresponding to the $x/\tilde{x}$-th primitive root of 1.[31] Note that the chirality fittingness (sphericity) of $\mathbf{S}_x(/\mathbf{S}_d)$ is not always equal to that of $\mathbf{S}_{\tilde{x}}(/\mathbf{C}_1)$. In the previous paper,[30] the relationships represented by eqs 7 and 8 have been concerned with markaracters. They have been restricted to state amplified irreducible representations. However, they can be easily transformed into the relationship between a **Q**-conjugacy representation and a dominat coset representation. Thus, eqs 7 and 8 are transformed into

$$\mathbf{S}_x(/\mathbf{S}_{x/\tilde{x}}) = \sum^{\delta|\tilde{x}} \Gamma_{x/\delta} \tag{11}$$

$$\Gamma_{x/\tilde{x}} \sum^{\delta|\tilde{x}} \mu(\delta,\tilde{x})\, \mathbf{S}_\delta(/\mathbf{C}1) \underset{=}{\text{amp}} \sum^{\delta|\tilde{x}} \mu(\delta,\tilde{x})\, \mathbf{S}_x(/\mathbf{S}_{x/\delta}) \tag{12}$$

where $\tilde{x} = x/d$. Since the subduction of $\Gamma_{x/\tilde{x}}$ to $\mathbf{S}_x$ (i.e. $\Gamma_{x/\tilde{x}} \downarrow \mathbf{S}_x$) is $\Gamma_{x/\tilde{x}}$ itself, we have the definition of a characteristic monomial with chirality fittingness (CM-CF) as follows:

$$\mathrm{ZC}(\Gamma_{x/\tilde{x}}\downarrow\mathbf{S}_x;\$_\delta) = \prod^{\delta|\tilde{x}} \$_\delta^{\mu(\delta,\tilde{x}x)} \tag{13}$$

Note that we place $\alpha(x/\delta, x) = 1$ and $\gamma(x/\delta, x) = \delta$ in eq 53 for this case.

Further subduction to every subgroup of $\mathbf{S}_d$ is obtained by introducing eq 49 into eq 12, i.e.,

$$\begin{aligned}\Gamma_{x/\tilde{x}} \downarrow \mathbf{S}_{d'} &= [\Gamma_{x/\tilde{x}} \downarrow \mathbf{S}_d] \downarrow \mathbf{S}_{d'} \\ &= \sum^{\delta|\tilde{x}} \mu(\delta, \tilde{x})\, \mathbf{S}_x(/\mathbf{S}_{x/\delta}) \downarrow \mathbf{S}_{d'} \\ &= \sum^{\delta|\tilde{x}} \mu(\delta, \tilde{x})\, \alpha(x/\delta,d')\, \mathbf{S}_{d'}(/\mathbf{S}_{(x/\delta,d')})\end{aligned} \tag{14}$$

By starting from eq 53 and eq 14, we define a characteristic monomial with chirality fittingness (CM-CF) as follows:

$$\begin{aligned}\mathrm{ZC}(\Gamma_{x/\tilde{x}} \downarrow \mathbf{S}_{d'}; \$_{\gamma(x/\delta,d')}) &= \prod^{\delta|\tilde{x}} (\mathrm{ZC}(\mathbf{S}_x(/\mathbf{S}_{x/\delta}) \downarrow \mathbf{S}_{d'}; \$_{\gamma(x/\delta,d'')}))^{\mu(\delta,\tilde{x})} \\ &= \prod^{\delta|\tilde{x}} \$_{\gamma(x/\delta,d')}^{\mu(\delta,\tilde{x})\alpha(x/\delta,d')},\end{aligned} \tag{15}$$

where we place \$ according to the chirality fittingness of $\mathbf{S}_{d'}(/\mathbf{S}_{(x/\delta d')})$: $\$ = a$ if homospheric, $\$ = b$ if hemispheric, and $\$ = c$ if enantiospheric. Note that eq 13 is a special case of eq 15.

Example 1. Let us consider the achiral cyclic group $\mathbf{S}_6$ of order 6. Equation 11 for this case provides the following equations:

$$\mathbf{S}_6(/\mathbf{C}_1) = \Gamma_{6/1} + \Gamma_{6/2} + \Gamma_{6/3} + \Gamma_{6/6} \tag{16}$$

$$\mathbf{S}_6(/\mathbf{C}_i) = \Gamma_{6/1} + \Gamma_{6/3} \tag{17}$$

$$\mathbf{S}_6(/\mathbf{C}_3) = \Gamma_{6/1} + \Gamma_{6/2} \tag{18}$$

$$\mathbf{S}_6(/\mathbf{S}_6) = \Gamma_{6/1} \tag{19}$$

where $\Gamma_{6/\delta}$ is the **Q**-conjugacy representation corresponding to the δ-th primitive root of 1. By solving these equations or by applying eq 12 to this case, we obtain

$$A_g:\quad \Gamma_{6/1} = \mu(1,1)\, \mathbf{S}_6(/\mathbf{S}_6) = \mathbf{S}_6(/\mathbf{S}_6) \ldots a_1 \tag{20}$$

$$A_u:\quad \Gamma_{6/2} = \mu(1, 2)\, \mathbf{S}_6(/\mathbf{S}_6) + \mu(2,2)\, \mathbf{S}_6(/\mathbf{C}_3) = -\mathbf{S}_6(/\mathbf{S}_6) + \mathbf{S}_6(/\mathbf{C}_3) \ldots a_1^{-1}c_2 \tag{21}$$

$$E_g:\quad \Gamma_{6/3} = \mu(1,3)\, \mathbf{S}_6(/\mathbf{C}_6) + \mu(3,3)\, \mathbf{S}_6(/\mathbf{C}_i) = -\mathbf{S}_6(/\mathbf{C}_6) + \mathbf{S}_6(/\mathbf{C}_i) \ldots a_1^{-1}a_3 \tag{22}$$

$$\begin{aligned}\mathrm{Eu}:\quad \Gamma_{6/6} &= \mu(1,6)\, \mathbf{S}_6(/\mathbf{S}_6) + \mu(2,6)\, \mathbf{S}_6(/\mathbf{C}_3) + \mu(3,6)\, \mathbf{S}_6(/\mathbf{C}_i) + \mu(6,6)\, \mathbf{S}_6(/\mathbf{C}_1) \\ &= \mathbf{S}_6(/\mathbf{S}_6) - \mathbf{S}_6(/\mathbf{C}_3) - \mathbf{S}_6(/\mathbf{C}_i) + \mathbf{S}_6(/\mathbf{C}_1) \ldots a_1c_2^{-1}\, a_3^{-1}c_6\end{aligned} \tag{23}$$

Table 9. CM-CF Table for $\mathbf{S}_6$ and $\mathbf{C}_{3h}$

$\mathbf{C}_{3h}$	$\mathbf{S}_6$		$\downarrow\mathbf{C}_1$ $\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_s$ $\downarrow\mathbf{C}_i$	$\downarrow\mathbf{C}_3$ $\downarrow\mathbf{C}_3$	$\downarrow\mathbf{C}_{3h}$ $\downarrow\mathbf{S}_6$
A'	A_g:	$\Gamma_{6/1}$	b_1	a_1	b_1	a_1
A''	A_u:	$\Gamma_{6/2}$	b_1	$a_1^{-1}c_2$	b_1	$a_1^{-1}c_2$
E'	E_g:	$\Gamma_{6/3}$	b_1^2	a_1^2	$b_1^{-1}b_3$	$a_1^{-1}a_3$
E''	E_u:	$\Gamma_{6/6}$	b_1^2	$a_1^{-1}c_2^2$	$b_1^{-1}b_3$	$a_1c_2^{-1}a_3^{-1}c_6$

Table 10. CM-CF Table for $\mathbf{C}_s$ and $\mathbf{C}_i$

$\mathbf{C}_i$	$\mathbf{C}_s$		$\downarrow\mathbf{C}_1$ $\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_i$ $\downarrow\mathbf{C}_s$
A_g	A':	$\Gamma_{2/1}$	b_1	a_1
A_u	A'':	$\Gamma_{2/2}$	b_1	$a_1^{-1}c_2$

Table 11. CM-CF Table for $\mathbf{C}_p$ ($p \geq 2$: Prime Number)

		$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_p$
A:	$\Gamma_{p/1}$	b_1	b_1
E:	$\Gamma_{p/p}$	b_1^{-1}	$b_1^{-1}b_p$

Table 12. CM-CF Table for $\mathbf{S}_4$

		$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{S}_4$
A:	$\Gamma_{4/1}$	b_1	b_1	a_1
B:	$\Gamma_{4/2}$	b_1	b_1	$a_1^{-1}c_2$
E:	$\Gamma_{4/4}$	b_1^2	$b_1^{-2}b_2^2$	$c_2^{-1}c_4$

Table 13. CM-CF Table for $\mathbf{S}_8$

		$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_4$	$\downarrow\mathbf{S}_8$
A:	$\Gamma_{8/1}$	b_1	b_1	b_1	a_1
B:	$\Gamma_{4/2}$	b_1	b_1	b_1	$a_1^{-1}c_2$
E_2:	$\Gamma_{8/4}$	b_1^2	b_1^2	$b_1^{-2}b_2^2$	$c_2^{-1}c_4$
$E_1 + E_3$:	$\Gamma_{8/8}$	b_1^4	$b_1^{-4}b_2^4$	$b_2^{-2}b_4^2$	$c_4^{-1}c_8$

The right-hand side of each equation gives the corresponding CM-CF, which is calculated from the data of USCIs collected in Table 5 by means of eq 15 ($\mathbf{S}_{d'} = \mathbf{S}_6$). The CM-CF obtained is listed in the end of each equation and collected in the $\downarrow\mathbf{S}_6$-column of Table 9.

The remaining columns of Table 9 are obtained by means of eq 15. This procedure can be simplified by using the USCI-CFs collected in Table 5. For example, the subduction $\Gamma_{6/3}\downarrow\mathbf{C}_3$ gives

$$\Gamma_{6/3}\downarrow\mathbf{C}_3 = -\mathbf{S}_6(/\mathbf{C}_6)\downarrow\mathbf{C}_3 + \mathbf{S}_6(/\mathbf{C}_i)\downarrow\mathbf{C}_3 \qquad (24)$$

The $\downarrow\mathbf{C}_3$-column of Table 5 gives b_1 for $\mathbf{S}_6(/\mathbf{C}_6)\downarrow\mathbf{C}_3$ and b_3 $\mathbf{S}_6(/\mathbf{C}_i)\downarrow\mathbf{C}_3$. Hence, we calculate the CM-CF to be $b_1^{-1}b_3$ for the subduction $\Gamma_{6/3}\downarrow\mathbf{C}_3$, where the powers of the CM-CF come from the coefficients appearing in the right-hand side of eq 24.

Table 10 shows the CM-CF table for $\mathbf{C}_s$ and $\mathbf{C}_i$. This is a special case of cyclic groups of prime-number order, as shown in Table 11. Tables 12−14 show the CM-CF tables for achiral cyclic groups $\mathbf{S}_4$, $\mathbf{S}_8$, and $\mathbf{S}_{10}$, respectively.

2.4.2. Characteristic Monomials with Chirality Fittingness for Finite Groups. Suppose that a **Q**-conjugacy character Γ_i of a finite group **G** is restricted to its cyclic subgroup $\mathbf{S}_x$ according to the following equation:

$$\Gamma_i\downarrow\mathbf{S}_x = \sum^{\tilde{x}|x} \beta_{x|\tilde{x}}\Gamma_{x|\tilde{x}} \qquad (25)$$

Table 14. CM-CF Table for $\mathbf{S}_{10}$ and $\mathbf{C}_{5h}$

$\mathbf{C}_{5h}$	$\mathbf{S}_{10}$		$\downarrow\mathbf{C}_1$ $\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_s$ $\downarrow\mathbf{C}_i$	$\downarrow\mathbf{C}_5$ $\downarrow\mathbf{C}_5$	$\downarrow\mathbf{C}_{5h}$ $\downarrow\mathbf{S}_{10}$
A'	A_g:	$\Gamma_{10/1}$	b_1	a_1	b_1	a_1
A''	A_u:	$\Gamma_{10/2}$	b_1	$a_1^{-1}c_2$	b_1	$a_1^{-1}c_2$
$E_1' + E_2'$	$E_{1g} + E_{2g}$	$\Gamma_{10/5}$	b_1^4	a_1^4	$b_1^{-1}b_5$	$b_1^{-1}b_5$
$E_1'' + E_2''$	$E_{1u} + E_{2u}$	$\Gamma_{10/10}$	b_1^4	$a_1^{-4}c_2^4$	$b_1^{-1}b_5$	$a_1c_2^{-1}a_5^{-1}c_{10}$

Then, we define a characteristic monomial with chirality fittingness (CM-CF) for $\Gamma_i\downarrow\mathbf{S}_x$ as follows by using eq 13:

$$\mathrm{ZC}(\Gamma_i\downarrow\mathbf{S}_x;\$_\delta) = \prod^{\tilde{x}|x}[\mathrm{ZC}(\Gamma_{x/\tilde{x}}\downarrow\mathbf{S}_x;\$_\delta)]^{\beta_{x//\tilde{x}}} \qquad (26)$$

$$= \prod^{\tilde{x}|x}[\prod^{\delta|\tilde{x}}\$_\delta^{\mu(\delta,\tilde{x})}]^{\beta_{x/\tilde{x}}} \qquad (27)$$

Since the subgroup $\mathbf{S}_x$ has been related to its subgroup $\mathbf{S}_{d'}$ by further restriction, eq 25 gives

$$\Gamma_i\downarrow\mathbf{S}_{d'} = [\Gamma_i\downarrow\mathbf{S}_x]\downarrow\mathbf{S}_{d'} = \sum^{\tilde{x}|x}\beta_{x/\tilde{x}}(\Gamma_{x/\tilde{x}}\downarrow\mathbf{S}_{d'}) \qquad (28)$$

Hence, we define a CM-CF for $\Gamma_i\downarrow\mathbf{S}_{d'}$ by using eq 15 as follows:

$$\mathrm{ZC}(\Gamma_i\downarrow\mathbf{S}_{d'};\$_{d(x/\delta,d')}) = \prod^{\tilde{x}|x}[\mathrm{ZC}(\Gamma_{x/\tilde{x}}\downarrow\mathbf{S}_{d'};\$_{d(x/\delta,d')})]^{\beta_{x/\tilde{x}}}$$

$$= \prod^{\tilde{x}|x}[\prod^{\tilde{x}|x}\$_{d(x/\delta,d')}^{\mu(\delta,\tilde{x})\alpha(n/\delta,d')}]^{\beta_{x|\tilde{x}}} \qquad (29)$$

As a result, eq 27 gives the data for the $\downarrow\mathbf{S}_x$-column in the table of CM-CFs for **G**, and eq 29 constructs the related columns corresponding to the respective subgroups of $\mathbf{S}_x$. The following example shows a procedure of constructing such a CM-CF table.

Example 2. The point group $\mathbf{D}_{2d}$ has a **Q**-conjugacy character table:

$$\mathbf{D}_{\mathbf{D}_{2d}} = \begin{array}{c} \\ A_1 \\ A_2 \\ B_1 \\ B_2 \\ E \end{array} \begin{array}{c} \begin{array}{ccccc} \downarrow\mathbf{C}_1 & \downarrow\mathbf{C}_2 & \downarrow\mathbf{C}_2' & \downarrow\mathbf{C}_s & \downarrow\mathbf{S}_4 \end{array} \\ \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 & -1 \\ 2 & -2 & 0 & 0 & 0 \end{pmatrix} \end{array} \qquad (30)$$

For the subduction of each representation to $\mathbf{C}'_2$ from the matrix $\mathbf{D}_{\mathbf{D}_{2d}}$ (eq 30), we select the columns related to $\mathbf{C}'_2$, i.e., the $\downarrow\mathbf{C}_1$-column and the $\downarrow\mathbf{C}'_2$-column. Thereby, we obtain a 4×2 matirix, which is multiplied by the inverse of the **Q**-conjugacy character table ($\mathbf{D}_{\mathbf{C}_2}{}^{-1}$) of $\mathbf{C}_2$ as follows:

$$\begin{pmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 1 \\ 1 & -1 \\ 2 & 0 \end{pmatrix} \begin{array}{c} \mathbf{D}_{\mathbf{C}_2}{}^{-1} \\ \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & -1/2 \end{pmatrix} \end{array} = \begin{array}{c} \\ A_1 \\ A_2 \\ B_1 \\ B_2 \\ E \end{array} \begin{array}{c} \begin{array}{cc} A & B \end{array} \\ \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix} \end{array} \begin{array}{c} \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \cdots \end{array} \begin{array}{cc} \downarrow\mathbf{C}_1 & \downarrow\mathbf{C}_2' \\ \hline b_1 & b_1 \\ b_1 & b_1^{-1}b_2 \\ b_1 & b_1 \\ b_1 & b_1^{-1}b_2 \\ b_1^2 & b_2 \end{array} \qquad (31)$$

We obtain CM-CFs as shown after dotted lines in eq 31.

Table 15. CM-CF for $\mathbf{D}_{2d}$

$\mathbf{D}_{2d}$	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_2'$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{S}_4$
A_1	b_1	b_1	b_1	a_1	a_1
A_2	b_1	b_1	$b_1^{-1}b_2$	$a_1^{-1}c_2$	a_1
B_1	b_1	b_1	b_1	$a_1^{-1}c_2$	$a_1^{-1}c_2$
B_2	b_1	b_1	$b_1^{-1}b_2$	a_1	$a_1^{-1}c_2$
E	b_1^2	$b_1^{-2}\,b_2^2$	b_2	c_2	$c_2^{-1}c_4$
N_j	$^1/_8$	$^1/_8$	$^1/_4$	$^1/_4$	$^1/_4$

For example, the **Q**-conjugacy representation E of $\mathbf{D}_{2d}$ yields $A + B$ of $\mathbf{C}_2$. Table 11 ($p = 2$) gives b_1 for A and $b_1^{-1}b_2$ for B ($=E$ when $p = 2$), which are multiplied to give $b_1 \times b_1^{-1}b_2 = b_2$.

Similarly, the subduction of each representation to $\mathbf{C}_s$ requires the V $\mathbf{C}_1$-column and the $\downarrow\mathbf{C}_s$-column of $\mathbf{D}_{\mathbf{D}_{2d}}$. Thereby, we have the following results:

$$\begin{pmatrix} 1 & 1 \\ 1 & -1 \\ 1 & -1 \\ 1 & 1 \\ 2 & 0 \end{pmatrix} \overset{\mathbf{D}_{\mathbf{C}_s}^{-1}}{\begin{pmatrix} ^1/_2 & ^1/_2 \\ ^1/_2 & -^1/_2 \end{pmatrix}} = \begin{array}{c} \\ A_1 \\ A_2 \\ B_1 \\ B_2 \\ E \end{array} \overset{\begin{array}{cc} A' & A'' \end{array}}{\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{pmatrix}} \begin{array}{c} \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \cdots \end{array} \begin{array}{cc} \downarrow\mathbf{C}_1 & \downarrow\mathbf{C}_2 \\ \hline b_1 & a_1 \\ b_1 & a_1^{-1}c_2 \\ b_1 & a_1^{-1}c_2 \\ b_1 & a_1 \\ b_1^2 & c_2 \end{array} \tag{32}$$

We obtain CM-CFs from the data of Table 10. For example, we have $E\downarrow\mathbf{C}_s = A' + A''$ in the bottom of the matrix in eq 32 so that a_1 for A' and $a_1^{-1}c_2$ for A'' (Table 10) gives the CM-CF, $a_1a_1^{-1}c_2 = c_2$. The resulting CM-CFs are shown after dotted lines in eq 32.

We select the $\downarrow\mathbf{C}_1$-, $\downarrow\mathbf{C}_2$-, and $\downarrow\mathbf{S}_4$-columns of $\mathbf{D}_{\mathbf{D}_{2d}}$ (eq 30) to form a 5 × 3 matrix. This matrix is multiplied by the inverse ($\mathbf{D}_{\mathbf{S}4}{}^{-1}$) of the **Q**-conjugacy character table of $\mathbf{S}_4$.

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & -1 \\ 2 & -2 & 0 \end{pmatrix} \overset{\mathbf{D}_{\mathbf{S}_4}{}^{-1}}{\begin{pmatrix} ^1/_4 & ^1/_4 & ^1/_4 \\ ^1/_4 & ^1/_4 & -^1/_4 \\ ^1/_2 & -^1/_2 & 0 \end{pmatrix}} = $$

$$\begin{array}{c} \\ A_1 \\ A_2 \\ B_1 \\ B_2 \\ E \end{array} \overset{\begin{array}{ccc} A & B & E \end{array}}{\begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}} \begin{array}{c} \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \cdots \end{array} \begin{array}{ccc} \downarrow\mathbf{C}_1 & \downarrow\mathbf{C}_2 & \downarrow\mathbf{S}_4 \\ \hline b_1 & b_1 & a_1 \\ b_1 & b_1 & a_1 \\ b_1 & b_1 & a_1^{-1}c_2 \\ b_1 & b_1 & a_1^{-1}c_2 \\ b_1^2 & b_1{}^2b_2{}^2 & c_2{}^{-1}c_4 \end{array} \tag{33}$$

We obtain CM-CFs from the data of Table 12, as shown after dotted lines in eq 33. All of the CM-CFs are collected to give a CM-CF table for $\mathbf{D}_{2d}$ (Table 15).

Similarly, we are able to prepare the CM-CF tables for **T** (Table 16), for $\mathbf{T}_d$ (Table 17), and for $\mathbf{T}_h$ (Table 18).

2.5. Combinatorial Enumeration by CM-CFs. We have reported a method of combinatorial enumeration based on characteristic monomials (CM),[25] where only achiral ligands are taken into consideration. This method is extended so as to treat achiral ligands as well as chiral ones by virtue of characteristic monomials with chirality fittingnes (CM-CFs) defined in the present paper. For this purpose, theorem 1.9

Table 16. CM-CF Table for **T**

T	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_3$
A	b_1	b_1	b_1
E	b_1^2	b_1^2	$b_1^{-1}b_3$
T	b_1^3	$b_1^{-1}\,b_2^2$	b_3
N_j	1/12	1/4	2/3

Table 17. CM-CF Table for $\mathbf{T}_d$

	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{S}_4$
A_1	b_1	b_1	a_1	b_1	a_1
A_2	b_1	b_1	$a_1^{-1}\,c_2^2$	b_1	$a_1^{-1}c_2$
E	b_1^2	b_1^2	c_2	$b_1^{-1}b_3$	c_2
T_1	b_1^3	$b_1^{-1}\,b_2^2$	$a_1^{-1}\,c_2^2$	b_3	$a_1c_2^{-1}c_4$
T_2	b_1^3	$b_1^{-1}\,b_2^2$	a_1c_2	b_3	$a_1^{-1}c_4$
N_j	$^1/_{24}$	$^1/_8$	$^1/_4$	$^1/_3$	$^1/_4$

Table 18. CM-CF Table for $\mathbf{T}_h$

	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{C}_i$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{S}_4$
A_g	b_1	b_1	a_1	a_1	b_1	a_1
A_u	b_1	b_1	$a_1^{-1}c_2$	$a_1^{-1}c_2$	b_1	$a_1^{-1}c_2$
E_g	b_1^2	b_1^2	a_1^2	a_1^2	$b_1^{-1}b_3$	$a_1^{-1}a_3$
E_u	b_1^2	b_1^2	$a_1^{-2}\,c_2^2$	$a_1^{-2}\,c_2^2$	$b_1^{-1}b_3$	$a_1c_2^{-1}\,a_3^{-1}c_6$
T_g	b_1^3	$b_1^{-1}\,b_2^2$	$a_1^{-1}\,c_2^2$	a_1^3	b_3	a_3
T_u	b_1^3	$b_1^{-1}\,b_2^2$	a_1c_2	$a_1^{-3}\,c_2^3$	b_3	$a_3^{-1}c_6$
N_u	$^1/_{24}$	$^1/_8$	$^1/_8$	$^1/_{24}$	$^1/_3$	$^1/_3$

of ref 25 concerning CMs shall be extended into a theorem concerning CM-CFs.

Let us consider a skeleton belonging to the point group **G**, which has a nonredundant set of dominant subgroups,

$$\mathrm{SCSG}_{\mathbf{G}}\{\mathbf{G}_1, \mathbf{G}_2, ..., \mathbf{G}_s\} \tag{34}$$

where the symbol $\mathbf{G}_i$ represents a cyclic subgroup. The positions of the skeleton are governed by a set of **Q**-conjugacy representations, i.e., $\sum_{l=1}^{s} a_l\Gamma_l$. By using the multiplicities a_l ($l = 1, 2, ..., s$) and the CM-CFs (eq 29), we have a cycle index with chirality fittingness (CI-CF) for the present case:

$$\mathrm{CIC}(\mathbf{G}, \$_{d_{jk}}) = \sum_{j=1}^{s} N_j \left(\sum_{l=1}^{s} (ZC(\Gamma_l\downarrow\mathbf{G}_j, \$_{d_{jk}}))^{a_l}\right) \tag{35}$$

where $\mathbf{G}_j$ is placed to be identical with $\mathbf{S}_{d'}$ in eq 29. The coefficient N_j used is the one obtained by the sum of each row in the inverse of the mark table.[25]

It should be noted here that the present CI-CF defined by eq 35 is equivalent to the one derived from USCIs (definition 19.7 of ref 18), though the former is based on **Q**-conjugacy representations and the latter is based on coset representations. This conclusion is deduced from the present procedure of converting USCI-CFs into CM-CFs for cyclic groups as well as finite groups.

Suppose the set of ligands,

$$\mathbf{X} = \{X_1, X_2, ..., X_{|\mathbf{x}|}\} \tag{36}$$

contains achiral and chiral ligands, where, if necessary, we use the symbol $X_i^{(a)}$ for an achiral ligand and $X_i^{(c)}$ for a chiral ligand. We place η_i ligands X_i ($i = 1, 2, ..., \upsilon$) on the n positions of a skeleton to give an isomer with the formula

$$W_\eta = \prod_{i=1}^{\upsilon} X_i^{\eta_i} \tag{37}$$

where we have a partition:

$$[\eta] = \sum_{i=1}^{\upsilon} \eta_i = n \tag{38}$$

The number (A_η) of isomers with the formula W_η (eq 37) is enumerated by the following theorem.

Theorem 4. *The number (A_η) of isomers with W_η is calculated by a generating function,*

$$\sum_{[\eta]} A_\eta W_\eta \ \mathrm{CIC}(\mathbf{G}, \$_{d_{jk}}) \tag{39}$$

where each dummy variable ($) of the CI-CF (eq 35) is substituted by one of ligand inventories,

$$a_{d_{jk}} = \sum_{l=1}^{|X|} (X_l^{(a)})^{d_{jk}} \tag{40}$$

$$b_{d_{jk}} = \sum_{l=1}^{|X|} X_l^{d_{jk}} \tag{41}$$

$$c_{d_{jk}} = \sum_{l=1}^{|X|} (X_l^{(a)})^{d_{jk}} + \sum_{l=1}^{|X|} (X_l^{(c)} \bar{X}_l^{(c)})^{d_{jk}/2} \tag{42}$$

where $X_l^{(a)}$ is an achiral ligand, while $X_l^{(c)}$ represents a chiral ligand.

Example 3. Let us consider an allene skeleton, the four positions of which are substituted by a set of four atoms selected from four achiral ligands (A, B, C, and D) and four chiral ligands (p, q, r, s and their enantiomers designated by the symbols p̄, q̄, r̄, and s̄). This enumeration is concerned with promolecules reported in the previous paper[32] and book,[18] where the subduced-cycle-index (SCI) method was used. The present MC-CF method is as effective as the previous SCI method in solving this enumeration, as shown in this example.

The fixed point vector (markaracter) is calculated to be (4, 0, 0, 2, 0) by counting fixed points for the cyclic subgroups of $\mathbf{D}_{2d}$ ($\mathbf{C}_1$, $\mathbf{C}_2$, $\mathbf{C}'_2$, $\mathbf{C}_s$, and $\mathbf{S}_4$). It is multiplied by the inverse ($\mathbf{D}_{\mathbf{D}_{2d}}^{-1}$) of the **Q**-conjugacy character table to give

$$(4, 0, 0, 2, 0) \overbrace{\begin{pmatrix} 1/8 & 1/8 & 1/8 & 1/8 & 1/4 \\ 1/8 & 1/8 & 1/8 & 1/8 & -1/4 \\ 1/4 & -1/4 & 1/4 & -1/4 & 0 \\ 1/4 & -1/4 & -1/4 & 1/4 & 0 \\ 1/4 & 1/4 & -1/4 & -1/4 & 0 \end{pmatrix}}^{\mathbf{D}_{\mathbf{D}_{2d}}^{-1}} = (1, 0, 0, 1, 1) \tag{43}$$

Since the resulting row vector indicates the multiplicities of **Q**-conjugacy representations in the order of the leftmost column of Table 15, the four positions are determined to be divided into $A_1 + B_2 + E$.

According to the results, the A_1-, B_2-, and E-rows of Table 15 and the coefficients collected in the bottom of the table are used to obtain the CI-CF for this case:

$$\begin{aligned} \mathrm{CIC}(\mathbf{D}_{2d}; a_d, b_d, c_d) &= \frac{1}{8}(b_1)(b_1)(b_1^2) + \frac{1}{8}(b_1)(b_1)(b_1^{-2}b_2^2) + \frac{1}{4}(b_1)(b_1^{-1}b_2)(b_2) + \frac{1}{4}(a_1)(a_1)(c_2) + \frac{1}{4}(a_1)(a_1^{-1})(c_2)(c_2^{-1})(c_4) \\ &= \frac{1}{8}b_1^4 + \frac{3}{8}b_2^2 + \frac{1}{4}a_1^2c_2 + \frac{1}{4}b_4 \end{aligned} \tag{44}$$

The ligand inventories are obtained to be

$$a_d = A^d + B^d + X^d + Y^d \tag{45}$$

$$b_d = A^d + B^d + X^d + Y^d + p^d + \bar{p}^d + q^d + \bar{q}^d r^d + \bar{r}^d s^d + \bar{s}^d \tag{46}$$

$$c_d = A^d + B^d + X^d + Y^d + 2p^{d/2}\bar{p}^{d/2} + 2q^{d/2}\bar{q}^{d/2} + 2r^{d/2}\bar{r}^{d/2} + 2s^{d/2}s^{d/2} \tag{47}$$

The inventories (eqs 45−47) are introduced into the CI-CF (eq 44) and the resulting equation is expanded to give a generating function:

$$\begin{aligned} f &= \mathrm{CIC}(\mathbf{C}_1; a_d, b_d, c_d) \\ &= (A^4 + B^4 + ...) + (A^3B + A^3X + ...) + \frac{1}{2}[(A^3p + A^3\bar{p}) + (A^3q + A^3\bar{q}) + ...] + 2(A^2B^2 + A^2X^2 + ...) + \\ &\quad 2(A^2BX + A^2BY + ...) + \frac{3}{2}[(A^2Bp + A^2B\bar{p}) + (A^2Bq + A^2B\bar{q}) + ...] + \frac{3}{2}[(A^2p^2 + A^2p^2) + (A^2q^2 + A^2\bar{q}^2) + ...] + \\ &\quad 2(A^2p\bar{p} + A^2q\bar{p} + ...) + \frac{3}{2}[(A^2pq + A^2\overline{pq}) + (B^2pq + B^2\overline{pq}) + ...] + 3ABXY + \frac{6}{2}[(ABXp + ABX\bar{p}) + (ABXq + \\ &\quad ABX\bar{q}) + ...] + \frac{3}{2}[(ABp^2 + AB\bar{p}^2) + (ABq2 + AB\bar{q}^2) + ...] + 4(ABp\bar{p} + ABq\bar{q} + ...) + \frac{6}{2}[(ABpq + AB\overline{pq}) + \\ &\quad (AXpq + AX\overline{pq}) + ...] + \frac{1}{2}[(Ap^3 + A\bar{q}^3) + (Aq^3 + A\bar{q}^3) + ...] + \frac{3}{2}[(Ap^2\bar{p} + Ap\bar{p}^2) + (Aq^2\bar{q} + Aq\bar{q}^2) + \\ &\quad ...] + \frac{1}{2}[(Ap^2q + A\bar{p}^2\bar{q}) + (Bp^2q + B\bar{p}^2\bar{q}) + ...] + \frac{6}{2}[(Ap\bar{p}q + Ap\overline{pq}) + (Bp\bar{p}q + Bp\overline{pq}) + ...] + \\ &\quad \frac{6}{2}[(Apqr + A\overline{pqr}) + (Bpqr + B\overline{pqr}) + ...] \ ... \end{aligned} \tag{48}$$

The results are consistent with those derived by alternative methods, which have been reported in Chapter 21 of ref 18.[33]

3. DISCUSSION

3.1. Isomer with Achiral Ligands Only. In the right-hand side of eq 48, a term containing achiral ligands only

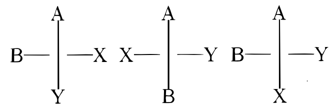


Figure 3. Allene derivatives with the formula ABXY.

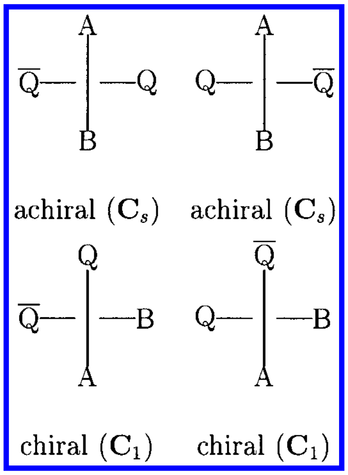


Figure 4. Allene derivatives with the formula ABq$\overline{\text{q}}$.

(A, B, X, and Y) corresponds to a chiral or an achiral isomer, where a pair of enantiomers is counted once as one isomer in the present enumeration. In such a case, the coefficient of the term directly indicates the number of such isomers. For example, there are three isomers with *ABXY*, since the coefficient of the term *ABXY* is equal to 3. The three isomers shown in Figure 3 are chiral, where an arbitrary enantiomer is depicted for the simplicity sake. These isomers correspond to structures **72**, **73**, and **74** listed in Figure 21.5 of ref 18. Obviously, they corresond to **3** derived from a methane skeleton.

3.2. Achiral Isomers with Chiral Ligands. Terms such as $A^2q\overline{q}$ and $ABq\overline{q}$ sometimes correspond to achiral isomers in which pairs of enantiomeric ligands compensate their chirality effects. In other words, the terms are ascribed to so-called mesoisomers. For example, the coefficient of $ABq\overline{q}$ is 4 as found in eq 48, which indicates that there are four isomers of the formula $ABq\overline{q}$. Among them, two $ABq\overline{q}$ isomers are meso isomers (achiral),[33] while the other two are chiral isomers, as shown in Figure 4. The former isomers correspond to structures **53** and **54** and the latter to **84** and **85** listed in Figure 21.5 of ref 18. Obviously, the former isomers (the top row of Figure 4) corresond to **4** and **5** derived from a methane skeleton.

3.3. Chiral Isomers with Chiral Ligands. Each coefficient of fraction type indicates that it is concerned with pairs of enantiomers, where their formulas have a different set of chiral ligands that are interchangeable under an improper operation. For example, the coefficient $^1/_2$ for ($A^3q + A^3\overline{q}$) reveals the presence of one pair of enantiomers (A^3q and $A^3\overline{q}$).[34] Similarly, there are six pairs of enantiomers ($ABXq$ and $ABX\overline{q}$) in terms of the factor $^6/_2$ for ($ABXq$ and $ABX\overline{q}$). To illustrated the results, Figure 5 shows the six isomers with the formula $ABXq$, where an arbitrary enantiomer is depicted as a representative of each pair of enantiomers ($ABXq$ and $ABX\overline{q}$). Stereochemically speaking, the six isomers shown in Figure 5 are diastereomers to each other. These isomers correspond to structures **75** to **80** listed in Figure 21.5 of ref 18.

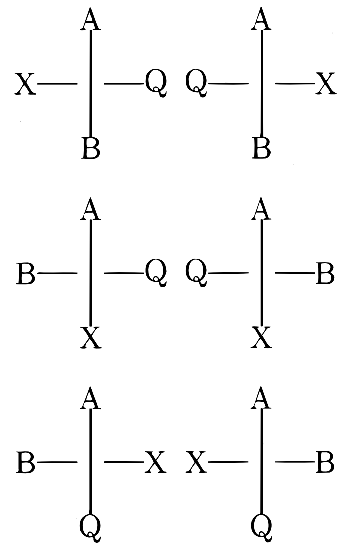


Figure 5. Allene derivatives with the formula ABXq.

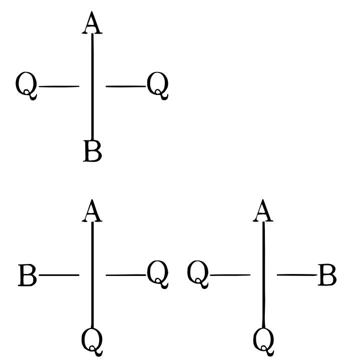


Figure 6. Allene derivatives with the formula ABq^2.

Figure 6 shows the six isomers with the formula ABq^2, where an arbitrary enantiomer is depicted as a representative of each pair of enantiomers (ABq^2 and $AB\overline{q}^2$). These isomers correspond to structures **81** to **83** listed in Figure 21.5 of ref 18. Obviously, the first isomer (the top row of Figure 6) corresonds to **2** derived from a methane skeleton.

4. CONCLUSION

After cyclic groups have been categorized into chiral and achiral, the achiral cyclic groups have been discussed in terms of chirality fittingness (sphericity). Thereby, characteristic monomials with chirality fittingness (CM-CFs) have been proposed for characterizing the desymmetrization of cyclic groups as well as of finite groups. A procedure of calculating CM-CFs for cyclic groups and finite groups has been described to tabulate them as CM-CF tables. A new method of combinatorial enumeration based on CM-CF tables has been developed.

APPENDIX A. SUBDUCTION FOR CYCLIC SUBGROUPS

A. 1. Unit Subduced Cycle Index with Chirality Fittingness for a Cyclic Group. Suppose that the group $\mathbf{S}_x$ is a cyclic point group. For a subgroup $\mathbf{S}_d$ of $\mathbf{S}_x$, there exists a coset representation $\mathbf{S}_x(/\mathbf{S}_d)$, which can be subduced into a subgroup $\mathbf{S}_{d'}$ as follows:

$$\mathbf{S}_x(/\mathbf{S}_d)\downarrow\mathbf{S}_{d'} = \sum_{g\in\Gamma}\mathbf{S}_{d'}(/g^{-1}\,\mathbf{S}_d g \cap \mathbf{S}_{d'}) = \alpha(d,d')\,\mathbf{S}_{d'}(/\mathbf{S}_d \cap \mathbf{S}_{d'}) = \alpha(d,d')\,\mathbf{S}_{d'}(/\,\mathbf{S}_{(d,d')}) \quad (49)$$

where Γ represents a transversal of the double-cosets decomposition of $\mathbf{S}_x$ by $\mathbf{S}_d$, and $\mathbf{S}_{d'}$, and we place $\mathbf{S}_{(d,d')} = \mathbf{S}_d \cap \mathbf{S}_{d'}$. Note that $g^{-1}\mathbf{S}_d g = \mathbf{S}_d$ because $\mathbf{S}_d$ is cyclic. The order of the cyclic group $\mathbf{S}_{(d,d')}$ is the greatest common divisor of the orders of the cyclic groups, $\mathbf{S}_d$ and $\mathbf{S}_{d'}$, i.e.,

$$|\mathbf{S}_{(d,d')}| = (|\mathbf{S}_d|, |\mathbf{S}_{d'}|) = (d, d') \quad (50)$$

Hence, the multiplicity $\alpha(d, d')$ is calculated to be

$$\alpha(d,d') = \frac{|\mathbf{S}_x||\mathbf{S}_{(d,d')}|}{|\mathbf{S}_d||\mathbf{S}_{d'}|} = \frac{x(d,d')}{dd'} \quad (51)$$

The coset representation $\mathbf{S}_{d'}(/\mathbf{S}_{(d,d')})$ in the right-hand side of eq 49 is capable of governing a $\gamma(d, d')$-membered orbit, where

$$\gamma(d,d') = |\mathbf{S}_{d'}|/|\mathbf{S}_{(d,d')}| = d'/(d,d') \quad (52)$$

Hence, we define a unit subduced cycle index with chirality fittingness (USCI-CF) as

$$\mathrm{ZC}(\mathbf{S}_x(/\mathbf{S}_d)\downarrow\mathbf{S}_{d'};\$_{\gamma(d,d')}) = \$_{\gamma(d,d')}^{\alpha(d,d')} \quad (53)$$

in which the subscript $\gamma(d, d')$ represents the size of the orbit and the superscript $\alpha(d, d')$ represents the multiplicity of the orbit. The dummy variable \$ in the USCI is selected according to the chirality fittingness (sphericity) of the orbit: *a* for a homospheric orbit, *b* for a hemispheric orbit, and *c* for a enantiospheric orbit.

A.2. Achiral Cyclic Groups of Type I. Let the point group $\mathbf{S}_x$ be an achiral cyclic group of even order x, where a rotoflection S_x is selected as a generator of the group $\mathbf{S}_x$. Then, the rotoflections (elements) of $\mathbf{S}_x$ are generated as follows:

$$\mathbf{S}_x = \{S_x, S_x^2, S_x^3, ..., S_x^x(=I)\} \quad (54)$$

In the present paper, such a point group as $\mathbf{S}_x$ (x: even) is called an achiral cyclic group of type I. Such an achiral group contains proper rotations and the same number of improper rotations, since its order x is even. Obviously, the generator S_x is an improper rotation. Hence, S_x^2 ($=\mathbf{C}_{x/2}$) is concluded to be a proper rotation. This generates the following chiral subgroup of order $x/2$.

$$\mathbf{C}_{x/2} = \{S_x^2, S_x^4, S_x^6, ..., S_x{}^n\ (=I)\} = \{C_{x/2}, C_{x/2}^2, C_{x/2}^3, ..., C_{x/2}{}^{x/2}(=I)\} \quad (55)$$

Thereby, we obtain a coset decomposition:

$$\mathbf{S}_x = \mathbf{C}_{x/2} + S_x\mathbf{C}_{x/2} \quad (56)$$

According to this decomposition, we have the coset representation represented by $\mathbf{S}_x(/\mathbf{C}_{x/2})$. Since $\mathbf{S}_x$ is achiral and $\mathbf{C}_{x/2}$ is chiral, the coset representation $\mathbf{S}_n(/\mathbf{C}_{x/2})$ is concluded to be enantiospheric.

A.3. Achiral Cyclic Groups of Type II. Let us now consider a rotoflection S_x (x: odd) is selected as a generator of the cyclic group $\mathbf{S}_x$ ($=\mathbf{C}_{xh}$). Then, the rotoflections (elements) of $\mathbf{S}_x$ ($=\mathbf{C}_{xh}$) are generated as follows:

$$\mathbf{C}_{xh} = \mathbf{S}_x\{S_x, S_x^2, ..., S_x^x, S_x^{x+1}, S_x^{x+2}, ..., S_x^{2x}\ (=I)\} \quad (57)$$

In the present paper, the point group $\mathbf{S}_x$ is called an achiral cyclic group of type II. The order of the resulting group $\mathbf{S}_x$ ($=\mathbf{C}_{xh}$) is equal to $2x$. Note that the element S_x^x represents a horizontal reflection (σ_h). Hereafter, the symbol $\mathbf{C}_{xh}$ is used. The achiral group $\mathbf{C}_{xh}$ (x: odd) contains proper rotations and the same number of improper rotations, since its order $2x$ is even.

Since the generator S_x is an improper rotation, S_x^2 (C_x^2) is concluded to be a proper rotation. This generates the following chiral subgroup of order x.

$$\begin{aligned}\mathbf{C}_x &= \{C_x^2, C_x^4, ..., C_x^{x-1}, C_x^{x+1}, C_x^{x+3}, ..., C_x^{2x}\ (=I)\}\\ &= \{C_x^2, C_x^4, ..., C_x^{x-1}, C_x, C_x^3, ..., C_x^x\ (=I)\}\\ &= \{C_x, C_x^2, ..., C_x^x\ (=I)\} \quad (58)\end{aligned}$$

It follows that the resulting cyclic group $\mathbf{C}_x$ is also generated from the generator C_x. Thereby, we obtain a coset decomposition:

$$\mathbf{C}_{xh} = \mathbf{S}_x = \mathbf{C}_x + S_x\mathbf{C}_x \quad (59)$$

According to this decomposition, we have the coset representation represented by $\mathbf{S}_x(/\mathbf{C}_x)$. Since $\mathbf{S}_x$ is achiral and $\mathbf{C}_x$ is chiral, the coset representation $\mathbf{S}_x(/\mathbf{C}_x)$ is concluded to be enantiospheric.

APPENDIX B. ORBITS FOR ACHIRAL CYCLIC GROUPS OF TYPE I

B.1. Enantiospheric and Homospheric Orbits. The discussion described in the preceding section can be extended to be applied to general cases of achiral cyclic groups of type I. An even positive integer x is factorized into prime factors as follows:

$$x = 2^m \times x_1^{n_1} \times x_2^{n_2} \times ... \quad (60)$$

where m, n_1, n_2, ... are integers satisfying $m \geq 1$, $n_1 \geq 0$, $n_2 \geq 0$, ... and x_1, x_2, ... are odd prime numbers.

It should be noted here that the element of order 2 may be chiral or achiral according to the order of a cyclic group of type I. In general, we have $S_x^{x/2} = i$ (inversion), if $m = 1$. The case of $\mathbf{S}_6$ described above exemplifies this proposition. On the other hand, we have $S_x^{x/2}$, if $m > 1$. For exmaple, the point group $\mathbf{S}_{12}$ ($= \langle S_{12}\rangle$) has a C_2 operation as the element of order 2, as found in the following list of the subgroups of $\mathbf{S}_{12}$:

$$\mathbf{S}_{12} = \{S_{12}, S_{12}^2, S_{12}^3, S_{12}^4, S_{12}^5, S_{12}^6, S_{12}^7, S_{12}^8, S_{12}^9, S_{12}^{10}, S_{12}^{11}, S_{12}^{12}\} = \{S_{12}, C_6, S_4, C_3, S_{12}^5, C_2, S_{12}^7, C_3^2, S_4^3, C_6^5, S_{12}^{11}, I\} \quad (61)$$

$$\mathbf{C}_6 = \{C_6, C_3, C_2, C_3^2, C_6^5, I\} \quad (62)$$

$$\mathbf{S}_4 = \{S_4, C_2, S_4^3, I\} \quad (63)$$

$$\mathbf{C}_3 = \{C_3, S_3^2, I\} \quad (64)$$

$$\mathbf{C}_2 = \{C_2, I\} \quad (65)$$

B.1.1. Homospheric Orbits and Achiral Subductions. Suppose that we select an odd divisor (y) of x to be

$$y = x_1^{n'_1} \times x_2^{n'_2} \times ... \quad (66)$$

where $n_i \geq n'_i \geq 0$ ($i = 1,2, ...$). Since y is odd, the element S_x^y ($=S_{x/y}$) is an improper rotation. Hence, it generates an achiral cyclic subgroup of order x/y as follows:

$$\mathbf{S}_{x/y} = \{S_x^y, S_x^{2y}, S_x^{3y}, ..., S_x^{(x/y)y}(=I)\} = \{S_{x/y}, S_{x/y}^2, S_{x/y}^3, ..., S_{x/y}^{x/y}(=I)\} \quad (67)$$

where the inteter x/y is calculated to be

$$x/y = 2^m \times x_1^{n_1-n'_1} \times x_2^{n_2-n'_2} \times ... \quad (68)$$

Since both $\mathbf{S}_x$ and $\mathbf{S}_{x/y}$ are achiral, the corresponding coset representation $\mathbf{S}_x(/\mathbf{S}_{x/y})$ is homospheric. The degree of the coset representation is represented by

$$|\mathbf{S}_x|/|\mathbf{S}_{x/y}| = x_1^{n'_1} \times x_2^{n'_2} ... \quad (69)$$

which is an odd integer.

Let us consider an odd integer represented by

$$y' = x_1^{n''_1} \times x_2^{n''_2} \times ... \quad (70)$$

The rotoflection $S_x^{y'} = S_{x/y'}$ generates an achiral subgroup $\mathbf{S}_{x/y'}$, the order of which is calculated to be

$$x/y' = 2^m \times x_1^{n_1-n''_1} \times x_2^{n_2-n''_2} \times ... \quad (71)$$

Let us now consider an achiral subduction of a homosheric orbit, which is represented by the symbol $\mathbf{S}_x(/\mathbf{S}_{x/y}) \downarrow \mathbf{S}_{x/y'}$. In light of theorem 2 of ref 35, we have

$$\mathbf{S}_x(/\mathbf{S}_{x/y}) \downarrow \mathbf{S}_{x/y'} = \sum_g \mathbf{S}_{x/y'}(/g^{-1}\mathbf{S}_{x/y}g \cap \mathbf{S}_{x/y'}) \quad (72)$$

where g runs over the transversal of the double coset decomposition of $\mathbf{S}_x$ by the subgroups $\mathbf{S}_{x/y}$ and $\mathbf{S}_{x/y'}$. Since $\mathbf{S}_{x/y}$ is cyclic, we have $g^{-1}\mathbf{S}_{x/y}g = \mathbf{S}_{x/y}$ for any g. Then, we place

$$\mathbf{S}_{x/y} \cap \mathbf{S}_{x/y'} = \mathbf{S}_x^{y''} = \mathbf{S}_{x/y''} \quad (73)$$

where x/y'' is the greatest common divisor of x/y and x/y', i.e.,

$$x/y'' = \gcd(x/y, x/y') = 2^m \times x_1^{n_1-n'''_1} \times x_2^{n_2-n'''_2} \times ... \quad (74)$$

Thereby, the integer y'' is calculated to be

$$y'' = \frac{x}{x/y''} = x_1^{n'''_1} \times x_2^{n'''_2} \times ... \quad (75)$$

which indicates that y'' is an odd integer. This means that $S_x^{y''}$ (i.e. $S_{x/y''}$) is an improper rotation and that $\mathbf{S}_{x/y''}$ generated from $S_x^{y''}$ is an achiral subgroup. As a result, eq 73 indicates that all of the terms in the summation of eq 72 are concluded to be identical with each other, being independent to g. Hence, eq 72 is transformed into

$$\mathbf{S}_x(/\mathbf{S}_{x/y}) \downarrow \mathbf{S}_{x/y'} = \alpha\mathbf{S}_{x/y'}(/\mathbf{S}_{x/y} \cap \mathbf{S}_{x/y'}) = \alpha\mathbf{S}_{x/y'}(/\mathbf{S}_{x/y''}) \quad (76)$$

where the multiplicity α is represented by

$$\alpha = \left(\frac{x}{x/y}\right) / \left(\frac{x/y'}{x/y''}\right) \times x_1^{n'_1+n''_1-n'''_1} \times x_2^{n'_2+n''_2-n'''_2} \times ... \quad (77)$$

which is an odd integer. Since both $\mathbf{S}_{x/y'}$ and $\mathbf{S}_{x/y''}$ are achiral, the coset representation $\mathbf{S}_{x/y'}(/\mathbf{S}_{x/y''})$ is determined to be homospheric. The degree of $\mathbf{S}_{x/y'}(/\mathbf{S}_{x/y''})$ is calculated to be

$$\frac{|\mathbf{S}_{x/y'}|}{|\mathbf{S}_{x/y''}|} = \frac{x/y'}{x/y''} = x_1^{n'''_1-n''_1} \times x_1^{n'''_2-n''_2} \times ... \quad (78)$$

which is an odd integer.

B.1.2. Homospheric Orbits and Chiral Subductions. The maximum chiral subgroup of the achiral cyclic group $\mathbf{S}_x$ (order x) is the group $\mathbf{C}_{x/2}$ of order $x/2$. Since the subgroup $\mathbf{S}_{x/y}$ is achiral, there exists its maximum chiral subgroup, i.e., $\mathbf{C}_{x/2y}$, which is a subgroup of $\mathbf{C}_{x/2}$. The following chiral subduction is easily obtained.

$$\mathbf{S}_x(/\mathbf{S}_{x/y}) \downarrow \mathbf{C}_{x/2} = \mathbf{C}_{x/2}(/\mathbf{C}_{x/2y}) \quad (79)$$

Note that the degrees of the participant coset representations satisfies

$$\frac{|\mathbf{S}_x|}{|\mathbf{S}_{x/y}|} = \frac{|\mathbf{C}_{x/2}|}{|\mathbf{C}_{x/2y}|} \quad (80)$$

By using the integer y' (eq 70), we consider a proper rotation $C_{x/2}^{y'} = \mathbf{C}_{x/2y'}$ that corresponds to the rotoflection $S_x^{y'} = S_{x/y'}$. The rotation $C_{x/2y'}$ generates a chiral group $\mathbf{C}_{x/2y'}$, which is the maximum chiral subgroup of $\mathbf{S}_{x/y'}$ ($=\langle S_{x/y'}\rangle$). From eq 79, we are able to obtain the following subduction:

$$\mathbf{S}_x(/\mathbf{S}_{x/y}) \downarrow \mathbf{C}_{x/2y'} = [\mathbf{S}_x(/\mathbf{S}_{x/y}) \downarrow \mathbf{C}_{x/2}] \downarrow \mathbf{C}_{x/2y'} = \mathbf{C}_{x/2}(/\mathbf{C}_{x/2y}) \downarrow \mathbf{C}_{x/2y'} \quad (81)$$

Thus, the chiral subduction of a homospheric coset representation, $\mathbf{S}_x(/S_{x/y}) \downarrow \mathbf{C}_{x/2y'}$, gives the same result as the chiral subduction concerning the corresponding maximum chiral subgroup, $\mathbf{C}_{x/2}(/\mathbf{C}_{x/2y}) \downarrow \mathbf{C}_{x/2y'}$.

B.1.3. Enantiospheric Orbits and Achiral Subductions. Suppose that we select an even divisor (z) of x to be

$$z = 2^{m'} \times x_1^{n'_1} \times x_2^{n'_2} \times ... \quad (82)$$

where $m \geq m' \geq 1$ and $n_i \geq n'_i \geq 0$ ($i = 1, 2, ...$). Then, the element S_x^z ($=C_{x/z}$) is a proper rotation, which generates a chiral cyclic group represented by

$$\mathbf{C}_{x/z} = \{S_x^z, S_x^{2z}, S_x^{3z}, ..., S_x^{(x/z)z} (=I)\} = \{C_{x/z}, C_{x/z}^2, C_{x/z}^2, ..., C_{x/z}^{x/z} (=I)\} \quad (83)$$

the order of which calculated to be

$$x/z = 2^{m-m'} \times x_1^{n_1-n'_1} \times x_2^{n_2-n'_2} \times ... \quad (84)$$

Note that x/z is an even integer if $m \geq m' \geq 1$ or an odd integer if $m = m'$. Since $\mathbf{S}_x$ is achiral and $\mathbf{C}_{x/z}$ is chiral, the coset representation $\mathbf{S}_x(/\mathbf{C}_{x/z})$ is enantiospheric. The degree of the coset representation is represented by

$$|\mathbf{S}_x|/|\mathbf{C}_{x/z}| = z = 2^{m'} \times x_1^{n'_1} \times x_2^{n'_2} \times ... \quad (85)$$

which is an even integer.

Let us now consider an achiral subduction of an enantiospheric orbit, which is represented by the symbol $\mathbf{S}_x(/\mathbf{C}_{x/z}) \downarrow \mathbf{S}_{x/y'}$, where y' is defined in eq 70. Theorem 2 of ref 35 is applied to this case, giving the following subduction:

$$\mathbf{S}_x(/\mathbf{C}_{x/z}) \downarrow \mathbf{S}_{x/y'} = \sum_g \mathbf{S}_{x/y'}(/g^{-1}\mathbf{C}_{x/z}g \cap \mathbf{S}_{x/y'}) \quad (86)$$

Since $\mathbf{C}_{x/z}$ is cyclic, we have $g^{-1}\mathbf{C}_{x/z}g = \mathbf{C}_{x/z}$. Then, we place

$$\mathbf{C}_{x/z} \cap \mathbf{S}_{x/y'} = \mathbf{C}_x^{z'} = \mathbf{C}_{x/z'} \quad (87)$$

where x/z' is the greatest common divisor of x/z and x/y'; i.e.,

$$x/z' = \gcd(x/z, x/y') = 2^{m-m'} \times x_1^{n_1-n'''_1} \times x_2^{n_2-n'''_2} \times ... \quad (88)$$

Thereby, the integer z' is calculated to be

$$z' = \frac{x}{x/z'} = 2^{m'} \times x_1^{n'''_1} \times x_2^{n'''_2} \times ... \quad (89)$$

which indicates that z' is an even integer. It follows that $S_x^{z'}(=C_{x/z'})$ is a proper rotation, which generates a chiral subgroup $\mathbf{C}_{x/z'}$. In a similar procedure for deriving eq 76, we have

$$\mathbf{S}_x(/\mathbf{C}_{x/z}) \downarrow \mathbf{S}_{x/y'} = \beta\mathbf{S}_{x/y'}(/\mathbf{C}_{x/z'} \cap \mathbf{S}_{x/y'}) = \beta\mathbf{S}_{x/y'}(/\mathbf{C}_{x/z'}) \quad (90)$$

where the multiplicity β is represented by

$$\beta = \left(\frac{x}{x/z}\right)/\left(\frac{x/y'}{x/z'}\right) \times x_1^{n'_1+n''_1-n'''_1} \times x_2^{n'_2+n''_2-n'''_2} \times ... \quad (91)$$

which is an odd integer. Since $\mathbf{S}_{x/y'}$ is achiral and $\mathbf{C}_{x/z'}$ is chiral, the coset representation $\mathbf{S}_{x/y'}(/\mathbf{C}_{x/z'})$ is enantiospheric. The degree of $\mathbf{S}_{x/y'}(/\mathbf{C}_{x/z'})$ is calculated to be

$$\frac{|\mathbf{S}_{x/y'}|}{|\mathbf{C}_{x/z'}|} = \frac{x/y'}{x/z'} = 2^{m'} \times x_1^{n'''_1-n''_1} \times x_2^{n'''_2-n''_2} \times ... \quad (92)$$

which is an even integer.

B.1.4. Enantiospheric Orbits and Chiral Subductions. Consider the enantiospheric coset representation $\mathbf{S}_x(/\mathbf{C}_{x/z})$, which is subduced into the maximum chiral subgroup $\mathbf{C}_{x/2}$:

$$\mathbf{S}_x(/\mathbf{C}_{x/z}) \downarrow \mathbf{C}_{x/2} = 2\mathbf{C}_{x/2}(/\mathbf{C}_{x/z}) \quad (93)$$

Note that the degrees of the participant coset representations satisfy

$$\frac{|\mathbf{S}_x|}{|\mathbf{S}_{x/y}|} = \frac{2|\mathbf{C}_{x/2}|}{|\mathbf{C}_{x/2y}|} \quad (94)$$

From eq 93, we are able to obtain the following subduction:

$$\mathbf{S}_x(/\mathbf{C}_{x/z}) \downarrow \mathbf{C}_{x/2y'} = [\mathbf{S}x(/\mathbf{C}_{x/z}) \downarrow \mathbf{C}_{x/2}] \downarrow \mathbf{C}_{x/2y'} = 2\mathbf{C}_{x/2}(/\mathbf{C}_{x/z}) \downarrow \mathbf{C}_{x/2y'} \quad (95)$$

This is twice the subduction represented by eq 81, if the group $\mathbf{C}_{x/z}$ in eq 95 is equalified to the group $\mathbf{C}_{x/2y}$ in eq 81.

APPENDIX C. ORBITS ACHIRAL CYCLIC GROUPS OF TYPE II

Let us now compare the cyclic group $\mathbf{C}_{xh}$ ($=\mathbf{S}_x$) with the cyclic group $\mathbf{S}_{2x}$, where x is odd. Since the generator S_x of the former corresponds to the generator S_{2x} of the latter, the element S_x^k corresponds to S_{2x}^k in one-to-one fashion. It follows that $\mathbf{C}_{xh}$ ($=\mathbf{S}_x$) is isomorphic to the cyclic group $\mathbf{S}_{2x}$, where x is odd. Moreover, each corresponding pair of elements has common proper/imporoper properties. Note that $S_x^x = \sigma_h$ and $S_{2x}^x = i$ and that $\mathbf{S}_{2x}$ (x: odd) is alternatively designated by the symbol $\mathbf{C}_{xi}$. Obviously, the maximum chiral subgroup $\mathbf{C}_x$ of $\mathbf{C}_{xh}$ is isomorphic to that of $\mathbf{C}_x$ of $\mathbf{C}_{xi}$ ($=\mathbf{S}_{2x}$). Hence, the discussions for cyclic groups of type I hold true for cyclic groups of type II. Thus, the subduction table and the related tables for $\mathbf{C}_{xh}$ (x: odd) are essentially equivalent to those for the cyclic groups $\mathbf{S}_{2x}$.

REFERENCES AND NOTES

(1) Pólya, G. Kombinatorische Anzahlbestimmungen für Gruppen, Graphen und chemische Verbindungen (Combinatorial Enumeration of Groups, Graphs, and Chemical Compounds). *Acta Math.* **1937**, *68*, 145−254.
(2) Redfield, J. H. The theory of group-reduced distributions. *Am. J. Math.* **1927**, *49*, 433−455.
(3) Rouvray, D. H. Isomer enumeration methods. *Chem. Soc. Rev.* **1974**, *3*, 355−372.
(4) Balaban, A. T. In *Chemical Group Theory. Introduction and Fundamentals*; Bonchev, D., Rouvray, D. H., Eds.; Gordon & Breach: Laussane, Switzerland, 1994; pp 159−208.
(5) Balaban, A. T., Ed. *Chemical Applications of Graph Theory*; Academic Press: London, 1976.
(6) Pólya, G.; Read, R. C. *Combinatorial Enumeration of Groups, Graphs, and Chemical Compounds*; Springer-Verlag: New York, 1987.
(7) Read, R. C. The enumeration of locally restricted graphs (i). *J. London Math. Soc.* **1959**, *34*, 417−436.
(8) Read, R. C. The enumeration of locally restricted graphs (ii). *J. London Math. Soc.* **1960**, *35*, 344−351.
(9) Read, R. C. The use of s-functions in combinatorial analysis. *Can. J. Math.* **1968**, *20*, 808−841.
(10) Foulkes, H. O. On Redfield's group reduction functions. *Can. J. Math.* **1963**, *15*, 272−284.
(11) Harary, F.; Palmer, E. The enumeration methods of Redfield. *Am. J. Math.* **1967**, *89*, 373−384.
(12) Davidson, R. A. Isomers and isomerization: Elements of Redfield's combinatorial theory. *J. Am. Chem. Soc.* **1981**, *103*, 312−314.
(13) Ruch, E.; Hässelbarth, W.; Richter, B. Doppelnebenklassen als Klassenbegriff und Nomenklaturprinzip für Isomere und ihre Abzählung. (Double Cosets as Class Concept and Nomenclature Principle for Isomers and their Enumeration). *Theor. Chim. Acta* **1970**, *19*, 288−300.
(14) Ruch, E.; Klein, D. J. Double cosets in chemistry and physics. *Theor. Chim. Acta* **1983**, *63*, 447−472.
(15) Hässelbarth, W. A note on Pólya enumeration theory. *Theor. Chim. Acta* **1984**, *66*, 91−110.
(16) Hässelbarth, W.; Ruch, E. *Isr. J. Chem.* **1977**, *15*, 112.
(17) Fujita, S. Subduction of coset representations. An application to enumeration of chemical structures. *Theor. Chim. Acta* **1989**, *76*, 247−268.

(18) Fujita, S. *Symmetry and Combinatorial Enumeration in Chemistry*; Springer-Verlag: Berlin−Heidelberg, 1991.
(19) Fujita, S. Enumeration of digraphs with a given automorphism group. *J. Math. Chem.* **1993**, *12*, 173−195.
(20) Fujita, S. Enumeration of chemical structures by subduction of coset representations. correlation of unit subduced cycle indices to Pólya's cycle indices. *J. Math. Chem.* **1990**, *5*, 99−120.
(21) Fujita, S. Subduction of coset representations. An application to enumeration of chemical structures with achiral and chiral ligands. *J. Math. Chem.* **1990**, *5*, 121−156.
(22) Fujita, S. Markaracter tables and **Q**-conjugacy character tables for cyclic subgroups. An application to combinatorial enumeration. *Bull. Chem. Soc. Jpn.* **1998**, *71*, 1587−1596.
(23) Fujita, S. Maturity of finite groups. An application to combinatorial enumeration of isomers. *Bull. Chem. Soc. Jpn.* **1998**, *71*, 2071−2080.
(24) Fujita, S. Inherent automorphism and **Q**-conjugacy character tables of finite groups. An application to combinatorial enumeration of isomers. *Bull. Chem. Soc. Jpn.* **1998**, *71*, 2309−2321.
(25) Fujita, S. Subduction of **Q**-conjugacy representations and characteristic monomials for combinatorial enumeration. *Theor. Chem. Acc*. **1998**, *99*, 224−230.
(26) Fujita, S. Direct subduction of **Q**-conjugacy representations to give characteristic monomials for combinatorial enumeration. *Theor. Chem. Acc.* **1998**, *99*, 404−410.
(27) Fujita, S. Characteristic monomial tables for enumeration of achiral and chiral isomers. *Bull. Chem. Soc. Jpn.* **1999**, *72*, 13−20.
(28) Fujita, S. Chirality fittingness of an orbit governed by a coset representation. Integration of point-group and permutation-group theories to treat local chirality and prochirality. *J. Am. Chem. Soc.* **1990**, *112*, 3390−3397.
(29) Fujita, S. Generalization of partial cycle indices and modified bisected mark tables for combinatorial enumeration. *Bull. Chem. Soc. Jpn.* **2000**, *73*, 329−339.
(30) Fujita, S. Möbius function and characteristic monomials for combinatorial enumeration. *Theor. Chem. Acc.* **1999**, *101*, 409−420.
(31) For the sake of simplicity, the symbol $\Gamma_{x/\tilde{x}}$ is used to designate a **Q**-conjugacy character as well as a **Q**-conjugacy representation, unless such usage gives confusion.
(32) Fujita, S. Promolecules for characterizing stereochemical relationships in nonrigid molecules. *Tetrahedron* **1991**, *47*, 31−46.
(33) The value listed at the intersection between the $ABp\bar{p}$-row and the $\mathbf{C}_s$-column of Table 21.3 (ref 18) should read “2”. The corresponding structural formulas have been correctly depicted as structures **53** and **54**.
(34) Although we assign a pair of symbols p (or q) and $\bar{p}$ (or $\bar{q}$) to a pair of enentiomeric ligands, the formulas (constitution) of such enantiomeric ligands are identical with each other. When we omit the discinction by an overline, we have, for example, $(1/2)(A^3p + A^3\bar{p}) = A^3p$.
(35) Fujita, S. Unit subduced cycle indices for combinatorial enumeration. *J. Graph Theory* **1994**, *18*, 349−371.

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