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Combinatorial Enumeration of Cubane Derivatives as Three-Dimensional Entities. III. Gross Enumeration by the Characteristic-Monomial Method

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Abstract

The CM (characteristic monomial) method developed by us (S. Fujita, *Theor. Chem. Acc.*, **99**, 224–230 (1998), S. Fujita, *J. Chem. Inf. Comput. Sci.*, **40**, 1101–1112 (2000)) is applied to enumeration of cubane derivatives with chiral and achiral proligands. For this purpose, CM-CFs (characteristic monomials with chirality fittingness) are calculated by emphasizing the interconvertivity between **Q**-conjugacy characters and markaracters. Thereby, a dominant CM-CF table is constructed so as to correspond to an irreducible **Q**-conjugacy character table in the present article (Part III of this series), just as a dominant USCI-CF (unit subduced-cycle index with chirality fittingness) table corresponds to a dominant markaracter table as discussed in Part II of this series. The present set of tables is used to prepare dominant and non-dominant USCI-CFs, which are in turn used to prepare SCI-CFs (subduced cycle indices with chirality fittingness) and CI-CFs (cycle indices with chirality fittingness). The CI-CFs of $\mathbf{O}_h$ and $\mathbf{O}$ for enumerating cubane derivatives as three-dimensional structural isomers and as steric isomers as well as for enumerating achiral and chiral cubane derivatives are clarified to be equivalent to those prepared by the proligand method (Part I of this series) as well as to those prepared by the markaracter method (Part II of this series). A Maple program source for calculating USCI-CFs from CM-CFs is given as an example of practical calculation.

1 Introduction

As discussed in Part II of this series reported in this journal, the concept of *marks* [1] has long been neglected in most textbooks on group theory, even on permutation groups [2–4], although the concept of marks is natural and more informative to discuss permutation representations, especially to discuss their applications to combinatorial enumeration. Instead, the concept of *characters* based on linear representations has been used to discuss permutation representations under excluding such applications to combinatorial enumeration. The USCI (unit subduced cycle index) approach developed by us [5] has casted a renewed light on the concept of marks, where the concepts of *subductions* of coset representations and unit subduced cycle indices (USCIs) have been introduced by starting from marks of coset representations as an essential set of permutation representations. These newly-developed concepts have been applied to combinatorial enumerations of chemical derivatives as three-dimensional (3D) objects after developing the concepts of *sphericities* and *chirality fittingness* [5]. The concept of *marks* has later been essentially qualified into the concept of *markaracters* [6], which, in turn, has been found to be a basis of dominant representations. After the related concepts to marks have been matched to markaracters, the qualified concepts have been applied to combinatorial enumerations [7] (cf. Part II of this series).

Because of easy manageability, the concept of characters has been a basis of linear representations as a predominant methodology in group theory and has worked as a main repertoire of most textbooks on group theory [8, 9], on chemical applications [10–13], on physical applications [14–17], and so on. However, the concept itself is short of capability to treat combinatorial enumeration as described in the preceding paragraph.

In order to cover this shortness, the CM (characteristic monomial) method developed by us has introduced the concept of *maturity* [18, 19] after clarifying the importance of **Q**-conjugacy representations and **Q**-conjugacy characters. Thereby, linear representations have been linked with coset representations so that the concept of *characteristic monomials* (CMs) and related concepts have been proposed to supply versatile tools for combinatorial enumeration [20–26]. The CM method has been extended to take account of *sphericities* and *chirality fittingness* to give CM-CFs (characteristic monomials with chirality fittingness), which are effective in combinatorial enumerations of chemical derivatives as 3D objects [27].

The purpose of the present series is to compare various methods of combinatorial enumeration, where we use the cubane skeleton of high symmetry ($\mathbf{O}_h$) as a common starting structure and we emphasize 3D structures of enumerated isomers as well as those of ligands to be substituted. In this paper, the CM method is applied to isomer enumerations of cubane derivatives, where both achiral and chiral ligands (more abstractly, proligands) are taken into consideration after introducing chirality fittingness. Thereby, the versatility of the CM method is emphasized even in the cubane skeleton of high symmetry ($\mathbf{O}_h$).

2 Characteristic Monomial Tables

2.1 Characteristic Monomial Table of $\mathbf{O}_h$

2.1.1 Via Multiplicity Vectors

According to the formulation reported by us [6, 18, 20], characters can be transformed into **Q**-conjugacy characters, where the concept of *maturity* works as a key concept [18]. Thereby, such (irreducible) character tables as collected in textbooks on group theory (e.g., [12]) can be converted into the corresponding **Q**-conjugacy markaracter tables by the procedure shown in [18, 20]. In particular, character tables for matured groups can be considered to be **Q**-conjugacy character tables as they are. Because the point group of $\mathbf{O}_h$ to be discussed mainly in the present article is matured, its character table (Table 1) itself is regarded as a **Q**-conjugacy character table, where each conjugacy class coressponds to each **Q**-conjugacy class.

Table 1: (**Q**-Conjugacy) Character Table of $\mathbf{O}_h$

$\widetilde{\mathrm{D}}_{\mathbf{O}_h}$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_2'$	$\mathbf{C}_s$	$\mathbf{C}_s'$	$\mathbf{C}_i$	$\mathbf{C}_3$	$\mathbf{C}_4$	$\mathbf{S}_4$	$\mathbf{C}_{3i}$
	I	$3C_2$	$6C_2$	$3\sigma_h$	$6\sigma_d$	i	$8C_3$	$6C_4$	$6S_4$	$8S_6$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	−1	1	−1	1	1	−1	−1	1
E_g	2	2	0	2	0	2	−1	0	0	−1
T_{1g}	3	−1	−1	−1	−1	3	0	1	1	0
T_{2g}	3	−1	1	−1	1	3	0	−1	−1	0
A_{1u}	1	1	1	−1	−1	−1	1	1	−1	−1
A_{2u}	1	1	−1	−1	1	−1	1	−1	1	−1
E_u	2	2	0	−2	0	−2	−1	0	0	1
T_{1u}	3	−1	−1	1	1	−3	0	1	−1	0
T_{2u}	3	−1	1	1	−1	−3	0	−1	1	0

Table 2: Markaracter Table of $\mathbf{O}_h$

$\widetilde{\mathrm{M}}_{\mathbf{O}_h}$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_2'$	$\mathbf{C}_s$	$\mathbf{C}_s'$	$\mathbf{C}_i$	$\mathbf{C}_3$	$\mathbf{C}_4$	$\mathbf{S}_4$	$\mathbf{C}_{3i}$
$\mathbf{O}_h(/\mathbf{C}_1)$	48	0	0	0	0	0	0	0	0	0
$\mathbf{O}_h(/\mathbf{C}_2)$	24	8	0	0	0	0	0	0	0	0
$\mathbf{O}_h(/\mathbf{C}_2')$	24	0	4	0	0	0	0	0	0	0
$\mathbf{O}_h(/\mathbf{C}_s)$	24	0	0	8	0	0	0	0	0	0
$\mathbf{O}_h(/\mathbf{C}_s')$	24	0	0	0	4	0	0	0	0	0
$\mathbf{O}_h(/\mathbf{C}_i)$	24	0	0	0	0	24	0	0	0	0
$\mathbf{O}_h(/\mathbf{C}_3)$	16	0	0	0	0	0	4	0	0	0
$\mathbf{O}_h(/\mathbf{C}_4)$	12	4	0	0	0	0	0	4	0	0
$\mathbf{O}_h(/\mathbf{S}_4)$	12	4	0	0	0	0	0	0	4	0
$\mathbf{O}_h(/\mathbf{C}_{3i})$	8	0	0	0	0	8	2	0	0	2

Each of the **Q**-conjugacy classes corresponds to a cyclic group, which is selected from a non-redundant set of cyclic subgroups (SCSG) according to [6], e.g.,

$$\mathrm{SCSG}_{\mathbf{O}_h} = \{\mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_2', \mathbf{C}_s, \mathbf{C}_s', \mathbf{C}_i, \mathbf{C}_3, \mathbf{C}_4, \mathbf{S}_4, \mathbf{C}_{3i}\} \tag{1}$$

for the point group $\mathbf{O}_h$. The respective cyclic subgroups correspond to the coset representations $\mathbf{O}_h(/\mathbf{G}_i)$ ($\mathbf{G}_i \in \mathrm{SCSG}_{\mathbf{O}_h}$), which are selected from the full set of coset representations for $\mathbf{O}_h(/\mathbf{G}_i)$ ($\mathbf{G}_i \in \mathrm{SSG}_{\mathbf{O}_h}$). The restricted set of coset representation, e.g., $\mathbf{O}_h(/\mathbf{G}_i)$ ($\mathbf{G}_i \in \mathrm{SCSG}_{\mathbf{O}_h}$), is called *dominant representations*, each of which is characterized by such a dominant markaracter as collected in a dominant markaracter table, e.g., Table 2.

The crux of the CM method is that **Q**-conjugacy characters can be regarded as markaracters [6]. This means that each row of of Table 1 can be regarded as a vector in a vector space spanned by the set of row vectors shown in the dominant markaracter table ($\widetilde{\mathrm{M}}_{\mathbf{O}_h}$ referred to shortly by the term *markaracter table*) shown in Table 2 (see Part II of this series). As a result, each row of of Table 1 is multiplied by the inverse markaracter table ($\widetilde{\mathrm{M}}_{\mathbf{O}_h}^{-1}$) to give a multiplicity vector shown in Table 3.

For example, the resulting multiplicity vector in the E_g-row of Table 3 means the following equation:

$$E_g = -\frac{1}{4}\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_1)} + \frac{1}{4}\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_2)} + \frac{1}{4}\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_s)} + \frac{1}{4}\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_i)} - \frac{1}{2}\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_{3i})}, \tag{2}$$

where $\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_1)}$ etc. denote the corresponding rows of Table 2. Thus, Eq. 2 is verified by the data of Table 2 as follows:

$$\begin{array}{rl}
-\frac{1}{4}\times & (48,0,0,0,0,\ 0,0,0,0,0) \\
+\frac{1}{4}\times & (24,8,0,0,0,\ 0,0,0,0,0) \\
+\frac{1}{4}\times & (24,0,0,8,0,\ 0,0,0,0,0) \\
+\frac{1}{4}\times & (24,0,0,0,0,24,0,0,0,0) \\
-\frac{1}{2}\times & (\ 8,0,0,0,0,\ 8,2,0,0,2) \\ \hline
\end{array}
\quad\Longrightarrow\quad
\begin{array}{rl}
& (-12,0,0,0,0,\ 0,\ 0,0,0,\ 0) \\
& (\ 6,2,0,0,0,\ 0,\ 0,0,0,\ 0) \\
& (\ 6,0,0,2,0,\ 0,\ 0,0,0,\ 0) \\
& (\ 6,0,0,0,0,\ 6,\ 0,0,0,\ 0) \\
& (\ -4,0,0,0,0,-4,-1,0,0,-1) \\ \hline
E_g = & (\ 2,2,0,2,0,\ 2,-1,0,0,-1)
\end{array} \tag{3}$$

Table 3: **Q**-Conjugacy Characters and Multiplicity Vectors for **Q**-Conjugacy Representations

	Q-conjugacy characters	$\times\widetilde{\mathrm{M}}_{\mathbf{O}_h}^{-1}$	multiplicity vectors
A_{1g}	$(1,1,1,1,1,1,1,1,1,1)$	$\Longrightarrow$	$(-\frac{3}{8},-\frac{1}{8},\frac{1}{4},\frac{1}{8},\frac{1}{4}-\frac{1}{8},0,\frac{1}{4},\frac{1}{4},\frac{1}{2})$
A_{2g}	$(1,1,-1,1,-1,1,1,-1,-1,1)$	$\Longrightarrow$	$(\frac{1}{8},\frac{3}{8},-\frac{1}{4},\frac{1}{8},-\frac{1}{4},-\frac{1}{8},0,-\frac{1}{4},-\frac{1}{4},\frac{1}{2})$
E_g	$(2,2,0,2,0,2,-1,0,0,-1)$	$\Longrightarrow$	$(-\frac{1}{4},\frac{1}{4},0,\frac{1}{4},0,\frac{1}{4},0,0,0,-\frac{1}{2})$
T_{1g}	$(3,-1,-1,-1,-1,3,0,1,1,0)$	$\Longrightarrow$	$(\frac{3}{8},-\frac{3}{8},-\frac{1}{4},-\frac{1}{8},-\frac{1}{4},\frac{1}{8},0,\frac{1}{4},\frac{1}{4},0)$
T_{2g}	$(3,-1,1,-1,1,3,0,-1,-1,0)$	$\Longrightarrow$	$(-\frac{1}{8},\frac{1}{8},\frac{1}{4},-\frac{1}{8},\frac{1}{4},\frac{1}{8},0,-\frac{1}{4},-\frac{1}{4},0)$
A_{1u}	$(1,1,1,-1,-1,-1,1,1,-1,-1)$	$\Longrightarrow$	$(-\frac{1}{8},\frac{1}{8},\frac{1}{4},-\frac{1}{8},-\frac{1}{4},\frac{1}{8},\frac{1}{2},\frac{1}{4},-\frac{1}{4},-\frac{1}{2})$
A_{2u}	$(1,1,-1,-1,1,-1,1,-1,1,-1)$	$\Longrightarrow$	$(-\frac{1}{8},\frac{1}{8},-\frac{1}{4},-\frac{1}{8},\frac{1}{4},\frac{1}{8},\frac{1}{2},-\frac{1}{4},\frac{1}{4},-\frac{1}{2})$
E_u	$(2,2,0,-2,0,-2,-1,0,0,1)$	$\Longrightarrow$	$(\frac{1}{4},\frac{1}{4},0,-\frac{1}{4},0,-\frac{1}{4},-\frac{1}{2},0,0,\frac{1}{2})$
T_{1u}	$(3,-1,-1,1,1,-3,0,1,-1,0)$	$\Longrightarrow$	$(\frac{1}{8},-\frac{1}{8},-\frac{1}{4},\frac{1}{8},\frac{1}{4},-\frac{1}{8},0,\frac{1}{4},-\frac{1}{4},0)$
T_{2u}	$(3,-1,1,1,-1,-3,0,-1,1,0)$	$\Longrightarrow$	$(\frac{1}{8},-\frac{1}{8},\frac{1}{4},\frac{1}{8},-\frac{1}{4},-\frac{1}{8},0,-\frac{1}{4},\frac{1}{4},0)$

The multiplicity vectors can be applied to a dominant USCI-CF table (cf. Table 3 of Part II for the $\mathbf{O}_h$ group). For example, the $\mathbf{S}_4$-column of the dominant USCI table of $\mathbf{O}_h$ contains c_4^{12} for the $\mathbf{O}_h(/\mathbf{C}_1)$-row, $c_2^4c_4^4$ for the $\mathbf{O}_h(/\mathbf{C}_2)$-row, c_4^6 for the $\mathbf{O}_h(/\mathbf{C}_s)$-row, c_4^6 for the $\mathbf{O}_h(/\mathbf{C}_i)$-row, and c_4^2 for the $\mathbf{O}_h(/\mathbf{C}_i)$-row, so that the resulting multiplicity vector in the E_g-row of Table 3 gives the following characteristic monomial with chirality fittingness (CM-CF) according to [27]:

$$\mathrm{Z}(E_g \downarrow \mathbf{S}_4; \$_d) = (c_4^{12})^{-1/4} \times (c_2^4c_4^4)^{1/4} \times (c_4^6)^{1/4} \times (c_4^6)^{1/4} \times (c_4^2)^{-1/2} = c_2, \qquad (4)$$

which corresponds to Eq. 2. This procedure is repeated to cover all of the multiplicity vectors collected in Table 3 and all of the columns in the dominant USCI table (Table 3 of Part II) so as to generate the CM-CF Table of $\mathbf{O}_h$ shown in Table 4. The CM-CF in Eq. 4 appears in the intersection of the E_g-row and the $\mathbf{S}_4$-column of Table 4. Note that Table 4 is obtained practically by using the Maple program listed in Appendix of Part II of this series, because respective rows of Table 1 (the left-hand side of Table 3) can be regarded as markaracters.

As shown in the top part of Table 4, the cyclic subgroups listed in $\mathrm{SCSG}_{\mathbf{O}_h}$ (Eq. 1) correspond to the **Q**-conjugacy classes, i.e., I; $3C_2$; $6C_2$; $3\sigma_h$; $6\sigma_d$; i; $8C_3$; $6C_4$; $6S_4$; and $8S_6$, where each coefficient indicates the number of elements contained in the **Q**-conjugacy class at issue. The bottom row shows the factor (N_j) of each **Q**-conjugacy class which is calculated by dividing the number of elements by 48 ($= |\mathbf{O}_h|$) [21, 27].

2.1.2 Via Direct Subductions

CM tables without chirality fittingness are alternatively constructed by means of direct subduction of **Q**-conjugacy representations [22]. The method of direct subduction has been extended to obtain the corresponding CM-CF Tables [27].

As an example, let us consider the subductions of **Q**-conjugacy characters (Table 1) into the cyclic subgroup $\mathbf{S}_4$. In a similar way to Example 2 of [27], a subduced **Q**-conjugacy character table is generated by selecting necessary columns ($\mathbf{C}_1$-, $\mathbf{C}_2$-, and $\mathbf{S}_4$-columns) from the **Q**-conjugacy character table (Table 1). The resulting matrix (the subduced **Q**-conjugacy character table) is multiplied by the inverse markaracter table of $\mathbf{S}_4$ ($\widetilde{\mathrm{M}}_{\mathbf{S}_4}^{-1}$) so as to give the following

Table 4: CM-CF Table of $\mathbf{O}_h$

	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}'_2$	$\mathbf{C}_s$	$\mathbf{C}'_s$	$\mathbf{C}_i$	$\mathbf{C}_3$	$\mathbf{C}_4$	$\mathbf{S}_4$	$\mathbf{C}_{3i}$
	I	$3C_2$	$6C_2$	$3\sigma_h$	$6\sigma_d$	i	$8C_3$	$6C_4$	$6S_4$	$8S_6$
A_{1g}	b_1	b_1	b_1	a_1	a_1	a_1	b_1	b_1	a_1	a_1
A_{2g}	b_1	b_1	$b_1^{-1}b_2$	a_1	$a_1^{-1}c_2$	a_1	b_1	$b_1^{-1}b_2$	$a_1^{-1}c_2$	a_1
E_g	b_1^2	b_1^2	b_2	a_1^2	c_2	a_1^2	$b_1^{-1}b_3$	b_2	c_2	$a_1^{-1}a_3$
T_{1g}	b_1^3	$b_1^{-1}b_2^2$	$b_1^{-1}b_2^2$	$a_1^{-1}c_2^2$	$a_1^{-1}c_2^2$	a_1^3	b_3	$b_1b_2^{-1}b_4$	$a_1c_2^{-1}c_4$	a_3
T_{2g}	b_1^3	$b_1^{-1}b_2^2$	b_1b_2	$a_1^{-1}c_2^2$	a_1c_2	a_1^3	b_3	$b_1^{-1}b_4$	$a_1^{-1}c_4$	a_3
A_{1u}	b_1	b_1	b_1	$a_1^{-1}c_2$	$a_1^{-1}c_2$	$a_1^{-1}c_2$	b_1	b_1	$a_1^{-1}c_2$	$a_1^{-1}c2$
A_{2u}	b_1	b_1	$b_1^{-1}b_2$	$a_1^{-1}c_2$	a_1	$a_1^{-1}c_2$	b_1	$b_1^{-1}b_2$	a_1	$a_1^{-1}c_2$
E_u	b_1^2	b_1^2	b_2	$a_1^{-2}c_2^2$	c_2	$a_1^{-2}c_2^2$	$b_1^{-1}b_3$	b_2	c_2	$a_1a_3^{-1}c_2^{-1}c_6$
T_{1u}	b_1^3	$b_1^{-1}b_2^2$	$b_1^{-1}b_2^2$	a_1c_2	a_1c_2	$a_1^{-3}c_2^3$	b_3	$b_1b_2^{-1}b_4$	$a_1^{-1}c_4$	$a_3^{-1}c_6$
T_{2u}	b_1^3	$b_1^{-1}b_2^2$	b_1b_2	a_1c_2	$a_1^{-1}c_2^2$	$a_1^{-3}c_2^3$	b_3	$b_1^{-1}b_4$	$a_1c_2^{-1}c_4$	$a_3^{-1}c_6$
N_j	$\frac{1}{48}$	$\frac{1}{16}$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{8}$	$\frac{1}{48}$	$\frac{1}{6}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{6}$

result:

$$\begin{array}{c} \\ A_{1g} \\ A_{2g} \\ E_g \\ T_{1g} \\ T_{2g} \\ A_{1u} \\ A_{2u} \\ E_u \\ T_{1u} \\ T_{2u} \end{array} \begin{array}{c} \begin{array}{ccc} \mathbf{C}_1 & \mathbf{C}_2 & \mathbf{S}_4 \end{array} \\ \left(\begin{array}{ccc} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & 2 & 0 \\ 3 & -1 & 1 \\ 3 & -1 & -1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \\ 2 & 2 & 0 \\ 3 & -1 & -1 \\ 3 & -1 & 1 \end{array}\right) \end{array} \underbrace{\begin{pmatrix} \frac{1}{4} & 0 & 0 \\ -\frac{1}{4} & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 1 \end{pmatrix}}_{\widetilde{\mathrm{M}}_{\mathbf{S}_4}^{-1}} = \begin{array}{c} \\ A_{1g} \downarrow \mathbf{S}_4 \\ A_{2g} \downarrow \mathbf{S}_4 \\ E_g \downarrow \mathbf{S}_4 \\ T_{1g} \downarrow \mathbf{S}_4 \\ T_{2g} \downarrow \mathbf{S}_4 \\ A_{1u} \downarrow \mathbf{S}_4 \\ A_{2u} \downarrow \mathbf{S}_4 \\ E_u \downarrow \mathbf{S}_4 \\ T_{1u} \downarrow \mathbf{S}_4 \\ T_{2u} \downarrow \mathbf{S}_4 \end{array} \begin{array}{c} \begin{array}{ccc} \mathbf{C}_1 & \mathbf{C}_2 & \mathbf{S}_4 \end{array} \\ \left(\begin{array}{ccc} 0 & 0 & 1 \\ 0 & 1 & -1 \\ 0 & 1 & 0 \\ 1 & -1 & 1 \\ 1 & 0 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & -1 \\ 1 & -1 & 1 \end{array}\right) \end{array} \begin{array}{c} \\ a_1 \\ a_1^{-1}c_2 \\ c_2 \\ a_1c_2^{-1}c_4 \\ a_1^{-1}c_4 \\ a_1^{-1}c_2 \\ a_1 \\ c_2 \\ a_1^{-1}c_4 \\ a_1c_2^{-1}c_4 \end{array} \tag{5}$$

where the first matrix in the left-hand side is the subduced $\mathbf{Q}$-conjugacy character table at issue (regarded as a kind of subduced markaracter table), the second one is $\widetilde{\mathrm{M}}_{\mathbf{S}_4}^{-1}$, and the matrix in the right-hand side is the subduction-multiplicity matrix at issue.

The subduction-multiplicity matrix (the right-hand side of Eq. 5) contains the multiplicities for the respective subductions. For example, the $T_{1g} \downarrow \mathbf{S}_4$-row indicates

$$T_{1g} \downarrow \mathbf{S}_4 = \mathbf{S}_4(/\mathbf{C}_1) - \mathbf{S}_4(/\mathbf{C}_2) + \mathbf{S}_4(/\mathbf{S}_4). \tag{6}$$

Equation 6 generates a USCI-CF $a_1c_2^{-1}c_4$ because the subscripts are calculated by using such relationships as $|\mathbf{S}_4|/|\mathbf{C}_1| = 4/1 = 4$, $|\mathbf{S}_4|/|\mathbf{C}_2| = 4/4 = 2$, and $|\mathbf{S}_4|/|\mathbf{S}_4| = 4/4 = 1$, where the coefficients appearing in the right-hand side are used as the powers of the respective components of the USCI-CF. Note that $\mathbf{S}_4(/\mathbf{C}_1)$, $\mathbf{S}_4(/\mathbf{C}_2)$, and $\mathbf{S}_4(/\mathbf{S}_4)$ are respectively characterized by the sphericity indices c_4, c_2, and a_1, because the $\mathbf{S}_4(/\mathbf{C}_1)$ and the $\mathbf{S}_4(/\mathbf{C}_2)$ are enantiospheric and because the $\mathbf{S}_4(/\mathbf{S}_4)$ is homospheric in accord with the USCI approach [5]. This is symbolically denoted as follows:

$$\mathrm{Z}(T_{1g} \downarrow \mathbf{S}_4; \$_d) = a_1c_2^{-1}c_4, \tag{7}$$

which appears at the intersection of the T_{1g}-row and the $\mathbf{S}_4$-column in Table 4, where the symbol $\$_d$ represents a set of a_d, b_d, and c_d. On similar lines, the other subductions are characterized by CM-CFs collected in the rightmost part of Eq. 5. The CM-CFs of Eq. 5 appear in the $\mathbf{S}_4$-column of Table 4.

2.2 Characteristic Monomial Table of O

Because the point group of $\mathbf{O}$, which is the maximum chiral subgroup of $\mathbf{O}_h$, is matured, its character table (Table 5) is regarded as a $\mathbf{Q}$-conjugacy character table.

Table 5: ($\mathbf{Q}$-Conjugacy) Character Table of $\mathbf{O}$

$\widetilde{\mathrm{D}}_{\mathbf{O}}$	$\mathbf{C}_1$ I	$\mathbf{C}_2$ $3C_2$	$\mathbf{C}'_2$ $6C_2$	$\mathbf{C}_3$ $8C_3$	$\mathbf{C}_4$ $6C_4$
A_1	1	1	1	1	1
A_2	1	1	-1	1	-1
E	2	2	0	-1	0
T_1	3	-1	-1	0	1
T_2	3	-1	1	0	-1

Table 6: Markaracter Table of $\mathbf{O}_h$

$\widetilde{\mathrm{M}}_{\mathbf{O}}$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}'_2$	$\mathbf{C}_3$	$\mathbf{C}_4$
$\mathbf{O}(/\mathbf{C}_1)$	24	0	0	0	0
$\mathbf{O}(/\mathbf{C}_2)$	12	4	0	0	0
$\mathbf{O}(/\mathbf{C}'_2)$	12	0	2	0	0
$\mathbf{O}(/\mathbf{C}_3)$	8	0	0	2	0
$\mathbf{O}(/\mathbf{C}_4)$	6	2	0	0	2

Each row of of Table 5 is regarded as a vector in a vector space spanned by the set of row vectors shown in the (dominant) markaracter table ($\widetilde{\mathrm{M}}_{\mathbf{O}}$) shown in Table 6 (cf. Part II of this series). As a result, each row of of Table 5 is multiplied by the inverse markaracter table ($\widetilde{\mathrm{M}}_{\mathbf{O}}^{-1}$) to give a multiplicity vector, which is used to calculate the corresponding CM-CF in a similar way to the case of $\mathbf{O}_h$. The results are collected in Table 7.

Table 7: CM-CF Table of $\mathbf{O}$

	$\mathbf{C}_1$ I	$\mathbf{C}_2$ $3C_2$	$\mathbf{C}'_2$ $6C_2$	$\mathbf{C}_3$ $8C_3$	$\mathbf{C}_4$ $6C_4$
A_1	b_1	b_1	b_1	b_1	b_1
A_2	b_1	b_1	$b_1^{-1}b_2$	b_1	$b_1^{-1}b_2$
E	b_1^2	b_1^2	b_2	$b_1^{-1}b_3$	b_2
T_1	b_1^3	$b_1^{-1}b_2^2$	$b_1b_2^2$	b_3	$b_1b_2^{-1}b_4$
T_2	b_1^3	$b_1^{-1}b_2^2$	b_1b_2	b_3	$b_1^{-1}b_4$
N_j	$\frac{1}{24}$	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{4}$

3 Characteristic-Monomial Method for Enumeration

3.1 Markaracters as Q-Conjugacy Characters

3.1.1 Dominant Markaracters as Q-Conjugacy Characters

In the preceding section, an irreducible **Q**-conjugacy character (e.g., each row of Table 1 for the point group $\mathbf{Q}_h$) is regarded as a vector in the vector space spanned by a set of dominant markaracters (e.g., the set of row vectors shown in Table 2), where the corresponding multiplicity vectors are collected in Table 3.

From an inverse point of view, a dominant markaracter (in this example, each row of Table 2) can be regarded as a vector in the vector space spanned by a set of irreducible **Q**-conjugacy characters (in this example, the set of row vectors shown in Table 1). For example, the $\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_1)}$-row of Table 2 corresponds to the following multiplicity vector:

$$\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_1)}\mathrm{D}_{\mathbf{O}_h}^{-1} = (48,0,0,0,0,0,0,0,0,0)\mathrm{D}_{\mathbf{O}_h}^{-1} = (1,1,2,3,3,1,1,2,3,3), \tag{8}$$

where the symbol $\mathrm{D}_{\mathbf{O}_h}^{-1}$ denotes the inverse of Table 1 (denoted by the symbol $\mathrm{D}_{\mathbf{O}_h}$). The concrete form of $\mathrm{D}_{\mathbf{O}_h}^{-1}$ is shown in Table 8. Because the coset representation $\mathbf{O}_h(/\mathbf{C}_1)$ represents the regular representation of $\mathbf{O}_h$, the multiplicity vector shown in the right-hand side of Eq. 8 is consistent with a well-known theorem which claims that each irreducible representation of degree n is contained n-times in the regular representation, i.e.,

$$\mathbf{O}_h(/\mathbf{C}_1) = A_{1g} + A_{2g} + 2E_g + 3T_{1g} + 3T_{2g} + A_{1u} + A_{2u} + 2E_u + 3T_{1u} + 3T_{2u}. \tag{9}$$

This equation shows that A_{1g} (or A_{2g}, or A_{1u}, or A_{2u}) of degree 1 appears once, E_g (or E_u) of degree 2 appears twice, and T_{1g} (or T_{2g}, or T_{1u}, or T_{2u}) of degree 3 appears three times.

Table 8: Inverse **Q**-Conjugacy Character Table of $\mathbf{O}_h$

$\mathrm{D}_{\mathbf{O}_h}^{-1}$		A_{1g}	A_{2g}	E_g	T_{1g}	T_{2g}	A_{1u}	A_{2u}	E_u	T_{1u}	T_{2u}
$\mathbf{C}_1$	I	$\frac{1}{48}$	$\frac{1}{48}$	$\frac{1}{24}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{48}$	$\frac{1}{48}$	$\frac{1}{24}$	$\frac{1}{16}$	$\frac{1}{16}$
$\mathbf{C}_2$	$3C_2$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{8}$	$-\frac{1}{16}$	$-\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{8}$	$-\frac{1}{16}$	$-\frac{1}{16}$
$\mathbf{C}_2'$	$6C_2$	$\frac{1}{8}$	$-\frac{1}{8}$	0	$-\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$-\frac{1}{8}$	0	$-\frac{1}{8}$	$\frac{1}{8}$
$\mathbf{C}_s$	$3\sigma_h$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{8}$	$-\frac{1}{16}$	$-\frac{1}{16}$	$-\frac{1}{16}$	$-\frac{1}{16}$	$-\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{16}$
$\mathbf{C}_s'$	$6\sigma_d$	$\frac{1}{8}$	$-\frac{1}{8}$	0	$-\frac{1}{8}$	$\frac{1}{8}$	$-\frac{1}{8}$	$\frac{1}{8}$	0	$\frac{1}{8}$	$-\frac{1}{8}$
$\mathbf{C}_i$	i	$\frac{1}{48}$	$\frac{1}{48}$	$\frac{1}{24}$	$\frac{1}{16}$	$\frac{1}{16}$	$-\frac{1}{48}$	$-\frac{1}{48}$	$-\frac{1}{24}$	$-\frac{1}{16}$	$-\frac{1}{16}$
$\mathbf{C}_3$	$8C_3$	$\frac{1}{6}$	$\frac{1}{6}$	$-\frac{1}{6}$	0	0	$\frac{1}{6}$	$\frac{1}{6}$	$-\frac{1}{6}$	0	0
$\mathbf{C}_4$	$6C_4$	$\frac{1}{8}$	$-\frac{1}{8}$	0	$\frac{1}{8}$	$-\frac{1}{8}$	$\frac{1}{8}$	$-\frac{1}{8}$	0	$\frac{1}{8}$	$-\frac{1}{8}$
$\mathbf{S}_4$	$6S_4$	$\frac{1}{8}$	$-\frac{1}{8}$	0	$\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$\frac{1}{8}$	0	$-\frac{1}{8}$	$\frac{1}{8}$
$\mathbf{C}_{3i}$	$8S_6$	$\frac{1}{6}$	$\frac{1}{6}$	$-\frac{1}{6}$	0	0	$-\frac{1}{6}$	$-\frac{1}{6}$	$\frac{1}{6}$	0	0

The procedure exemplified by Eq. 8 is repeated to cover the respective rows of Table 2 so as to give the corresponding multiplicity vectors shown in Table 9. For the purpose of practical calculation, Table 2 ($\widetilde{\mathrm{M}}_{\mathbf{O}_h}$) is regarded as a matrix and multiplied by the inverse (Table 8, $\mathrm{D}_{\mathbf{O}_h}^{-1}$), i.e.,

$$\widetilde{\mathrm{M}}_{\mathbf{O}_h}\mathrm{D}_{\mathbf{O}_h}^{-1}. \tag{10}$$

The resulting matrix is the same as the right-hand side of Table 9. The calculation of Eq. 10 is conducted by the Maple system, where the following Maple program (the file name "CM01.mpl") is read from the Maple display window:

```
#CM01.mpl
#Q-conjugacy multiplicity of dominant representations
#read "c:/fujita0/CM01.mpl";

with(linalg);

DOh := matrix(10,10,
[[1,1,1,1,1,1,1,1,1,1],
[1,1,-1,1,-1,1,1,-1,-1,1],
[2,2,0,2,0,2,-1,0,0,-1],
[3,-1,-1,-1,-1,3,0,1,1,0],
[3,-1,1,-1,1,3,0,-1,-1,0],
[1,1,1,-1,-1,-1,1,1,-1,-1],
[1,1,-1,-1,1,-1,1,-1,1,-1],
[2,2,0,-2,0,-2,-1,0,0,1],
[3,-1,-1,1,1,-3,0,1,-1,0],
[3,-1,1,1,-1,-3,0,-1,1,0]]);

InvDOh := inverse(DOh);

MOh := matrix(10,10,
[[48,0,0,0,0,0,0,0,0,0],
[24,8,0,0,0,0,0,0,0,0],
[24,0,4,0,0,0,0,0,0,0],
[24,0,0,8,0,0,0,0,0,0],
[24,0,0,0,4,0,0,0,0,0],
[24,0,0,0,0,24,0,0,0,0],
[16,0,0,0,0,0,4,0,0,0],
[12,4,0,0,0,0,0,4,0,0],
[12,4,0,0,0,0,0,0,4,0],
[8,0,0,0,0,8,2,0,0,2]]);

MultiDomi:=evalm(MOh &* InvDOh);
```

As for the point group **O**, the inverse point of view is also effective. Thus, a dominant markaracter (each row of Table 6) can be regarded as a vector in the vector space spanned by a set of irreducible **Q**-conjugacy characters (the set of row vectors shown in Table 5). In a similar way to $\mathbf{O}_h$, the inverse $\mathrm{D}_{\mathbf{O}}^{-1}$ for the **O** group (Table 10) is used to calculate multiplicity vectors collected in Table 11. Note that the coset representation $\mathbf{O}(/\mathbf{C}_1)$ as the regular representation is characterized by the multiplicity vector calculated as follows:

$$\widetilde{\mathrm{M}}_{\mathbf{O}(/\mathbf{C}_1)}\mathrm{D}_{\mathbf{O}}^{-1} = (24,0,0,0,0)\mathrm{D}_{\mathbf{O}}^{-1} = (1,1,2,3,3), \tag{11}$$

which corresponds to the following reduction:

$$\mathbf{O}(/\mathbf{C}_1) = A_1 + A_2 + 2E + 3T_1 + 3T_2, \tag{12}$$

where each irreducible representation of degree n is contained n-times in the regular representation. Thus, A_1 (or A_2) of degree 1 appears once, E of degree 2 appears twice, and T_1 (or T_2) of degree 3 appears three times.

Table 9: Markaracters and Multiplicity Vectors for Dominant Representations ($\mathbf{O}_h$)

Markaracters		$\times D^{-1}_{\mathbf{O}_h}$	multiplicity vectors
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}_1)}$	$= (48,0,0,0,0,0,0,0,0,0)$	$\Longrightarrow$	$(1,1,2,3,3,1,1,2,3,3)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}_2)}$	$= (24,8,0,0,0,0,0,0,0,0)$	$\Longrightarrow$	$(1,1,2,1,1,1,1,2,1,1)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}'_2)}$	$= (24,0,4,0,0,0,0,0,0,0)$	$\Longrightarrow$	$(1,0,1,1,2,1,0,1,1,2)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}_s)}$	$= (24,0,0,8,0,0,0,0,0,0)$	$\Longrightarrow$	$(1,1,2,1,1,0,0,0,2,2)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}'_s)}$	$= (24,0,0,0,4,0,0,0,0,0)$	$\Longrightarrow$	$(1,0,1,1,2,0,1,1,2,1)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}_i)}$	$= (24,0,0,0,0,24,0,0,0,0)$	$\Longrightarrow$	$(1,1,2,3,3,0,0,0,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}_3)}$	$= (16,0,0,0,0,0,4,0,0,0)$	$\Longrightarrow$	$(1,1,0,1,1,1,1,0,1,1)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}_4)}$	$= (12,4,0,0,0,0,0,4,0,0)$	$\Longrightarrow$	$(1,0,1,1,0,1,0,1,1,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{S}_4)}$	$= (12,4,0,0,0,0,0,0,4,0)$	$\Longrightarrow$	$(1,0,1,1,0,0,1,1,0,1)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}_{3i})}$	$= (8,0,0,0,0,8,2,0,0,2)$	$\Longrightarrow$	$(1,1,0,1,1,0,0,0,0,0)$

Table 10: Inverse **Q**-Conjugacy Character Table of **O**

$D^{-1}_{\mathbf{O}}$		A_1	A_2	E	T_1	T_2
$\mathbf{C}_1$	I	$\frac{1}{24}$	$\frac{1}{24}$	$\frac{1}{12}$	$\frac{1}{8}$	$\frac{1}{8}$
$\mathbf{C}_2$	$3C_2$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{4}$	$-\frac{1}{8}$	$-\frac{1}{8}$
$\mathbf{C}'_2$	$6C_2$	$\frac{1}{4}$	$-\frac{1}{4}$	0	$-\frac{1}{4}$	$\frac{1}{4}$
$\mathbf{C}_3$	$8C_3$	$\frac{1}{3}$	$\frac{1}{3}$	$-\frac{1}{3}$	0	0
$\mathbf{C}_4$	$6C_4$	$\frac{1}{4}$	$-\frac{1}{4}$	0	$\frac{1}{4}$	$-\frac{1}{4}$

Table 11: Markaracters and Multiplicity Vectors for Dominant Representations (**O**)

Markaracters		$\times D^{-1}_{\mathbf{O}}$	multiplicity vectors
$\widetilde{M}_{\mathbf{O}(/\mathbf{C}_1)}$	$= (24,0,0,0,0)$	$\Longrightarrow$	$(1,1,2,3,3)$
$\widetilde{M}_{\mathbf{O}(/\mathbf{C}_2)}$	$= (12,4,0,0,0)$	$\Longrightarrow$	$(1,1,2,1,1)$
$\widetilde{M}_{\mathbf{O}(/\mathbf{C}'_2)}$	$= (12,0,2,0,0)$	$\Longrightarrow$	$(1,0,1,1,2)$
$\widetilde{M}_{\mathbf{O}(/\mathbf{C}_3)}$	$= (8,0,0,2,0)$	$\Longrightarrow$	$(1,1,0,1,1)$
$\widetilde{M}_{\mathbf{O}(/\mathbf{C}_4)}$	$= (6,2,0,0,2)$	$\Longrightarrow$	$(1,0,1,1,0)$

As found in Table 11, the coset representation $\mathbf{O}(/\mathbf{C}_3)$ as a dominant representation is characterized by the markaracter ($\widetilde{\mathrm{M}}_{\mathbf{O}(/\mathbf{C}_3)}$), which generates a multiplicity vector as follows:

$$\widetilde{\mathrm{M}}_{\mathbf{O}(/\mathbf{C}_3)}\mathrm{D}_{\mathbf{O}}^{-1} = (8,0,0,2,0)\mathrm{D}_{\mathbf{O}}^{-1} = (1,1,0,1,1). \tag{13}$$

The resulting multiplicity vector corresponds to the following reduction:

$$\mathbf{O}(/\mathbf{C}_3) = A_1 + A_2 + T_1 + T_2. \tag{14}$$

3.1.2 Non-Dominant Markaracters as Q-Conjugacy Characters

After the inverse viewpoint is adopted, non-dominant markaracters (cf. Part II of this series) can be treated on the same line as the dominant markaracters described above. For example, the coset representation $\mathbf{O}_h(/\mathbf{C}_{3v})$ as a non-dominant representation is characterized by the markaracter ($\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_{3v})}$), which generates a multiplicity vector as follows:

$$\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_{3v})}\mathrm{D}_{\mathbf{O}_h}^{-1} = (8,0,0,0,4,0,2,0,0,0)\mathrm{D}_{\mathbf{O}_h}^{-1} = (1,0,0,0,1,0,1,0,1,0). \tag{15}$$

The resulting multiplicity vector corresponds to the following reduction:

$$\mathbf{O}_h(/\mathbf{C}_{3v}) = A_{1g} + T_{2g} + A_{2u} + T_{1u}. \tag{16}$$

In a similar way, other non-dominant representations are assigned to multiplicity vectors collected in Table 12.

Non-dominant markaracters for the point group $\mathbf{O}$ (cf. Part II of this series) are also treated on the same line as the cases of $\mathbf{O}_h$. The resulting multiplicity vectors are collected in Table 13.

3.2 USCI-CFs Calculated From CM-CF Tables

3.2.1 Dominant USCI-CFs from CM-CFs

The multiplicity vector shown in the $\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_3)}$-row of Table 9 corresponds to the following reduction:

$$\mathbf{O}_h(/\mathbf{C}_3) = A_{1g} + A_{2g} + T_{1g} + T_{2g} + A_{1u} + A_{2u} + T_{1u} + T_{2u}. \tag{17}$$

Let us consider the subduction of the dominant representation $\mathbf{O}_h(/\mathbf{C}_3)$ into a subgroup $\mathbf{S}_4$. Then, we obtain:

$$\begin{aligned}\mathbf{O}_h(/\mathbf{C}_3)\downarrow\mathbf{S}_4 \;=\;& A_{1g}\downarrow\mathbf{S}_4 + A_{2g}\downarrow\mathbf{S}_4 + T_{1g}\downarrow\mathbf{S}_4 + T_{2g}\downarrow\mathbf{S}_4\\ &+ A_{1u}\downarrow\mathbf{S}_4 + A_{2u}\downarrow\mathbf{S}_4 + T_{1u}\downarrow\mathbf{S}_4 + T_{2u}\downarrow\mathbf{S}_4.\end{aligned} \tag{18}$$

By referring to the data collected in the $\mathbf{S}_4$-column of the CM-CF table of $\mathbf{O}_h$ (Table 4), the USCI-CF corresponding to $\mathbf{O}_h(/\mathbf{C}_3)\downarrow\mathbf{S}_4$ is calculated as follows:

$$\begin{aligned}&\mathrm{Z}(\mathbf{O}_h(/\mathbf{C}_3)\downarrow\mathbf{S}_4;\$_d)\\ &= \mathrm{Z}(\mathbf{O}_h(A_{1g}\downarrow\mathbf{S}_4;\$_d)\mathrm{Z}(\mathbf{O}_h(A_{2g}\downarrow\mathbf{S}_4;\$_d)\mathrm{Z}(\mathbf{O}_h(T_{1g}\downarrow\mathbf{S}_4;\$_d)\mathrm{Z}(\mathbf{O}_h(T_{2g}\downarrow\mathbf{S}_4;\$_d)\\ &\quad\times\mathrm{Z}(\mathbf{O}_h(A_{1u}\downarrow\mathbf{S}_4;\$_d)\mathrm{Z}(\mathbf{O}_h(A_{2u}\downarrow\mathbf{S}_4;\$_d)\mathrm{Z}(\mathbf{O}_h(T_{1u}\downarrow\mathbf{S}_4;\$_d)\mathrm{Z}(\mathbf{O}_h(T_{2u}\downarrow\mathbf{S}_4;\$_d)\\ &= (a_1)(a_1^{-1}c_2)(a_1c_2^{-1}c_4)(a_1^{-1}c_4)(a_1^{-1}c_2)(a_1)(a_1^{-1}c_4)(a_1c_2^{-1}c_4) = c_4^4.\end{aligned} \tag{19}$$

Table 12: Markaracters and Multiplicity Vectors for Non-Dominant Representations ($\mathbf{O}_h$)

markaracter		$\times D_{\mathbf{O}_h}^{-1}$	multiplicity vectors
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{D}_2)}$	$= (12,12,0,0,0,0,0,0,0,0)$	$\Longrightarrow$	$(1,1,2,0,0,1,1,2,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{D}'_2)}$	$= (12,4,4,0,0,0,0,0,0,0)$	$\Longrightarrow$	$(1,0,1,0,1,1,0,1,0,1)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}_{2v})}$	$= (12,4,0,8,0,0,0,0,0,0)$	$\Longrightarrow$	$(1,1,2,0,0,0,0,0,1,1)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}'_{2v})}$	$= (12,4,0,0,4,0,0,0,0,0)$	$\Longrightarrow$	$(1,0,1,0,1,0,1,1,1,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}''_{2v})}$	$= (12,0,2,4,2,0,0,0,0,0)$	$\Longrightarrow$	$(1,0,1,0,1,0,0,0,1,1)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}_{2h})}$	$= (12,4,0,4,0,12,0,0,0,0)$	$\Longrightarrow$	$(1,1,2,1,1,0,0,0,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}'_{2h})}$	$= (12,0,2,0,2,12,0,0,0,0)$	$\Longrightarrow$	$(1,0,1,1,2,0,0,0,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{D}_3)}$	$= (8,0,4,0,0,0,2,0,0,0)$	$\Longrightarrow$	$(1,0,0,0,1,1,0,0,0,1)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}_{3v})}$	$= (8,0,0,0,4,0,2,0,0,0)$	$\Longrightarrow$	$(1,0,0,0,1,0,1,0,1,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{D}_4)}$	$= (6,6,2,0,0,0,0,2,0,0)$	$\Longrightarrow$	$(1,0,1,0,0,1,0,1,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}_{4v})}$	$= (6,2,0,4,2,0,0,2,0,0)$	$\Longrightarrow$	$(1,0,1,0,0,0,0,0,1,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{C}_{4h})}$	$= (6,2,0,2,0,6,0,2,2,0)$	$\Longrightarrow$	$(1,0,1,1,0,0,0,0,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{D}_{2d})}$	$= (6,6,0,0,2,0,0,0,2,0)$	$\Longrightarrow$	$(1,0,1,0,0,0,1,1,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{D}'_{2d})}$	$= (6,2,2,4,0,0,0,0,2,0)$	$\Longrightarrow$	$(1,0,1,0,0,0,0,0,0,1)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{D}_{2h})}$	$= (6,6,0,6,0,6,0,0,0,0)$	$\Longrightarrow$	$(1,1,2,0,0,0,0,0,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{D}'_{2h})}$	$= (6,2,2,2,2,6,0,0,0,0)$	$\Longrightarrow$	$(1,0,1,0,1,0,0,0,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{T})}$	$= (4,4,0,0,0,0,4,0,0,0)$	$\Longrightarrow$	$(1,1,0,0,0,1,1,0,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{D}_{3d})}$	$= (4,0,2,0,2,4,1,0,0,1)$	$\Longrightarrow$	$(1,0,0,0,1,0,0,0,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{D}_{4h})}$	$= (3,3,1,3,1,3,0,1,1,0)$	$\Longrightarrow$	$(1,0,1,0,0,0,0,0,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{O})}$	$= (2,2,2,0,0,0,2,2,0,0)$	$\Longrightarrow$	$(1,0,0,0,0,1,0,0,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{T}_h)}$	$= (2,2,0,2,0,2,2,0,0,2)$	$\Longrightarrow$	$(1,1,0,0,0,0,0,0,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{T}_d)}$	$= (2,2,0,0,2,0,2,0,2,0)$	$\Longrightarrow$	$(1,0,0,0,0,0,1,0,0,0)$
$\widetilde{M}_{\mathbf{O}_h(/\mathbf{O}_h)}$	$= (1,1,1,1,1,1,1,1,1,1)$	$\Longrightarrow$	$(1,0,0,0,0,0,0,0,0,0)$

Table 13: Markaracters and Multiplicity Vectors for Non-Dominant Representations ($\mathbf{O}$)

markaracter		$\times D_{\mathbf{O}}^{-1}$	multiplicity vectors
$\widetilde{M}_{\mathbf{O}(/\mathbf{D}_2)}$	$= (6,6,0,0,0)$	$\Longrightarrow$	$(1,1,2,0,0)$
$\widetilde{M}_{\mathbf{O}(/\mathbf{D}'_2)}$	$= (6,2,2,0,0)$	$\Longrightarrow$	$(1,0,1,0,1)$
$\widetilde{M}_{\mathbf{O}(/\mathbf{D}_3)}$	$= (4,0,2,1,0)$	$\Longrightarrow$	$(1,0,0,0,1)$
$\widetilde{M}_{\mathbf{O}(/\mathbf{D}_4)}$	$= (3,3,1,0,1)$	$\Longrightarrow$	$(1,0,1,0,0)$
$\widetilde{M}_{\mathbf{O}(/\mathbf{T})}$	$= (2,2,0,2,0)$	$\Longrightarrow$	$(1,1,0,0,0)$
$\widetilde{M}_{\mathbf{O}(/\mathbf{O})}$	$= (1,1,1,1,1)$	$\Longrightarrow$	$(1,0,0,0,0)$

Table 14: Dominant USCI-CF Table of $\mathbf{O}_h$

	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}'_2$	$\mathbf{C}_s$	$\mathbf{C}'_s$	$\mathbf{C}_i$	$\mathbf{C}_3$	$\mathbf{C}_4$	$\mathbf{S}_4$	$\mathbf{C}_{3i}$
	I	$3C_2$	$6C_2$	$3\sigma_h$	$6\sigma_d$	i	$8C_3$	$6C_4$	$6S_4$	$8S_6$
$\mathbf{O}_h(/\mathbf{C}_1)$	b_1^{48}	b_2^{24}	b_2^{24}	c_2^{24}	c_2^{24}	c_2^{24}	b_3^{16}	b_4^{12}	c_4^{12}	c_6^{8}
$\mathbf{O}_h(/\mathbf{C}_2)$	b_1^{24}	$b_1^{8}b_2^{8}$	b_2^{12}	c_2^{12}	c_2^{12}	c_2^{12}	b_3^{8}	$b_2^{4}b_4^{4}$	$c_2^{4}c_4^{4}$	c_6^{4}
$\mathbf{O}_h(/\mathbf{C}'_2)$	b_1^{24}	b_2^{12}	$b_1^{4}b_2^{10}$	c_2^{12}	c_2^{12}	c_2^{12}	b_3^{8}	b_4^{6}	c_4^{6}	c_6^{4}
$\mathbf{O}_h(/\mathbf{C}_s)$	b_1^{24}	b_2^{12}	b_2^{12}	$a_1^{8}c_2^{8}$	c_2^{12}	c_2^{12}	b_3^{8}	b_4^{6}	c_4^{6}	c_6^{4}
$\mathbf{O}_h(/\mathbf{C}'_s)$	b_1^{24}	b_2^{12}	b_2^{12}	c_2^{12}	$a_1^{4}c_2^{10}$	c_2^{12}	b_3^{8}	b_4^{6}	c_4^{6}	c_6^{4}
$\mathbf{O}_h(/\mathbf{C}_i)$	b_1^{24}	b_2^{12}	b_2^{12}	c_2^{12}	c_2^{12}	a_1^{24}	b_3^{8}	b_4^{6}	c_4^{6}	a_3^{8}
$\mathbf{O}_h(/\mathbf{C}_3)$	b_1^{16}	b_2^{8}	b_2^{8}	c_2^{8}	c_2^{8}	c_2^{8}	$b_1^{4}b_3^{4}$	b_4^{4}	c_4^{4}	$c_2^{2}c_6^{2}$
$\mathbf{O}_h(/\mathbf{C}_4)$	b_1^{12}	$b_1^{4}b_2^{4}$	b_2^{6}	c_2^{6}	c_2^{6}	c_2^{6}	b_3^{4}	$b_1^{4}b_4^{2}$	$c_2^{2}c_4^{2}$	c_6^{2}
$\mathbf{O}_h(/\mathbf{S}_4)$	b_1^{12}	$b_1^{4}b_2^{4}$	b_2^{6}	c_2^{6}	c_2^{6}	c_2^{6}	b_3^{4}	$b_2^{2}b_4^{2}$	$a_1^{4}c_4^{2}$	c_6^{2}
$\mathbf{O}_h(/\mathbf{C}_{3i})$	b_1^{8}	b_2^{4}	b_2^{4}	c_2^{4}	c_2^{4}	a_1^{8}	$b_1^{2}b_3^{2}$	b_4^{2}	c_4^{2}	$a_1^{2}a_3^{2}$
N_j	$\frac{1}{48}$	$\frac{1}{16}$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{8}$	$\frac{1}{48}$	$\frac{1}{6}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{6}$

When this procedure is repeated by considering Table 9 and Table 4, we obtain the dominant USCI-CF table shown in Table 14, which is essentially identical with Table 3 of Part II. Obviously, this treatment is the reverse of the treatment described in Section 2.

Practically, the full data of Table 14 were calculated by using the Maple system [28], where a Maple file named "cm5A.mpl" (extension .mpl), whose source list is shown in Appendix, was used for calculation. After the file was stored in a working directory named "c:/fujita0/", the following commands were input from the display of the Maple system:

```
>restart;
>read "c:/fujita0/cm05A.mpl";
```

Similar discussions on the relationship between CM-CFs and dominant USCI-CFs are available with respect to the point group **O** by using the CM-CF table of **O** (Table 7) and the multiplicity vectors listed in Table 11.

3.2.2 Non-Dominant USCI-CFs from CM-CFs

The discussions in the preceding paragraph can be applied to non-dominant markaracters listed in Table 12. For example, the multiplicity vector shown in the $\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_{3v})}$-row of Table 12 (Eq. 15) corresponds to the reduction shown in Eq. 16. The subduction into $\mathbf{S}_4$ is represented by the following equation:

$$\mathbf{O}_h(/\mathbf{C}_{3v}) \downarrow \mathbf{S}_4 = A_{1g} \downarrow \mathbf{S}_4 + T_{2g} \downarrow \mathbf{S}_4 + A_{2u} \downarrow \mathbf{S}_4 + T_{1u} \downarrow \mathbf{S}_4. \quad (20)$$

By starting from the data collected in the $\mathbf{S}_4$-column of the CM-CF table of $\mathbf{O}_h$ (Table 4), the USCI-CF corresponding to $\mathbf{O}_h(/\mathbf{C}_{3v}) \downarrow \mathbf{S}_4$ is calculated as follows:

$$\mathrm{Z}(\mathbf{O}_h(/\mathbf{C}_{3v}) \downarrow \mathbf{S}_4; \$_d)$$

$$
\begin{aligned}
&= \mathrm{Z}(\mathbf{O}_h(A_{1g} \downarrow \mathbf{S}_4;\$_d)\mathrm{Z}(\mathbf{O}_h(T_{2g} \downarrow \mathbf{S}_4;\$_d) \\
&\quad \times \mathrm{Z}(\mathbf{O}_h(A_{2u} \downarrow \mathbf{S}_4;\$_d)\mathrm{Z}(\mathbf{O}_h(T_{1u} \downarrow \mathbf{S}_4;\$_d) \\
&= (a_1)(a_1^{-1}c_4)(a_1)(a_1^{-1}c_4) = c_4^2. \qquad (21)
\end{aligned}
$$

This procedure is repeated to give the USCI-CFs of $\mathbf{O}_h(/\mathbf{C}_{3v})$ as follows:

$$(b_1^8, b_2^4, b_2^4, c_2^4, a_1^4c_2^2, c_2^4, b_1^2b_3^2, b_4^2, c_4^2, c_2c_6). \qquad (22)$$

When this procedure is repeated by considering Table 12 and Table 4, we obtain the non-dominant USCI-CF table shown in Table 15, which is essentially identical with Table 5 of Part II.

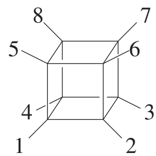
It should be noted that the process of calculating non-dominant USCI-CFs (e.g., Eq. 16 → Eq. 20 → Eq. 21) is essentially equivalent to the process calculating dominant USCI-CFs (e.g., Eq. 17 → Eq. 18 → Eq. 19), because we start from the common CM-CF table (Table 4). Hence, the full data of Table 15 were calculated by using the same Maple file (cm5A.mpl) listed in Appendix.

Similar discussions on the relationship between CM-CFs and dominant USCI-CFs for the point group **O** are obtained by starting from the CM-CF table of **O** (Table 7) and the multiplicity vectors listed in Table 13.

3.3 Enumeration of Cubane Derivatives

3.3.1 Cubane Derivatives as 3D Structural Isomers

The numbering of a cubane skeleton belonging to the $\mathbf{O}_h$-point group is shown in **1** (Figure 1). The 8 positions generates 48 permutations on the action of the 48 elements of $\mathbf{O}_h$, where they



1

Figure 1: Numbering of the eight positions of cubane (**1**)

construct a permutation representation **P**. The markaracter for characterizing **P** is obtained by counting fixed positions on the action of each cyclic subgroup. For example, let us examine the point group $\mathbf{C}'_s = \{I, \sigma_{d(6)}\}$, which is concerned with the mirror plane containing the positions 2, 4, 6, and 8 in the cubane skeleton (**1**). Permutations (as products of cycles) corresponding to the $\mathbf{C}'_s$ group are selected from **P** as follows:

I	(1)(2)(3)(4)(5)(6)(7)(8)
$\sigma_{d(6)}$	$\overline{(2)(4)(6)(8)(1\ 3))(5\ 7)}$
fixed positions	(2), (4), (6) and (8)

Table 15: Non-Dominant USCI-CF Table of $\mathbf{O}_h$

	$\mathbf{C}_1$ I	$\mathbf{C}_2$ $3C_2$	$\mathbf{C}'_2$ $6C_2$	$\mathbf{C}_s$ $3\sigma_h$	$\mathbf{C}'_s$ $6\sigma_d$	$\mathbf{C}_i$ i	$\mathbf{C}_3$ $8C_3$	$\mathbf{C}_4$ $6C_4$	$\mathbf{S}_4$ $6S_4$	$\mathbf{C}_{3i}$ $8S_6$
$\mathbf{O}_h(/\mathbf{D}_2)$	b_1^{12}	b_1^{12}	b_2^6	c_2^6	c_2^6	c_2^6	b_3^4	b_2^6	c_2^6	c_6^2
$\mathbf{O}_h(/\mathbf{D}'_2)$	b_1^{12}	$b_1^4b_2^4$	$b_1^4b_2^4$	c_2^6	c_2^6	c_2^6	b_3^4	$b_2^2b_4^2$	$c_2^2c_4^2$	c_6^2
$\mathbf{O}_h(/\mathbf{C}_{2v})$	b_1^{12}	$b_1^4b_2^4$	b_2^6	$a_1^8c_2^2$	c_2^6	c_2^6	b_3^4	$b_2^2b_4^2$	$c_2^2c_4^2$	c_6^2
$\mathbf{O}_h(/\mathbf{C}'_{2v})$	b_1^{12}	$b_1^4b_2^4$	b_2^6	c_2^6	$a_1^4c_2^4$	c_2^6	b_3^4	$b_2^2b_4^2$	$c_2^2c_4^2$	c_6^2
$\mathbf{O}_h(/\mathbf{C}''_{2v})$	b_1^{12}	b_2^6	$b_1^2b_2^5$	$a_1^4c_2^4$	$a_1^2c_2^5$	c_2^6	b_3^4	b_4^3	c_4^3	c_6^2
$\mathbf{O}_h(/\mathbf{C}_{2h})$	b_1^{12}	$b_1^4b_2^4$	b_2^6	$a_1^4c_2^4$	c_2^6	a_1^{12}	b_3^4	$b_2^2b_4^2$	$c_2^2c_4^2$	a_3^4
$\mathbf{O}_h(/\mathbf{C}'_{2h})$	b_1^{12}	b_2^6	$b_1^2b_2^5$	c_2^6	$a_1^2c_2^5$	a_1^{12}	b_3^4	b_4^3	c_4^3	a_3^4
$\mathbf{O}_h(/\mathbf{D}_3)$	b_1^8	b_2^4	$b_1^4b_2^2$	c_2^4	c_2^4	c_2^4	$b_1^2b_3^2$	b_4^2	c_4^2	c_2c_6
$\mathbf{O}_h(/\mathbf{C}_{3v})$	b_1^8	b_2^4	b_2^4	c_2^4	$a_1^4c_2^2$	c_2^4	$b_1^2b_3^2$	b_4^2	c_4^2	c_2c_6
$\mathbf{O}_h(/\mathbf{D}_4)$	b_1^6	b_1^6	$b_1^2b_2^2$	c_2^3	c_2^3	c_2^3	b_3^2	$b_1^2b_2^2$	c_2^3	c_6
$\mathbf{O}_h(/\mathbf{C}_{4v})$	b_1^6	$b_1^2b_2^2$	b_2^3	$a_1^4c_2$	$a_1^2c_2^2$	c_2^3	b_3^2	$b_1^2b_4$	c_2c_4	c_6
$\mathbf{O}_h(/\mathbf{C}_{4h})$	b_1^6	$b_1^2b_2^2$	b_2^3	$a_1^2c_2^2$	c_2^3	a_1^6	b_3^2	$b_1^2b_4$	$a_1^2c_4$	a_3^2
$\mathbf{O}_h(/\mathbf{D}_{2d})$	b_1^6	b_1^6	b_2^3	c_2^3	$a_1^2c_2^2$	c_2^3	b_3^2	b_2^3	$a_1^2c_2^2$	c_6
$\mathbf{O}_h(/\mathbf{D}'_{2d})$	b_1^6	$b_1^2b_2^2$	$b_1^2b_2^2$	$a_1^4c_2$	c_2^3	c_2^3	b_3^2	b_2b_4	$a_1^2c_4$	c_6
$\mathbf{O}_h(/\mathbf{D}_{2h})$	b_1^6	b_1^6	b_2^3	a_1^6	c_2^3	a_1^6	b_3^2	b_2^3	c_2^3	a_3^2
$\mathbf{O}_h(/\mathbf{D}'_{2h})$	b_1^6	$b_1^2b_2^2$	$b_1^2b_2^2$	$a_1^2c_2^2$	$a_1^2c_2^2$	a_1^6	b_3^2	b_2b_4	c_2c_4	a_3^2
$\mathbf{O}_h(/\mathbf{T})$	b_1^4	b_1^4	b_2^2	c_2^2	c_2^2	c_2^2	b_1^4	b_2^2	c_2^2	c_2^2
$\mathbf{O}_h(/\mathbf{D}_{3d})$	b_1^4	b_2^2	$b_1^2b_2$	c_2^2	$a_1^2c_2$	a_1^4	b_1b_3	b_4	c_4	a_1a_3
$\mathbf{O}_h(/\mathbf{D}_{4h})$	b_1^3	b_1^3	b_1b_2	a_1^3	a_1c_2	a_1^3	b_3	b_1b_2	a_1c_2	a_3
$\mathbf{O}_h(/\mathbf{O})$	b_1^2	b_1^2	b_1^2	c_2	c_2	c_2	b_1^2	b_1^2	c_2	c_2
$\mathbf{O}_h(/\mathbf{T}_h)$	b_1^2	b_1^2	b_2	a_1^2	c_2	a_1^2	b_1^2	b_2	c_2	a_1^2
$\mathbf{O}_h(/\mathbf{T}_d)$	b_1^2	b_1^2	b_2	c_2	a_1^2	c_2	b_1^2	b_2	a_1^2	c_2
$\mathbf{O}_h(/\mathbf{O}_h)$	b_1	b_1	b_1	a_1	a_1	a_1	b_1	b_1	a_1	a_1
N_j	$\frac{1}{48}$	$\frac{1}{16}$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{8}$	$\frac{1}{48}$	$\frac{1}{6}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{6}$

where the overbar represents the inversion of chirality. Note that each of the fixed positions (2, 4, 6, and 8) is capable of accommodating an achiral proligand only (achirality determined in isolation) in accord with chirality fittingness [5]. Because the four positions are fixed as designated by one-cycles, the value 4 is placed as the $\mathbf{C}'_s$-component of the markaracter $\widetilde{\mathrm{M}}_{\mathbf{P}}$. This procedure is repeated to cover all of the cyclic subgroups up to conjugation so as to give the markaracter:

$$\widetilde{\mathrm{M}}_{\mathbf{P}} = (8,0,0,0,4,0,2,0,0,0), \tag{23}$$

which is identical with the $\widetilde{\mathrm{M}}_{\mathbf{O}_h(/\mathbf{C}_{3v})}$-row of Table 12 (Eq. 15). As a result, the USCI-CFs listed in Eq. 22 (the $\mathbf{O}_h(/\mathbf{C}_{3v})$-row of Table 15) are regarded as the corresponding SCI-CFs, because the permutation representation $\mathbf{P}$ consists of a single orbit. Hence, Eq. 35 of [27] is adopted to treat this case so as to generate the following CI-CF:

$$\begin{aligned} \text{CI-CF}(\mathbf{P}, \$_d) &= \frac{1}{48}b_1^8 + \frac{1}{16}b_2^4 + \frac{1}{8}b_2^4 + \frac{1}{16}c_2^4 + \frac{1}{8}a_1^4c_2^2 + \frac{1}{48}c_2^4 + \frac{1}{6}b_1^2b_3^2 + \frac{1}{8}b_4^2 + \frac{1}{8}c_4^2 + \frac{1}{6}c_2c_6 \\ &= \frac{1}{48}b_1^8 + \frac{3}{16}b_2^4 + \frac{1}{6}b_1^2b_3^2 + \frac{1}{8}b_4^2 + \frac{1}{12}c_2^4 + \frac{1}{6}c_2c_6 + \frac{1}{8}a_1^4c_2^2 + \frac{1}{8}c_4^2 \end{aligned} \tag{24}$$

by applying the data of the N_j-row of Table 7 to the SCI-CFs (Eq. 22).

Let us consider an inventory of proligands:

$$\mathbf{L} = \{\mathrm{H,A,B,C,W,X,Y,Z};\ \mathrm{p},\overline{\mathrm{p}};\ \mathrm{q},\overline{\mathrm{q}}\}, \tag{25}$$

where H, A, B, C, W, X, Y, and Z are achiral proligands in isolation, while p, q, $\overline{\mathrm{p}}$, and $\overline{\mathrm{q}}$ are chiral proligands in isolation. The pair of a letter (e.g., p) and its overlined counterpart (e.g., $\overline{\mathrm{p}}$) represents an enantiomeric pair. According to Theorem 4 of [27], we use the following inventory functions:

$$a_d = \mathrm{H}^d + \mathrm{A}^d + \mathrm{B}^d + \mathrm{C}^d + \mathrm{W}^d + \mathrm{X}^d + \mathrm{Y}^d + \mathrm{Z}^d \tag{26}$$

$$b_d = \mathrm{H}^d + \mathrm{A}^d + \mathrm{B}^d + \mathrm{C}^d + \mathrm{W}^d + \mathrm{X}^d + \mathrm{Y}^d + \mathrm{Z}^d + \mathrm{p}^d + \overline{\mathrm{p}}^d + \mathrm{q}^d + \overline{\mathrm{q}}^d \tag{27}$$

$$c_d = \mathrm{H}^d + \mathrm{A}^d + \mathrm{B}^d + \mathrm{C}^d + \mathrm{W}^d + \mathrm{X}^d + \mathrm{Y}^d + \mathrm{Z}^d + 2\mathrm{p}^{d/2}\overline{\mathrm{p}}^{d/2} + 2\mathrm{q}^{d/2}\overline{\mathrm{q}}^{d/2}. \tag{28}$$

They are introduced into Eq. 24 to give a generating function where the coefficient of each term $\mathrm{H}^h\mathrm{A}^a\mathrm{B}^b\mathrm{C}^c\mathrm{W}^w\mathrm{X}^x\mathrm{Y}^y\mathrm{Z}^z\mathrm{p}^p\overline{\mathrm{p}}^{\overline{p}}\mathrm{q}^q\overline{\mathrm{q}}^{\overline{q}}$ represents the number of cubane derivatives as 3D-structural isomers having h of H, a of A, b of B, c of C, W of W, x of X, y of Y, z of Z, p of p, $\overline{p}$ of $\overline{\mathrm{p}}$ q of q, and $\overline{q}$ of $\overline{\mathrm{q}}$. As for practical calculations, see Parts I and II of this series.

3.3.2 Cubane Derivatives as Steric Isomers

To count cubane derivatives as steric isomers, the cubane skeleton (**1**) is considered to belong to the point group **O**. The 8 positions of **1** generates 24 permutations on the action of the 24 elements of **O** where they construct a permutation representation $\mathbf{P}'$. The markaracter for characterizing $\mathbf{P}'$ is obtained by counting fixed positions on the action of each cyclic subgroup:

$$\widetilde{\mathrm{M}}_{\mathbf{P}'} = (8,0,0,2,0), \tag{29}$$

which has already appeared in Eq. 13 and in Table 11. The corresponding multiplicity vector indicates the reduction shown in Eq. 14. The right-hand side of Eq. 14 is combined with the data of the CM-CF table of **O** (Table 7) so as to generate the USCI-CFs for $\mathbf{O}(/\mathbf{C}_3)$:

$$(b_1^8, b_2^4, b_2^4, b_1^2b_3^2, b_4^2). \tag{30}$$

Because the permutation representation $\mathbf{P}'$ consists of a single orbit corresponding to $\mathbf{O}(/\mathbf{C}_3)$, each USCI-CF itself can be regarded as its SCI-CF. Hence, Eq. 35 of [27] is adopted to treat this case so as to generate the following CI-CF:

$$\begin{aligned} \text{CI-CF}(\mathbf{P}', b_d) &= \frac{1}{24}b_1^8 + \frac{1}{8}b_2^4 + \frac{1}{4}b_2^4 + \frac{1}{3}b_1^2 b_3^2 + \frac{1}{4}b_4^2 \\ &= \frac{1}{24}b_1^8 + \frac{3}{8}b_2^4 + \frac{1}{3}b_1^2 b_3^2 + \frac{1}{4}b_4^2 \end{aligned} \tag{31}$$

by using the data shown in Eq. 30 and the N_j-row of Table 7. Note that Eq. 31 contains the SI b_d only. When the ligand inventory **L** (Eq. 25) is adopted to count cubane derivatives as steric isomers, the ligand-inventory function b_d (Eq. 27) is introduced into the right-hand side of Eq. 31 according to Theorem 4 of [27]. Then, the expansion of the resulting function gives a generating function for counting cubane derivatives as steric isomers. As for practical calculations, see Parts I and II of this series.

3.3.3 Achiral Cubane Derivatives

When the symbol A represents the number of achiral derivatives and the symbol C represents the number of enantiomeric pairs (a pair of enantiomers is separately counted once), The CI-CF$(\mathbf{P}, \$_d)$ (Eq. 24) is equal to A + C, while the CI-CF$(\mathbf{P}', b_d)$ (Eq. 31) is equal to A + 2C. Hence, the CI-CF$^{(a)}(\mathbf{P}, \$_d)$ for obtaining the number of achiral derivatives is evaluated as follows:

$$\begin{aligned} \text{CI-CF}^{(a)}(\mathbf{P}, \$_d) &= 2\text{CI-CF}(\mathbf{P}, \$_d) - \text{CI-CF}(\mathbf{P}', b_d) \\ &= \frac{1}{6}c_2^4 + \frac{1}{3}c_2 c_6 + \frac{1}{4}a_1^4 c_2^2 + \frac{1}{4}c_4^2. \end{aligned} \tag{32}$$

When the ligand inventory **L** (Eq. 25) is adopted to count achiral cubane derivatives, the ligand-inventory functions a_d and c_d (Eqs. 26 and 28) are introduced into the right-hand side of Eq. 32. As for practical calculations, see Parts I and II of this series.

3.3.4 Enantiomeric Pairs of Cubane Derivatives

On a similar line to the preceding paragraphs, the CI-CF$^{(c)}(\mathbf{P}, \$_d)$ for obtaining the number of enantiomeric pairs is evaluated as follows:

$$\begin{aligned} \text{CI-CF}^{(e)}(\mathbf{P}, \$_d) &= \text{CI-CF}(\mathbf{P}', b_d) - \text{CI-CF}(\mathbf{P}, \$_d) \\ &= \frac{1}{48}b_1^8 + \frac{3}{16}b_2^4 + \frac{1}{6}b_1^2 b_3^2 + \frac{1}{8}b_4^2 - \frac{1}{12}c_2^4 - \frac{1}{6}c_2 c_6 - \frac{1}{8}a_1^4 c_2^2 - \frac{1}{8}c_4^2. \end{aligned} \tag{33}$$

When the ligand inventory **L** (Eq. 25) is adopted to count enantiomeric pairs of chiral cubane derivatives, the ligand-inventory functions a_d, b_d, and c_d (Eqs. 26–28) are introduced into the right-hand side of Eq. 33. As for practical calculations, see Parts I and II of this series.

3.4 Cycle Indices Calculated by Other Methods

The crux of the CM method is the recognition that markaracters can be regarded as **Q**-conjugacy characters and vice versa. Thereby, USCI-CFs (unit subduced cycle indices with chirality fittingness) based on markaracters can be derived by starting from dominant CM-CFs based on irreducible **Q**-conjugacy characters, as discussed in this article (Part III of this series). From the inverse viewpoint, CM-CFs can be in turn calculated by starting from dominant USCI-CFs, as discussed in Part II of this series. This means that SCI-CFs (subduced cycle indices with chirality fittingness) and CI-CFs (cycle indices with chirality fittingness) are equivalent in both the methods. In addition, the proligand method discussed in Part I of this series, is found to be based on **Q**-conjugacy so as to be linked with the CM method. The proligand method is also linked with the markaracter method, because a set of conjugate subgroups corresponds to a set of **Q**-conjugacy classes. As a result, the SCI-CFs and CI-CFs obtained by the proligand method are equivalent to those of the CM method and to those of the markaracter method. Such general propositions are exemplified by the CI-CFs shown in Eq. 24 (3D-structural isomers), Eq. 31 (steric isomers), Eq. 32 (achiral derivatives), and Eq. 33 (chiral derivatives) for counting cubane derivatives under the action of $\mathbf{O}_h$ (or **O**).

4 Conclusions

To show the versatility of the CM (characteristic monomial) method developed by us [21, 27], the CM-CF tables of $\mathbf{O}_h$ and **O** are prepared for the purpose of enumerating cubane derivatives, where CM-CFs (characteristic monomials with chirality fittingness) are calculated to treat achiral and chiral ligands. The crux of the CM method is the recognition that markaracters can be regarded as **Q**-conjugacy characters and vice versa. Thereby, USCI-CFs (unit subduced cycle indices with chirality fittingness) based on markaracters can be derived by starting from CM-CFs based on **Q**-conjugacy characters. The calculated USCI-CFs can be applied to prepare SCI-CFs (subduced cycle indices with chirality fittingness), which are further used to prepare CI-CFs (cycle indices with chirality fittingness). The CI-CFs for enumerating cubane derivatives as 3D-structural isomers and steric isomers as well as for enumerating achiral and chiral cubane derivatives are clarified to be equivalent to those prepared by the proligand method (Part I of this series) as well as to those prepared by the markaracter method (Part II of this series). A Maple program source for calculating USCI-CFs from CM-CFs is given as an example of practical calculation.

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Appendix

Maple Program for Generating the Data of Tables 14 and 15

```
#cm05A.mpl
#SCI-CFs for dominant and non-dominant parts
#read "c:/fujita0/fujita/stereochm11/cubaneCM/calc/cm05A.mpl";

with(linalg);

DOh := matrix(10,10,
[[1,1,1,1,1,1,1,1,1,1],
[1,1,-1,1,-1,1,1,-1,-1,1],
[2,2,0,2,0,2,-1,0,0,-1],
[3,-1,-1,-1,-1,3,0,1,1,0],
[3,-1,1,-1,1,3,0,-1,-1,0],
[1,1,1,-1,-1,-1,1,1,-1,-1],
[1,1,-1,-1,1,-1,1,-1,1,-1],
[2,2,0,-2,0,-2,-1,0,0,1],
[3,-1,-1,1,1,-3,0,1,-1,0],
[3,-1,1,1,-1,-3,0,-1,1,0]]);

InvDOh := inverse(DOh);

ndSCIcf := proc(m::vector)
local v, SCIcf;
v:=evalm(m &* InvDOh);
```

```
SCIcf:=vector(10);
SCIcf[1]:=sort(
(b1^(v[1]))*(b1^(v[2]))*(b1^(2*v[3]))*(b1^(3*v[4]))*
(b1^(3*v[5]))*(b1^(v[6]))*(b1^(v[7]))*(b1^(2*v[8]))*
(b1^(3*v[9]))*(b1^(3*v[10])),[b1,b2]);
SCIcf[2]:=sort(
(b1^(v[1]))*(b1^(v[2]))*(b1^(2*v[3]))*
(b1^((-1)*v[4]))*(b2^(2*v[4]))*
(b1^((-1)*v[5]))*(b2^(2*v[5]))*
(b1^(v[6]))*(b1^(v[7]))*(b1^(2*v[8]))*
(b1^((-1)*v[9]))*(b2^(2*v[9]))*
(b1^((-1)*v[10]))*(b2^(2*v[10])),[b1,b2]);
SCIcf[3]:=sort(
(b1^(v[1]))*(b1^((-1)*v[2]))*(b2^(v[2]))*
(b2^(v[3]))*(b1^((-1)*v[4]))*(b2^(2*v[4]))*
(b1^(v[5]))*(b2^(v[5]))*
(b1^(v[6]))*(b1^((-1)*v[7]))*(b2^(v[7]))*
(b2^(v[8]))*(b1^((-1)*v[9]))*(b2^(2*v[9]))*
(b1^(v[10]))*(b2^(v[10])),[b1,b2]);
SCIcf[4]:=sort(
(a1^(v[1]))*(a1^(v[2]))*(a1^(2*v[3]))*
(a1^((-1)*v[4]))*(c2^(2*v[4]))*
(a1^((-1)*v[5]))*(c2^(2*v[5]))*
(a1^((-1)*v[6]))*(c2^(v[6]))*
(a1^((-1)*v[7]))*(c2^(v[7]))*
(a1^((-2)*v[8]))*(c2^(2*v[8]))*
(a1^(v[9]))*(c2^(v[9]))*(a1^(v[10]))*(c2^(v[10])), [a1,c2]);
SCIcf[5]:=sort(
(a1^(v[1]))*(a1^((-1)*v[2]))*(c2^(v[2]))*
(c2^(v[3]))*(a1^((-1)*v[4]))*(c2^(2*v[4]))*
(a1^(v[5]))*(c2^(v[5]))*(a1^((-1)*v[6]))*(c2^(v[6]))*
(a1^(v[7]))*(c2^(v[8]))*(a1^(v[9]))*(c2^(v[9]))*
(a1^((-1)*v[10]))*(c2^(2*v[10])),[a1,c2]);
SCIcf[6]:=sort(
(a1^(v[1]))*(a1^(v[2]))*(a1^(2*v[3]))*(a1^(3*v[4]))*
(a1^(3*v[5]))*(a1^((-1)*v[6]))*(c2^(v[6]))*
(a1^((-1)*v[7]))*(c2^(v[7]))*
(a1^((-2)*v[8]))*(c2^(2*v[8]))*
(a1^((-3)*v[9]))*(c2^(3*v[9]))*
(a1^((-3)*v[10]))*(c2^(3*v[10])), [a1,c2]);
SCIcf[7]:=sort(
(b1^(v[1]))*(b1^(v[2]))*
(b1^((-1)*v[3]))*(b3^(v[3]))*
(b3^(v[4]))*(b3^(v[5]))*(b1^(v[6]))*(b1^(v[7]))*
(b1^((-1)*v[8]))*(b3^(v[8]))*
(b3^(v[9]))*(b3^(v[10])),[b1,b2,b3]);
SCIcf[8]:=sort(
(b1^(v[1]))*(b1^((-1)*v[2]))*(b2^(v[2]))*
(b2^(v[3]))*(b1^(v[4]))*(b2^((-1)*v[4]))*(b4^(v[4]))*
(b1^((-1)*v[5]))*(b4^(v[5]))*(b1^(v[6]))*
(b1^((-1)*v[7]))*(b2^(v[7]))*(b2^(v[8]))*
(b1^(v[9]))*(b2^((-1)*v[9]))*(b4^(v[9]))*
(b1^((-1)*v[10]))*(b4^(v[10])), [b1,b2,b3,b4]);
SCIcf[9]:=sort(
(a1^(v[1]))*
(a1^((-1)*v[2]))*(c2^(v[2]))*(c2^(v[3]))*
(a1^(v[4]))*(c2^((-1)*v[4]))*(c4^(v[4]))*
(a1^((-1)*v[5]))*(c4^(v[5]))*
(a1^((-1)*v[6]))*(c2^(v[6]))*
(a1^(v[7]))*(c2^(v[8]))*(a1^((-1)*v[9]))*(c4^(v[9]))*
(a1^(v[10]))*(c2^((-1)*v[10]))*(c4^(v[10])), [a1,c2,c4]);
```

```
SCIcf[10]:=sort(
(a1^(v[1]))*(a1^(v[2]))*(a1^((-1)*v[3]))*(a3^(v[3]))*
(a3^(v[4]))*(a3^(v[5]))*(a1^((-1)*v[6]))*(c2^(v[6]))*
(a1^((-1)*v[7]))*(c2^(v[7]))*
(a1^(v[8]))*(a3^((-1)*v[8]))*(c2^((-1)*v[8]))*(c6^(v[8]))*
(a3^((-1)*v[9]))*(c6^(v[9]))*
(a3^((-1)*v[10]))*(c6^(v[10])),[a1,a3,c2,c6]);

printf("%a, %a, %a, %a, %a, %a, %a, %a, %a, %a",
SCIcf[1],SCIcf[2],SCIcf[3],SCIcf[4],
SCIcf[5],SCIcf[6],SCIcf[7],SCIcf[8],
SCIcf[9],SCIcf[10]);
end proc:

#dominant USCIs
m:= vector([48,0,0,0,0,0,0,0,0,0]); ndSCIcf(m);
m:= vector([24,8,0,0,0,0,0,0,0,0]); ndSCIcf(m);
m:= vector([24,0,4,0,0,0,0,0,0,0]); ndSCIcf(m);
m:= vector([24,0,0,8,0,0,0,0,0,0]); ndSCIcf(m);
m:= vector([24,0,0,0,4,0,0,0,0,0]); ndSCIcf(m);
m:= vector([24,0,0,0,0,24,0,0,0,0]); ndSCIcf(m);
m:= vector([16,0,0,0,0,0,4,0,0,0]); ndSCIcf(m);
m:= vector([12,4,0,0,0,0,0,4,0,0]); ndSCIcf(m);
m:= vector([12,4,0,0,0,0,0,0,4,0]); ndSCIcf(m);
m:= vector([8,0,0,0,0,8,2,0,0,2]); ndSCIcf(m);

#non-dominant USCIs
m:= vector([12,12,0,0,0,0,0,0,0,0]); ndSCIcf(m);
m:= vector([12,4,4,0,0,0,0,0,0,0]); ndSCIcf(m);
m:= vector([12,4,0,8,0,0,0,0,0,0]); ndSCIcf(m);
m:= vector([12,4,0,0,4,0,0,0,0,0]); ndSCIcf(m);
m:= vector([12,0,2,4,2,0,0,0,0,0]); ndSCIcf(m);
m:= vector([12,4,0,4,0,12,0,0,0,0]); ndSCIcf(m);
m:= vector([12,0,2,0,2,12,0,0,0,0]); ndSCIcf(m);
m:= vector([8,0,4,0,0,0,2,0,0,0]); ndSCIcf(m);
m:= vector([8,0,0,0,4,0,2,0,0,0]); ndSCIcf(m);
m:= vector([6,6,2,0,0,0,0,2,0,0]); ndSCIcf(m);
m:= vector([6,2,0,4,2,0,0,2,0,0]); ndSCIcf(m);
m:= vector([6,2,0,2,0,6,0,2,2,0]); ndSCIcf(m);
m:= vector([6,6,0,0,2,0,0,0,2,0]); ndSCIcf(m);
m:= vector([6,2,2,4,0,0,0,0,2,0]); ndSCIcf(m);
m:= vector([6,6,0,6,0,6,0,0,0,0]); ndSCIcf(m);
m:= vector([6,2,2,2,2,6,0,0,0,0]); ndSCIcf(m);
m:= vector([4,4,0,0,0,0,4,0,0,0]); ndSCIcf(m);
m:= vector([4,0,2,0,2,4,1,0,0,1]); ndSCIcf(m);
m:= vector([3,3,1,3,1,3,0,1,1,0]); ndSCIcf(m);
m:= vector([2,2,2,0,0,0,2,2,0,0]); ndSCIcf(m);
m:= vector([2,2,0,2,0,2,2,0,0,2]); ndSCIcf(m);
m:= vector([2,2,0,0,2,0,2,0,2,0]); ndSCIcf(m);
m:= vector([1,1,1,1,1,1,1,1,1,1]); ndSCIcf(m);
```