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Restricted Enumerations by the Unit-Subduced-Cycle-Index (USCI) Approach. III. The Restricted-Partial-Cycle-Index (RPCI) Method for Treating Interactions Between Two or More Orbits

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Abstract

The restricted partial-cycle-index (RPCI) method has been developed by starting from the partial-cycle-index (PCI) method of the unit-subduced-cycle-index (USCI) approach (S. Fujita, "Symmetry and Combinatorial Enumeration in Chemistry", Springer-Verlag (1991)), where enumerated derivatives are generated by means of vertex substitution (monodentate ligands) and/or edge substitution (bidentate ligands) under a restriction condition that occupation of a common vertex (or occupation of adjacent edges) is avoided. Thus, restricted partial cycle indices with chirality fittingness (PCI-CFs) are derived from unit subduced cycle indices with chirality fittingness (USCI-CFs) via restricted subduced cycle indices with chirality fittingness (SCI-CFs). The resulting restricted PCI-CFs enable us to enumerate derivatives under the restricted condition in a symmetry-itemized fashion. The restricted PCI-CFs are further transformed into restricted cycle indices with chirality fittingness (restricted CI-CFs) for gross enumerations of total, achiral, chiral derivatives. A maple program for the RPCI method is reported as an appendix.

1 Introduction

The partial-cycle-index (PCI) method [1, 2] is one of the four methods supported by the unit-subduced-cycle-index (USCI) approach [3, 4], where partial cycle indices without and with chirality fittingness (PCIs and PCI-CFs) are derived from unit subduced cycle indices without and with chirality fittingness (USCIs and USCI-CFs) via subduced cycle indices without and with chirality fittingness (SCIs and SCI-CFs) and used to provide generating functions for symmetry-itemized enumerations.

In Part II of this series, we have extended the fixed-point matrix (FPM) method [57], which is another method of the USCI approach, so as to be capable of treating restricted cases in which occupation of a common vertex (by a monodentate ligand and a bidentate ligand) or occupation of adjacent edges (by two bidentate ligands) is avoided. In the model adopted by the restricted FPM method (Part II), such restricted cases are considered to stem from interactions between two or more orbits of vertices and/or edges. Then, superposed occupation at a vertex due to such interactions is rejected by converting SCI-CFs (or SCIs) into restricted SCI-CFs (or restricted SCIs), which are used to evaluate a fixed-point matrix (FPM), as formulated in Part II. As a continuation of Part II, a parallel extension of the PCI method is desirable for the purpose of expanding facilities of the USCI approach.

In the present paper, the restricted PCI (RPCI) method will be proposed on the basis of the restricted SCI-CFs described in Part II, where symmetry-itemized enumerations under restricted conditions can be conducted. Moreover, restricted cycle indices without and with chirality fittingness (CIs and CI-CFs) are derived from the restricted PCIs and PCI-CFs, so as to conduct gross enumerations of total, achiral, and chiral derivatives. Although we have discussed another version of the RPCI method for treating restricted cases of a slightly different type in Part I of this series, the consideration of restriction conditions has been based on factorizations of SCI-CFs (or SCIs), which are not fully systematic from a practical point of view. Hence, the present RPCI method aims at a more systematic consideration of restriction conditions as a continuation of the methodology described in Part II.

2 Symmetry-Itemized Restricted Enumerations

2.1 Restricted Partial Cycle Indices With Chirality Fittingness

The subduced cycle index with chirality fittingness (SCI-CF) defined by Def. 19.3 of [3] has been transformed into the corresponding restricted SCI-CF for the subgroup $\mathbf{G}_j$ ($\subset \mathbf{G}$) in terms of Lemma 1 of Part II of this series, i.e., $\overline{\text{SCI-CF}}(\mathbf{G}_j; \$^{(i\alpha)}_{d_{jk}})$. The restricted SCI-CF has been used to evaluate the marks (the numbers of fixed points, $\rho_{\theta j}$) for restricted enumerations, as shown in Lemma 2 of Part II. The marks have been collected to form a restricted fixed-point matrix (FPM), which is in turn multiplied by the inverse mark table of $\mathbf{G}$ to give the numbers of derivatives, as formulated in the FPM method (Part II of this series).

Remember that usual SCI-CFs provide the basis of the FPM method as well as the basis of the PCI method, as formulated in our monograph [3]. This implies that restricted SCI-CFs are capable of providing a restricted version of the PCI method, because they have already been demonstrated as the basis of the restricted FPM method in Part II of this series. As a result, just as the usual SCI-CFs are transformed into partial cycle indices with chirality fittingness (PCI-CFs) as shown in Def. 19.6 of [3], the restricted SCI-CFs can be transformed into restricted partial cycle indices with chirality fittingness ($\overline{\text{PCI-CF}}(\mathbf{G}_i; \$_{d_{jk}}^{(i\alpha)})$):

Definition 1 (Restricted PCI-CFs) The restricted PCI-CFs are defined as follows:

$$\overline{\text{PCI-CF}}(\mathbf{G}_i; \$_{d_{jk}}^{(i\alpha)}) = \sum_{j=1}^{s} \overline{m}_{ji} \overline{\text{SCI-CF}}(\mathbf{G}_j; \$_{d_{jk}}^{(i\alpha)}) \tag{1}$$

for $i = 1, 2, \ldots, s$, where the restricted SCI-CF in the right-hand side has been given in Lemma 1 of Part II of this series.

Note that $\mathbf{G}_i$ is tentatively fixed in the right-hand side of Eq. 1 but covers all of the subgroups selected from the non-redundant set of subgroups ($\text{SSG}_{\mathbf{G}}$) of the group $\mathbf{G}$:

$$\text{SSG}_{\mathbf{G}} = \{\mathbf{G}_1(= \mathbf{C}_1), \mathbf{G}_2, \cdots, \mathbf{G}_i, \ldots, \mathbf{G}_s(= \mathbf{G})\}. \tag{2}$$

The summation $\sum_{j=1}^{s}$ in the right-hand side of Eq. 1 is concerned with $\mathbf{G}_j$, which also covers all of the subgroups of the $\text{SSG}_{\mathbf{G}}$.

The usual PCI-CFs described in Theorem 19.6 of [3] are easily replaced by the restricted PCI-CFs defined by Def. 1. Thus, the following derivation is traceable by starting from Theorem 1 of Part II:

$$\begin{aligned} \sum_{[\theta]} B_{\theta i} W_\theta &= \sum_{[\theta]} \sum_{j=1}^{s} \rho_{\theta j} \overline{m}_{ji} W_\theta = \sum_{j=1}^{s} \overline{m}_{ji} \sum_{[\theta]} \rho_{\theta j} W_\theta \\ &= \sum_{j=1}^{s} \overline{m}_{ji} \overline{\text{SCI-CF}}(\mathbf{G}_j; \$_{d_{jk}}^{(i\alpha)}) = \overline{\text{PCI-CF}}(\mathbf{G}_i; \$_{d_{jk}}^{(i\alpha)}), \end{aligned} \tag{3}$$

where Lemma 2 of Part II is used to evaluate marks implicitly, i.e., $\sum_{[\theta]} \rho_{\theta j} W_\theta$. The word “implicitly” is used to show that the equations contained in Lemma 2 of Part II are not been expanded during the derivation of Eq. 3 but afterward expanded at the step of the last equation. This delayed expansion provides the same effect as the introduction of inventory functions into the last equation of Eq. 3. As a result, we reach the following theorem.

Theorem 1 (Enumerations by Restricted PCI-CFs) Generating functions for obtaining the numbers $B_{\theta i}$ of $\mathbf{G}_i$-derivatives with weight W_θ under the restricted condition are calculated by the following equations:

$$\sum_{[\theta]} B_{\theta i} W_\theta = \overline{\text{PCI-CF}}(\mathbf{G}_i; \$_{d_{jk}}^{(i\alpha)}) \tag{4}$$

for $i = 1, 2, \ldots, s$, where the variables $\$_{d_{jk}}^{(i\alpha)}$ ($\$ = a, b, c$) are substituted by

$$a_{d_{jk}}^{(i\alpha)} = \sum_{\ell=1}^{|\mathrm{X}|} w_{i\alpha}(\mathrm{X}_\ell^{(a)})^{d_{jk}} \tag{5}$$

$$b_{d_{jk}}^{(i\alpha)} = \sum_{\ell=1}^{|\mathrm{X}|} w_{i\alpha}(\mathrm{X}_\ell)^{d_{jk}} \tag{6}$$

$$c_{d_{jk}}^{(i\alpha)} = \sum_{\ell=1}^{|\mathrm{X}|} w_{i\alpha}(\mathrm{X}_\ell^{(a)})^{d_{jk}} + 2 \sum_{\ell=1}^{|\mathrm{X}|} \left(w_{i\alpha}(\mathrm{X}_\ell^{(c)}) w_{i\alpha}(\overline{\mathrm{X}}_\ell^{(c)}) \right)^{d_{jk}/2}, \tag{7}$$

where the notations succeed Part II and our monograph [3]. Hereafter, the enumeration based on Theorem 1 is called *the restricted PCI (RPCI) method.*

To memorize Eq. 1 of Def. 1, let us define the vector of SCI-CFs ($\overline{\text{SCIV}}$) and the vector of PCI-CFs ($\overline{\text{PCIV}}$) as follows:

$$\overline{\text{SCIV}} = (\overline{\text{SCI-CF}}(\mathbf{G}_1;\$_{d_{jk}}^{(i\alpha)}), \overline{\text{SCI-CF}}(\mathbf{G}_2;\$_{d_{jk}}^{(i\alpha)}), \ldots, \overline{\text{SCI-CF}}(\mathbf{G}_j;\$_{d_{jk}}^{(i\alpha)}), \ldots, \overline{\text{SCI-CF}}(\mathbf{G}_s;\$_{d_{jk}}^{(i\alpha)})) \quad (8)$$

$$\overline{\text{PCIV}} = (\overline{\text{PCI-CF}}(\mathbf{G}_1;\$_{d_{jk}}^{(i\alpha)}), \overline{\text{PCI-CF}}(\mathbf{G}_2;\$_{d_{jk}}^{(i\alpha)}), \ldots, \overline{\text{PCI-CF}}(\mathbf{G}_i;\$_{d_{jk}}^{(i\alpha)}), \ldots, \overline{\text{PCI-CF}}(\mathbf{G}_s;\$_{d_{jk}}^{(i\alpha)})). \quad (9)$$

Then, Eq. 1 is transformed into the following vector-matrix representation:

$$\overline{\text{PCIV}} = \overline{\text{SCIV}} \times M_{\mathbf{G}}^{-1}, \quad (10)$$

where the symbol $M_{\mathbf{G}}^{-1}$ denotes the inverse mark table of $\mathbf{G}$.

2.2 Restricted Partial Cycle Indices (Without Chirality Fittingness)

Just as the usual PCI-CFs are transformed into PCIs (without chirality fittingness) [3], restricted PCI-CFs defined by Def. 1 can be degenerated into restricted PCIs (without chirality fittingness) by putting $\$_{d_{jk}}^{(i\alpha)} = s_{d_{jk}}^{(i\alpha)}$, i.e., $a_{d_{jk}}^{(i\alpha)} = c_{d_{jk}}^{(i\alpha)} = c_{d_{jk}}^{(i\alpha)} = s_{d_{jk}}^{(i\alpha)}$. This degeneration means that the chiralilty/achirality of a (pro)ligand is neglected so that three-dimensional structures are degenerated into graphs in one extreme. To do this degeneration, the restricted SCI-CFs given in Lemma 1 of Part II of this series, i.e., $\overline{\text{SCI-CF}}(\mathbf{G}_j;\$_{d_{jk}}^{(i\alpha)})$, is degenerated into the restricted SCIs, i.e., $\overline{\text{SCI}}(\mathbf{G}_j;s_{d_{jk}}^{(i\alpha)})$, which is used to the following definition in a parallel way to Def. 1:

Definition 2 (Restricted PCIs (without chirality fittingness)) The restricted PCIs are defined as follows:

$$\overline{\text{PCI}}(\mathbf{G}_i;s_{d_{jk}}^{(i\alpha)}) = \sum_{j=1}^{s} \overline{m}_{ji}\overline{\text{SCI}}(\mathbf{G}_j;s_{d_{jk}}^{(i\alpha)}) \quad (11)$$

for $i = 1,2,\ldots,s$, where the restricted SCI in the right-hand side, i.e., $\overline{\text{SCI}}(\mathbf{G}_j;s_{d_{jk}}^{(i\alpha)})$, is derived from the restricted SCI-CF given in Lemma 1 of Part II of this series by putting $\$_{d_{jk}}^{(i\alpha)} = s_{d_{jk}}^{(i\alpha)}$.

Obviously, $\overline{\text{PCI}}(\mathbf{G}_i;s_{d_{jk}}^{(i\alpha)}) = \overline{\text{PCI-CF}}(\mathbf{G}_i;\$_{d_{jk}}^{(i\alpha)})$, when we place $\$_{d_{jk}}^{(i\alpha)} = s_{d_{jk}}^{(i\alpha)}$. It follows that Theorem 1 is degenerated into the following theorem by placing $\$_{d_{jk}}^{(i\alpha)} = s_{d_{jk}}^{(i\alpha)}$, i.e., $a_{d_{jk}}^{(i\alpha)} = c_{d_{jk}}^{(i\alpha)} = c_{d_{jk}}^{(i\alpha)} = s_{d_{jk}}^{(i\alpha)}$.

Theorem 2 (Enumerations by Restricted PCIs) Generating functions for obtaining the numbers $B_{\theta i}$ of $\mathbf{G}_i$-derivatives with weight W_θ under the restricted condition and without considering the chirality/achirality of substituents are calculated by the following equations:

$$\sum_{[\theta]} B_{\theta i} W_\theta = \overline{\text{PCI}}(\mathbf{G}_i;s_{d_{jk}}^{(i\alpha)}) \quad (12)$$

for $i = 1, 2, \ldots, s$, where the variable $s_{d_{jk}}^{(i\alpha)}$ is substituted by

$$s_{d_{jk}}^{(i\alpha)} = \sum_{\ell=1}^{|\mathrm{X}|} w_{i\alpha} (\mathrm{X}_{\ell}^{(a)})^{d_{jk}}. \tag{13}$$

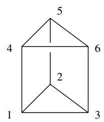
The words "without considering the chirality/achirality of substituents" indicate that Theorem 2 is effective in graph enumerations. The enumeration based on Theorem 2 is also called *the restricted PCI (RPCI) method.*

2.3 Illustrative Example

2.3.1 Restricted PCI-CFs for the Trigonal Prismatic Skeleton

The same problem of Part II on counting derivatives of a trigonal prismatic skeleton (**1**) under the restricted condition is alternatively solved by using restricted PCI-CFs formulated above:

> Consider the vertices and the edges of a trigonal prismatic skeleton (**1**) as substitution sites. Monodentate ligands (X, p, and $\overline{\mathrm{p}}$), where X is an achiral ligand and p/$\overline{\mathrm{p}}$ represents an enantiomeric pair of chiral monodentate ligands, are placed on the vertices and bidentate ligands (Z's) are placed on the edges under the restricted condition that no occupation of common vertices (or no occupation of adjacent edges) occurs. Evaluate the numbers of such derivatives.



1

Figure 1: Trigonal prismatic skeleton

The point group $\mathbf{D}_{3h}$ of the trigonal prismatic skeleton (**1**) is characterized by the following non-redundant set of subgroups:

$$\mathrm{SSG}_{\mathbf{D}_{3h}} = \{\mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_s, \mathbf{C}'_s, \mathbf{C}_3, \mathbf{C}_{2v}, \mathbf{C}_{3v}, \mathbf{C}_{3h}, \mathbf{D}_3, \mathbf{D}_{3h}\}. \tag{14}$$

The restricted SCI-CFs necessary to the present RPCI method (cf. Def. 1) are cited from the Table 1 of Part II of this series as follows:

$$\begin{aligned}
\overline{\text{SCI-CF}}(\mathbf{C}_1; \$_d, \tilde{\$}_d, \hat{\$}_d) &= b_1^6 + 6b_1^2\tilde{b}_1\hat{b}_1 + 3b_1^2\hat{b}_1^2 + 9b_1^2\tilde{b}_1^2 + 3b_1^4\hat{b}_1 \\
&\quad + 6b_1^4\tilde{b}_1 + 3\tilde{b}_1^2\hat{b}_1 + \hat{b}^3 && (15) \\
\overline{\text{SCI-CF}}(\mathbf{C}_2; \$_d, \tilde{\$}_d, \hat{\$}_d) &= b_2^3 + b_2^2\hat{b}_1 + 3b_2\tilde{b}_2 + b_2\hat{b}_2 + \tilde{b}_2\hat{b}_1 + \hat{b}_1\hat{b}_2 && (16) \\
\overline{\text{SCI-CF}}(\mathbf{C}_s; \$_d, \tilde{\$}_d, \hat{\$}_d) &= a_1^2c_2^2 + 2c_2\tilde{a}_1\hat{a}_1 + 2a_1^2c_2\tilde{a}_1 + a_1^2\tilde{a}_1^2 + c_2^2\hat{a}_1 \\
&\quad + \tilde{a}_1^2\hat{a}_1 + a_1^2\hat{c}_2 + \tilde{a}_1\hat{c}_2 && (17) \\
\overline{\text{SCI-CF}}(\mathbf{C}'_s; \$_d, \tilde{\$}_d, \hat{\$}_d) &= c_2^3 + \hat{a}_1^3 + 3\tilde{c}_2\hat{a}_1 + 3c_2\tilde{c}_2 + 3c_2^2\hat{a}_1 + 3c_2\hat{a}_1^2 && (18)
\end{aligned}$$

$$
\begin{aligned}
\overline{\text{SCI-CF}}(\mathbf{C}_3; \$_d, \tilde{\$}_d, \hat{\$}_d) &= b_3^2 + \hat{b}_3 && (19)\\
\overline{\text{SCI-CF}}(\mathbf{C}_{2v}; \$_d, \tilde{\$}_d, \hat{\$}_d) &= a_2c_4 + a_2\tilde{a}_2 + a_2\hat{a}_2 + \hat{a}_1\hat{a}_2 + \tilde{a}_2\hat{a}_1 + c_4\hat{a}_1 && (20)\\
\overline{\text{SCI-CF}}(\mathbf{C}_{3v}; \$_d, \tilde{\$}_d, \hat{\$}_d) &= a_3^2 + \hat{a}_3 && (21)\\
\overline{\text{SCI-CF}}(\mathbf{C}_{3h}; \$_d, \tilde{\$}_d, \hat{\$}_d) &= c_6 + \hat{a}_3 && (22)\\
\overline{\text{SCI-CF}}(\mathbf{D}_3; \$_d, \tilde{\$}_d, \hat{\$}_d) &= b_6 + \hat{b}_3 && (23)\\
\overline{\text{SCI-CF}}(\mathbf{D}_{3h}; \$_d, \tilde{\$}_d, \hat{\$}_d) &= a_6 + \hat{a}_3 && (24)
\end{aligned}
$$

Note that the symbol $\$_{d_{jk}}^{(i\alpha)}$ ($\$ = a, b, c$) in the right-hand side of Eq. 1 is replaced by $\$_d$ ($\$ = a, b, c$) for suborbits generated from the orbit of vertices governed by $\mathbf{D}_{3h}(/\mathbf{C}_s)$, by $\tilde{\$}_d$ ($\tilde{\$} = \tilde{a}, \tilde{b}, \tilde{c}$) for suborbits generated from the orbit of edges governed by $\mathbf{D}_{3h}(/\mathbf{C}_s)$, and by $\hat{\$}_d$ ($\hat{\$} = \hat{a}, \hat{b}, \hat{c}$) for suborbits generated from the orbit of edges governed by $\mathbf{D}_{3h}(/\mathbf{C}_{2v})$.

According to Eq. 1 of Def. 1, the restricted SCI-CFs (Eqs. 15–24) and the inverse mark table of $\mathbf{D}_{3h}$ [3, 8] give the following set of restricted PCI-CFs:

$$
\begin{aligned}
\overline{\text{PCI-CF}}(\mathbf{C}_1; \$_d, \tilde{\$}_d, \hat{\$}_d) &= \frac{1}{12}\overline{\text{SCI-CF}}(\mathbf{C}_1; \$_d, \tilde{\$}_d, \hat{\$}_d) - \frac{1}{4}\overline{\text{SCI-CF}}(\mathbf{C}_2; \$_d, \tilde{\$}_d, \hat{\$}_d)\\
&\quad - \frac{1}{4}\overline{\text{SCI-CF}}(\mathbf{C}_s; \$_d, \tilde{\$}_d, \hat{\$}_d) - \frac{1}{12}\overline{\text{SCI-CF}}(\mathbf{C}'_s; \$_d, \tilde{\$}_d, \hat{\$}_d)\\
&\quad - \frac{1}{12}\overline{\text{SCI-CF}}(\mathbf{C}_3; \$_d, \tilde{\$}_d, \hat{\$}_d) + \frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{C}_{2v}; \$_d, \tilde{\$}_d, \hat{\$}_d)\\
&\quad + \frac{1}{4}\overline{\text{SCI-CF}}(\mathbf{C}_{3v}; \$_d, \tilde{\$}_d, \hat{\$}_d) + \frac{1}{12}\overline{\text{SCI-CF}}(\mathbf{C}_{3h}; \$_d, \tilde{\$}_d, \hat{\$}_d)\\
&\quad + \frac{1}{4}\overline{\text{SCI-CF}}(\mathbf{D}_3; \$_d, \tilde{\$}_d, \hat{\$}_d) - \frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{D}_{3h}; \$_d, \tilde{\$}_d, \hat{\$}_d)\\
&= \frac{1}{6}\hat{b}_3 - \frac{1}{6}\hat{a}_3 + \frac{1}{12}c_6 + \frac{1}{4}b_6 + \frac{1}{4}b_1^2\hat{b}_1^2 + \frac{3}{4}b_1^2\tilde{b}_1^2 + \frac{1}{4}b_1^4\hat{b}_1\\
&\quad + \frac{1}{2}b_1^4\tilde{b}_1 + \frac{1}{4}\tilde{b}_1^2\hat{b}_1 - \frac{1}{4}b_2^2\hat{b}_1 - \frac{1}{4}\tilde{b}_2\hat{b}_1 - \frac{1}{4}b_2\hat{b}_2 - \frac{1}{4}\hat{b}_1\hat{b}_2\\
&\quad - \frac{3}{4}b_2\tilde{b}_2 - \frac{1}{4}a_1^2\tilde{a}_1^2 - \frac{1}{4}a_1^2c_2^2 - \frac{1}{2}c_2^2\hat{a}_1 - \frac{1}{4}\tilde{a}_1^2\hat{a}_1 - \frac{1}{4}a_1^2\hat{c}_2\\
&\quad - \frac{1}{4}\hat{a}_1\hat{c}_2 - \frac{1}{4}\tilde{c}_2\hat{a}_1 - \frac{1}{4}c_2\tilde{c}_2 - \frac{1}{4}c_2\hat{a}_1^2 + \frac{1}{2}a_2\hat{a}_2 + \frac{1}{2}a_2c_4\\
&\quad + \frac{1}{2}\hat{a}_1\hat{a}_2 + \frac{1}{2}a_2\tilde{a}_2 + \frac{1}{2}\tilde{a}_2\hat{a}_1 + \frac{1}{2}c_4\hat{a}_1 + \frac{1}{12}b_1^6\\
&\quad + \frac{1}{12}\hat{b}_1^3 - \frac{1}{4}b_2^3 - \frac{1}{12}c_2^3 - \frac{1}{12}\hat{a}_1^3 - \frac{1}{12}b_3^2 + \frac{1}{4}a_3^2 + \frac{1}{2}b_1^2\tilde{b}_1\hat{b}_1\\
&\quad - \frac{1}{2}c_2\tilde{a}_1\hat{a}_1 - \frac{1}{2}a_1^2c_2\tilde{a}_1 - \frac{1}{2}a_6 && (25)\\
\overline{\text{PCI-CF}}(\mathbf{C}_2; \$_d, \tilde{\$}_d, \hat{\$}_d) &= \frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{C}_2; \$_d, \tilde{\$}_d, \hat{\$}_d) - \frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{C}_{2v}; \$_d, \tilde{\$}_d, \hat{\$}_d)\\
&\quad - \frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{D}_3; \$_d, \tilde{\$}_d, \hat{\$}_d) + \frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{D}_{3h}; \$_d, \tilde{\$}_d, \hat{\$}_d)\\
&= \frac{1}{2}b_2^3 + \frac{1}{2}b_2^2\hat{b}_1 + \frac{3}{2}b_2\tilde{b}_2 + \frac{1}{2}\tilde{b}_2\hat{b}_1 + \frac{1}{2}b_2\hat{b}_2 + \frac{1}{2}\hat{b}_1\hat{b}_2 - \frac{1}{2}a_2\hat{a}_2\\
&\quad - \frac{1}{2}a_2c_4 - \frac{1}{2}a_2\tilde{a}_2 - \frac{1}{2}\hat{a}_1\hat{a}_2 - \frac{1}{2}\tilde{a}_2\hat{a}_1 - \frac{1}{2}c_4\hat{a}_1 - \frac{1}{2}\hat{b}_3 - \frac{1}{2}b_6\\
&\quad + \frac{1}{2}\hat{a}_3 + \frac{1}{2}a_6 && (26)
\end{aligned}
$$

$$
\begin{aligned}
\overline{\text{PCI-CF}}(\mathbf{C}_s;\$_d,\tilde{\$}_d,\hat{\$}_d) &= \frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{C}_s;\$_d,\tilde{\$}_d,\hat{\$}_d)-\frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{C}_{2v};\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&\quad -\frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{C}_{3v};\$_d,\tilde{\$}_d,\hat{\$}_d)+\frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{D}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&= c2\tilde{a}_1\hat{a}_1+a1^2c_2\tilde{a}_1+\frac{1}{2}a_1^2c_2^2+\frac{1}{2}a_1^2\tilde{a}_1^2+\frac{1}{2}c_2^2\hat{a}_1+\frac{1}{2}\tilde{a}_1^2\hat{a}_1\\
&\quad +\frac{1}{2}a_1^2\hat{c}_2+\frac{1}{2}\hat{a}_1\hat{c}_2-\frac{1}{2}a_2\hat{a}_2-\frac{1}{2}a_2c_4-\frac{1}{2}a_2\tilde{a}_2-\frac{1}{2}\hat{a}_1\hat{a}_2\\
&\quad -\frac{1}{2}\tilde{a}_2\hat{a}_1-\frac{1}{2}c_4\hat{a}_1-\frac{1}{2}a_3^2+\frac{1}{2}a_6 \qquad (27)\\
\overline{\text{PCI-CF}}(\mathbf{C}'_s;\$_d,\tilde{\$}_d,\hat{\$}_d) &= \frac{1}{6}\overline{\text{SCI-CF}}(\mathbf{C}'_s;\$_d,\tilde{\$}_d,\hat{\$}_d)-\frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{C}_{2v};\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&\quad -\frac{1}{6}\overline{\text{SCI-CF}}(\mathbf{C}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d)+\frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{D}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&= \frac{1}{6}c_2^3+\frac{1}{6}\hat{a}_1^3+\frac{1}{2}\tilde{c}_2\hat{a}_1+\frac{1}{2}c_2\tilde{c}_2+\frac{1}{2}c_2^2\hat{a}_1+\frac{1}{2}c_2\hat{a}_1^2\\
&\quad -\frac{1}{2}a_2\hat{a}_2-\frac{1}{2}a_2c_4-\frac{1}{2}a_2\tilde{a}_2-\frac{1}{2}\hat{a}_1\hat{a}_2-\frac{1}{2}\tilde{a}_2\hat{a}_1-\frac{1}{2}c_4\hat{a}_1\\
&\quad +\frac{1}{3}\hat{a}_3-\frac{1}{6}c_6+\frac{1}{2}a_6 \qquad (28)\\
\overline{\text{PCI-CF}}(\mathbf{C}_3;\$_d,\tilde{\$}_d,\hat{\$}_d) &= \frac{1}{4}\overline{\text{SCI-CF}}(\mathbf{C}_3;\$_d,\tilde{\$}_d,\hat{\$}_d)-\frac{1}{4}\overline{\text{SCI-CF}}(\mathbf{C}_{3v};\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&\quad -\frac{1}{4}\overline{\text{SCI-CF}}(\mathbf{C}_3h;\$_d,\tilde{\$}_d,\hat{\$}_d)-\frac{1}{4}\overline{\text{SCI-CF}}(\mathbf{D}_3;\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&\quad +\frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{D}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&= \frac{1}{4}b_3^2-\frac{1}{4}a_3^2-\frac{1}{4}c_6-\frac{1}{4}b_6+\frac{1}{2}a_6 \qquad (29)\\
\overline{\text{PCI-CF}}(\mathbf{C}_{2v};\$_d,\tilde{\$}_d,\hat{\$}_d) &= \overline{\text{SCI-CF}}(\mathbf{C}_{2v};\$_d,\tilde{\$}_d,\hat{\$}_d)-\overline{\text{SCI-CF}}(\mathbf{C}_{2v};\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&= a_2\hat{a}_2+a_2c_4+a_2\tilde{a}_2+\hat{a}_1\hat{a}_2+\tilde{a}_2\hat{a}_1+c_4\hat{a}_1-\hat{a}_3-a_6 \qquad (30)\\
\overline{\text{PCI-CF}}(\mathbf{C}_{3v};\$_d,\tilde{\$}_d,\hat{\$}_d) &= \frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{C}_{3v};\$_d,\tilde{\$}_d,\hat{\$}_d)-\frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{D}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&= \frac{1}{2}a_3^2-\frac{1}{2}a_6 \qquad (31)\\
\overline{\text{PCI-CF}}(\mathbf{C}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d) &= \frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{C}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d)-\frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{D}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&= \frac{1}{2}c_6-\frac{1}{2}a_6 \qquad (32)\\
\overline{\text{PCI-CF}}(\mathbf{D}_3;\$_d,\tilde{\$}_d,\hat{\$}_d) &= \frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{D}_3;\$_d,\tilde{\$}_d,\hat{\$}_d)-\frac{1}{2}\overline{\text{PCI-CF}}(\mathbf{D}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&= \frac{1}{2}\hat{b}_3+\frac{1}{2}b_6-\frac{1}{2}\hat{a}_3-\frac{1}{2}a_6 \qquad (33)\\
\overline{\text{PCI-CF}}(\mathbf{D}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d) &= \overline{\text{SCI-CF}}(\mathbf{D}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&= \hat{a}_3+a_6 \qquad (34)
\end{aligned}
$$

The inventory functions for vertex substitution is obtained by applying Eqs. 5–7 of Theorem 1 to the present case. Thereby, the following inventory functions are obtained:

$$\begin{aligned} a_d &= 1+\mathrm{X}^d &(35)\\ b_d &= 1+\mathrm{X}^d+\mathrm{p}^d+\overline{\mathrm{p}}^d &(36)\\ c_d &= 1+\mathrm{X}^d+2\mathrm{p}^{d/2}\overline{\mathrm{p}}^{d/2} &(37)\end{aligned}$$

On the other hand, the inventory function for edge substitution is obtained by applying Eqs. 5–7 of Theorem 1 to the present case.

$$\begin{aligned} \tilde{a}_d=\tilde{b}_d=\tilde{c}_d &= \mathrm{Z}^d &(38)\\ \hat{a}_d=\hat{b}_d=\hat{c}_d &= \mathrm{Z}^d &(39)\end{aligned}$$

The inventory functions for vertex substitution (Eqs. 35–37) as well as the inventory functions for edge substitution (Eqs. 38 and 39) are introduced into the restricted PCI-CFs (Eqs. 25–34). The resulting equations are expanded to give the following generating functions of respective subsymmetries (cf. $\mathrm{SSG}_{\mathbf{D}_{3h}}$ of Eq. 14) for counting derivatives under the restricted condition:

$$\begin{aligned} f(\mathbf{C}_1) = {} & \mathrm{X}^3+\frac{1}{2}(\mathrm{p}+\overline{\mathrm{p}})+\frac{1}{2}(\mathrm{p}^2+\overline{\mathrm{p}}^2)+\frac{3}{2}(\mathrm{p}^3+\overline{\mathrm{p}}^3)+\mathrm{p}\overline{\mathrm{p}}+5\mathrm{p}^2\overline{\mathrm{p}}^2+\mathrm{p}^3\overline{\mathrm{p}}^3+\frac{5}{2}(\mathrm{Xp}+\mathrm{X}\overline{\mathrm{p}})\\ & +5(\mathrm{X}^2\mathrm{p}+\mathrm{X}^2\overline{\mathrm{p}})+5(\mathrm{Xp}^2+\mathrm{X}\overline{\mathrm{p}}^2)+5(\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{p}\overline{\mathrm{p}}^2)+8\mathrm{Xp}\overline{\mathrm{p}}+12\mathrm{X}^2\mathrm{p}\overline{\mathrm{p}}\\ & +15(\mathrm{Xp}^2\overline{\mathrm{p}}+\mathrm{Xp}\overline{\mathrm{p}}^2)+\frac{1}{2}(\mathrm{p}^4+\overline{\mathrm{p}}^4)+5(\mathrm{Xp}^3+\mathrm{X}\overline{\mathrm{p}}^3)+5(\mathrm{X}^3\mathrm{p}+\mathrm{X}^3\overline{\mathrm{p}})\\ & +6(\mathrm{X}^2\mathrm{p}^2+\mathrm{X}^2\overline{\mathrm{p}}^2)+5(\mathrm{p}\overline{\mathrm{p}}^3+\mathrm{p}^3\overline{\mathrm{p}})+8\mathrm{X}^3\mathrm{p}\overline{\mathrm{p}}+\mathrm{X}^4\mathrm{p}\overline{\mathrm{p}}+5\mathrm{X}^2\mathrm{p}^2\overline{\mathrm{p}}^2+13\mathrm{Xp}^2\overline{\mathrm{p}}^2\\ & +15(\mathrm{X}^2\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{X}^2\mathrm{p}\overline{\mathrm{p}}^2)+10(\mathrm{Xp}\overline{\mathrm{p}}^3+\mathrm{Xp}^3\overline{\mathrm{p}})+\frac{5}{2}(\mathrm{Xp}^4+\mathrm{X}\overline{\mathrm{p}}^4)+5(\mathrm{X}^2\mathrm{p}^3+\mathrm{X}^2\overline{\mathrm{p}}^3)\\ & +\frac{5}{2}(\mathrm{X}^4\mathrm{p}+\mathrm{X}^4\overline{\mathrm{p}})+5(\mathrm{X}^3\mathrm{p}^2+\mathrm{X}^3\overline{\mathrm{p}}^2)+5(\mathrm{p}^3\overline{\mathrm{p}}^2+\mathrm{p}^2\overline{\mathrm{p}}^3)+\frac{1}{2}(\mathrm{p}^5+\overline{\mathrm{p}}^5)\\ & +\frac{5}{2}(\mathrm{p}\overline{\mathrm{p}}^4+\mathrm{p}^4\overline{\mathrm{p}})+\frac{1}{2}(\mathrm{X}^2\mathrm{p}^4+\mathrm{X}^2\overline{\mathrm{p}}^4)+\frac{3}{2}(\mathrm{X}^3\mathrm{p}^3+\mathrm{X}^3\overline{\mathrm{p}}^3)+\frac{1}{2}(\mathrm{X}^5\mathrm{p}+\mathrm{X}^5\overline{\mathrm{p}})\\ & +\frac{1}{2}(\mathrm{X}^4\mathrm{p}^2+\mathrm{X}^4\overline{\mathrm{p}}^2)+\frac{1}{2}(\mathrm{Xp}^5+\mathrm{X}\overline{\mathrm{p}}^5)+5(\mathrm{X}^3\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{X}^3\mathrm{p}\overline{\mathrm{p}}^2)+5(\mathrm{X}^2\mathrm{p}\overline{\mathrm{p}}^3+\mathrm{X}^2\mathrm{p}^3\overline{\mathrm{p}})\\ & +5(\mathrm{Xp}^3\overline{\mathrm{p}}^2+\mathrm{Xp}^2\overline{\mathrm{p}}^3)+\frac{5}{2}(\mathrm{Xp}\overline{\mathrm{p}}^4+\mathrm{Xp}^4\overline{\mathrm{p}})+\frac{1}{2}(\mathrm{p}^4\overline{\mathrm{p}}^2+\mathrm{p}^2\overline{\mathrm{p}}^4)+\frac{1}{2}(\mathrm{p}\overline{\mathrm{p}}^5+\mathrm{p}^5\overline{\mathrm{p}})\\ & +\{2\mathrm{X}+2\mathrm{X}^2+2\mathrm{X}^3+3(\mathrm{p}+\overline{\mathrm{p}})+4(\mathrm{p}^2+\overline{\mathrm{p}}^2)+3(\mathrm{p}^3+\overline{\mathrm{p}}^3)+6\mathrm{p}\overline{\mathrm{p}}+3\mathrm{p}^2\overline{\mathrm{p}}^2\\ & +9(\mathrm{Xp}+\mathrm{X}\overline{\mathrm{p}})+9(\mathrm{X}^2\mathrm{p}+\mathrm{X}^2\overline{\mathrm{p}})+9\mathrm{X}(\mathrm{p}^2+\mathrm{X}\overline{\mathrm{p}}^2)+9(\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{p}\overline{\mathrm{p}}^2)+16\mathrm{Xp}\overline{\mathrm{p}}\\ & +6\mathrm{X}^2\mathrm{p}\overline{\mathrm{p}}+9(\mathrm{Xp}^2\overline{\mathrm{p}}+\mathrm{Xp}\overline{\mathrm{p}}^2)+\frac{1}{2}(\mathrm{p}^4+\overline{\mathrm{p}}^4)+3(\mathrm{Xp}^3+\mathrm{X}\overline{\mathrm{p}}^3)+3(\mathrm{X}^3\mathrm{p}+\mathrm{X}^3\overline{\mathrm{p}})\\ & +4(\mathrm{X}^2\mathrm{p}^2+\mathrm{X}^2\overline{\mathrm{p}}^2)+3(\mathrm{p}\overline{\mathrm{p}}^3+\mathrm{p}^3\overline{\mathrm{p}})\}\mathrm{Z}\\ & +\{2\mathrm{X}+3(\mathrm{Xp}+\mathrm{X}\overline{\mathrm{p}})+\frac{1}{2}(\mathrm{p}^2+\overline{\mathrm{p}}^2)+\mathrm{p}\overline{\mathrm{p}}+3(\mathrm{p}+\overline{\mathrm{p}})\}\mathrm{Z}^2 & (40)\end{aligned}$$

$$\begin{aligned} f(\mathbf{C}_2) = {} & \mathrm{X}^2+\mathrm{X}^4+3(\mathrm{X}^2\mathrm{p}^2+\mathrm{X}^2\overline{\mathrm{p}}^2)+\frac{3}{2}(\mathrm{p}^2\overline{\mathrm{p}}^4+\mathrm{p}^4\overline{\mathrm{p}}^2)+\frac{3}{2}(\mathrm{p}^2+\overline{\mathrm{p}}^2)\\ & +\frac{3}{2}(\mathrm{X}^4\mathrm{p}^2+\mathrm{X}^4\overline{\mathrm{p}}^2)+\frac{3}{2}(\mathrm{X}^2\mathrm{p}^4+\mathrm{X}^2\overline{\mathrm{p}}^4)+\frac{3}{2}(\mathrm{p}^4+\overline{\mathrm{p}}^4)+2\mathrm{p}^2\overline{\mathrm{p}}^2+2\mathrm{X}^2\mathrm{p}^2\overline{\mathrm{p}}^2\\ & +\{\mathrm{X}^2+(\mathrm{X}^2\mathrm{p}^2+\mathrm{X}^2\overline{\mathrm{p}}^2)+(\mathrm{p}^2+\overline{\mathrm{p}}^2)+\frac{1}{2}(\mathrm{p}^4+\overline{\mathrm{p}}^4)\}\mathrm{Z}\end{aligned}$$

$$
\begin{aligned}
& +\{1+X^2+2(p^2+\overline{p}^2)\}Z^2 && (41)\\
f(\mathbf{C}_s) &= X+X^2+X^3+X^4+4Xp^2\overline{p}^2+X^2p^2\overline{p}^2+4X^3p\overline{p}+4Xp\overline{p} \\
& +4X^2p\overline{p}+2p\overline{p}+X^5+2X^4p\overline{p}+p^2\overline{p}^2 \\
& +\{1+2X+3X^2+2X^3+X^4+4Xp\overline{p}+4X^2p\overline{p}+4p\overline{p}+p^2\overline{p}^2\}Z \\
& +\{1+2X+X^2+2p\overline{p}\}Z^2 && (42)\\
f(\mathbf{C}'_s) &= p^2\overline{p}^2+X^2p^2\overline{p}^2+2X^2p\overline{p}+p\overline{p}+X^4p\overline{p}+p^3\overline{p}^3 \\
& +(X^2+p^2\overline{p}^2+2p\overline{p}+2X^2p\overline{p})Z+2p\overline{p}Z^2 && (43)\\
f(\mathbf{C}_3) &= \frac{1}{2}(p^3+\overline{p}^3)+\frac{1}{2}(X^3p^3+X^3\overline{p}^3) && (44)\\
f(\mathbf{C}_{2v}) &= X^2+X^4+2X^2p^2\overline{p}^2+2p^2\overline{p}^2+\{1+X^4+2p^2\overline{p}^2\}Z+(2+2X^2)Z^2+Z^3 && (45)\\
f(\mathbf{C}_{3v}) &= X^3 && (46)\\
f(\mathbf{C}_{3h}) &= p^3\overline{p}^3 && (47)\\
f(\mathbf{D}_3) &= \frac{1}{2}(p^6+\overline{p}^6) && (48)\\
f(\mathbf{D}_{3h}) &= 1+X^6+Z^3 && (49)
\end{aligned}
$$

The processes of calculating generating functions by the RPCI method are programmed by using the Maple programming language [9]. The source list of a sample program for obtaining Eqs. 40–49 (named “prismPCI2-2-1BR.mpl”) is attached as an Appendix.

The coefficient of the term $X^k p^l \overline{p}^m Z^n$ appearing in the generating function for each subgroup $\mathbf{G}_i$ of $\mathbf{D}_{3h}$ (Eqs. 40–49) represents the number of $\mathbf{G}_i$-derivatives with the formula $X^k p^l \overline{p}^m Z^n$. Such terms as containing p and $\overline{p}$ (chiral ligands) should be commented to explain the features of the present enumeration, where each enantiomeric pair of chiral ligands is counted once.

The coefficient 2 of the term $p^2\overline{p}^2$ in Eq. 41 shows the presence of two enantiomeric pairs of $\mathbf{C}_2$-derivatives (**2/$\overline{\mathbf{2}}$** and **3/$\overline{\mathbf{3}}$**), as shown in Fig. 2, where p is represented by a black solid circle and $\overline{p}$ is represented by a gray solid circle. Note that the two-fold axis of the subgroup $\mathbf{C}_2$ runs through the midpoint of the edge $\{1,4\}$ and the center of the face $\{2,3,5,6\}$. Because the term $p^2\overline{p}^2$ is converted into itself ($\overline{p}^2p^2$) by a mirror-image operation, the term $2p^2\overline{p}^2$ is formally interpreted as $2\times\frac{1}{2}(p^2\overline{p}^2+\overline{p}^2p^2)=2p^2\overline{p}^2$. Thus, an enantiomeric pair as a unit corresponds to $\frac{1}{2}(p^2\overline{p}^2+\overline{p}^2p^2)=p^2\overline{p}^2$.

On the other hand, the term $\frac{3}{2}(p^2+\overline{p}^2)$ in Eq. 41 should be interpreted to be $3\times\frac{1}{2}(p^2+\overline{p}^2)$, so that there are three enantiomeric pairs of $\mathbf{C}_2$-derivatives (**4/$\overline{\mathbf{4}}$**, **5/$\overline{\mathbf{5}}$**, and **6/$\overline{\mathbf{6}}$**), as shown in Fig. 2. Thus, an enantiomeric pair as a unit corresponds to $\frac{1}{2}(p^2+\overline{p}^2)$ in terms of the present formulation, because the term p^2 is converted into $\overline{p}^2$ by a mirror-image operation vice versa. On a similar line, the term $(p^2+\overline{p}^2)Z$ in Eq. 41 should be interpreted to be $2\times\frac{1}{2}(p^2+\overline{p}^2)Z$, so that there are two enantiomeric pairs of $\mathbf{C}_2$-derivatives (**7/$\overline{\mathbf{7}}$** and **8/$\overline{\mathbf{8}}$**) as shown in Fig. 2.

When the term $p^2\overline{p}^2$ or $p^2\overline{p}^2Z$ corresponds to achiral derivatives, its coefficient represents the number of such achiral derivatives. For example, the term $p^2\overline{p}^2$ or $p^2\overline{p}^2Z$ in Eq. 42 shows the presence of one achiral derivative (**9** or **10**), as shown in Fig. 3. Note that the mirror plane of the subgroup $\mathbf{C}_s$ contains the edge $\{1,4\}$ and bisects the edges $\{2,3\}$ and $\{5,6\}$. Similarly, the term $p^2\overline{p}^2$ or $p^2\overline{p}^2Z$ in Eq. 43 shows the presence of one achiral derivative (**11** or **12**), as shown in Fig. 3. Note that the mirror plane of the subgroup $\mathbf{C}'_s$ bisects the edges $\{1,4\}$, $\{2,5\}$, and $\{3,6\}$.

In several cases, there appear phenomena akin to pseudoasymmetric cases. Thus, the term $2p^2\overline{p}^2$ in Eq. 45 shows the presence of two achiral $\mathbf{C}_{2v}$-derivatives (**13** and **14**), which are dia-

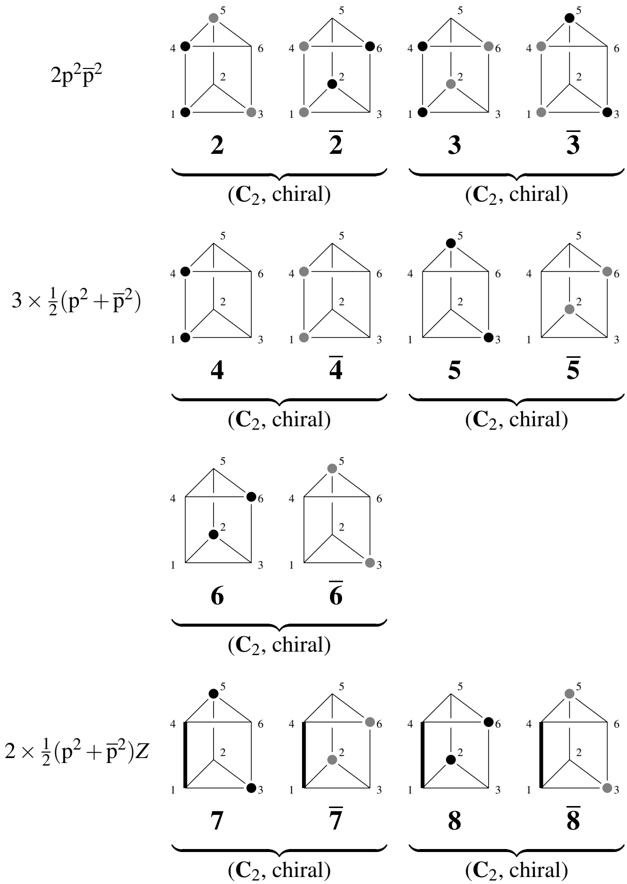
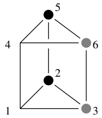


Figure 2: **C**$_2$-Derivatives with chiral ligands, where a chiral ligand p is represented by a black solid circle and its enantiomeric ligand $\overline{p}$ is represented by a gray solid circle. A bidentate ligand (Z) is represented by a boldfaced straight line. Two structures linked by an underbrace indicate an enantiomeric pair, which is counted once in the present methodology of enumerations.

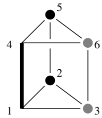
$p^2\overline{p}^2$



9

($\mathbf{C}_s$, achiral)

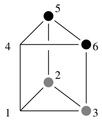
$p^2\overline{p}^2Z$



10

($\mathbf{C}_s$, achiral)

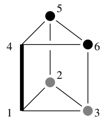
$p^2\overline{p}^2$



11

($\mathbf{C}'_s$, achiral)

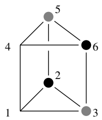
$p^2\overline{p}^2Z$



12

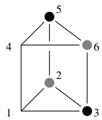
($\mathbf{C}'_s$, achiral)

$2p^2\overline{p}^2$



13

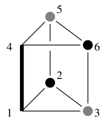
($\mathbf{C}_{2v}$, achiral)



14

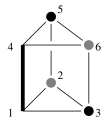
($\mathbf{C}_{2v}$, achiral)

$2p^2\overline{p}^2Z$



15

($\mathbf{C}_{2v}$, achiral)



16

($\mathbf{C}_{2v}$, achiral)

Figure 3: $\mathbf{C}_s$-, $\mathbf{C}'_s$-, and $\mathbf{C}_{2v}$-Derivatives with chiral ligands, where a chiral ligand p is represented by a black solid circle and its enantiomeric ligand $\overline{p}$ is represented by a gray solid circle. A bidentate ligand (Z) is represented by a boldfaced straight line.

stereomeric to each other so as to be regarded as an extended pseudoasymmetric case. Note that the two-fold axis of the subgroup $\mathbf{C}_{2v}$ runs through the midpoint of the edge $\{1,4\}$ and the center of the face $\{2,3,5,6\}$ and that one mirror plane of the subgroup $\mathbf{C}_{2v}$ contains the edge $\{1,4\}$ and bisects the edges $\{2,3\}$ and $\{5,6\}$ and the other mirror plane is a horizontal one bisecting the thee edges $\{1,4\}$, $\{2,5\}$, and $\{3,6\}$. Similarly, the term $2p^2\overline{p}^2Z$ in Eq. 45 shows the presence of two achiral $\mathbf{C}_{2v}$-derivatives (**15** and **16**), which are also diastereomeric to each other so as to be regarded as an extended pseudoasymmetric case.

As a matter of course, the results reported in Part II of this series (by the fixed-point matrix (FPM) method) are contained in Eqs. 40–49 as the coefficients of the terms 1, Z, Z^2, Z^3, $p\overline{p}$, $Xp\overline{p}$, $p\overline{p}Z$, and $Xp\overline{p}Z$. For example, the coefficients of the term Z^3 are 1 for $\mathbf{C}_{2v}$ (Eq. 45), 1 for $\mathbf{D}_{3h}$ (Eq. 49), and equal to zero for the other subgroups. This is identical with the result (the $[\theta]_1$-row) of the isomer-counting matrix (ICM) shown in Eq. 42 of Part II.

3 Gross Enumerations under the Restricted Condition

3.1 Total Numbers Under the Restricted Condition

According to Eq. 43 of Part II, the total number B_θ can be calculated by summing up $B_{\theta i}$ over all of the subgroups $\mathbf{G}_i$ ($i = 1,2,\ldots,s$) contained in the $\mathrm{SSG}_{\mathbf{G}}$ (Eq. 2):

$$B_\theta = \sum_{i=1}^{s} B_{\theta i} = \sum_{i=1}^{s}\sum_{j=1}^{s} \rho_{\theta j}\overline{m}_{ji} = \sum_{j=1}^{s} \rho_{\theta j}\left(\sum_{i=1}^{s}\overline{m}_{ji}\right). \tag{50}$$

On a similar line to Eq. 3, Eq. 50 can be converted into an expression for giving generating functions concerned with the weight (formula) W_θ:

$$\begin{aligned}\sum_{[\theta]} B_\theta W_\theta &= \sum_{[\theta]}\sum_{j=1}^{s} \rho_{\theta j}\left(\sum_{i=1}^{s}\overline{m}_{ji}\right) W_\theta = \sum_{j=1}^{s}\left(\sum_{i=1}^{s}\overline{m}_{ji}\right)\sum_{[\theta]}\rho_{\theta j} W_\theta \\ &= \sum_{j=1}^{s}\left(\sum_{i=1}^{s}\overline{m}_{ji}\right)\overline{\text{SCI-CF}}(\mathbf{G}_j;\$_{d_{jk}}^{(i\alpha)}) \overset{\text{def.}}{\equiv} \overline{\text{CI-CF}}(\mathbf{G};\$_{d_{jk}}^{(i\alpha)})\end{aligned} \tag{51}$$

The last part of Eq. 51 shows a definition of the restricted cycle index with chirality fittingness (CI-CF), which is proved easily to be equal to the sum of the restricted PCI-CFs shown in Def. 1, because the sum concerning i and the sum concerning j are interchangeable in their order of summing up. Then, we have the following definition:

Definition 3 (Restricted CI-CF for Counting Total Derivatives) The restricted CI-CF is defined as follows:

$$\overline{\text{CI-CF}}(\mathbf{G};\$_{d_{jk}}^{(i\alpha)}) = \sum_{i=1}^{s}\overline{\text{PCI-CF}}(\mathbf{G}_i;\$_{d_{jk}}^{(i\alpha)}) = \sum_{j=1}^{s}\left(\sum_{i=1}^{s}\overline{m}_{ji}\right)\overline{\text{SCI-CF}}(\mathbf{G}_j;\$_{d_{jk}}^{(i\alpha)}), \tag{52}$$

where the restricted SCI-CF in the right-hand side has been given in Lemma 1 of Part II of this series.

The delayed expansion described in Eq. 3 to give Theorem 1 can be also applied to Eq. 51. Thereby, we obtain a theorem for enumerations by the restricted CI-CF:

Theorem 3 (Gross Enumeration of Total Numbers by the Restricted CI-CF) Generating functions for obtaining the total numbers B_θ of derivatives with weight W_θ under the restricted condition are calculated by the following equations:

$$\sum_{[\theta]} B_\theta W_\theta = \overline{\text{CI-CF}}(\mathbf{G};\$_{d_{jk}}^{(i\alpha)}), \tag{53}$$

where the variables $\$_{d_{jk}}^{(i\alpha)}$ ($\$ = a,b,c$) are substituted by Eqs. 5–7.

It should be noted that the sum $\sum_{i=1}^{s}\overline{m}_{ji}$ for $\mathbf{G}_j$ vanishes to zero when $\mathbf{G}_j$ is a non-cyclic subgroup [10, 11]. This means that the restricted CI-CF (Def. 3) is concerned with cyclic subgroups only. To exemplify the disappearance of non-cyclic subgroups, we continue the enumeration of trigonal prismatic derivatives as follows.

The values of $\sum_{i=1}^{s} \overline{m}_{ji}$ for the group $\mathbf{D}_{3h}$ have already been reported in the "total"-column of the matrix for gross enumeration (Eq. 49 of Part II of this series). According to Def. 3, the restricted SCI-CFs for cyclic subgroups are selected from the restricted SCI-CFs (Eqs. 15–24) so as to give the following restricted CI-CF:

$$\begin{aligned}
\overline{\text{CI-CF}}(\mathbf{D}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d) &= \frac{1}{12}\overline{\text{SCI-CF}}(\mathbf{C}_1;\$_d,\tilde{\$}_d,\hat{\$}_d)+\frac{1}{4}\overline{\text{SCI-CF}}(\mathbf{C}_2;\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&\quad+\frac{1}{4}\overline{\text{SCI-CF}}(\mathbf{C}_s;\$_d,\tilde{\$}_d,\hat{\$}_d)+\frac{1}{12}\overline{\text{SCI-CF}}(\mathbf{C}'_s;\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&\quad+\frac{1}{6}\overline{\text{SCI-CF}}(\mathbf{C}_3;\$_d,\tilde{\$}_d,\hat{\$}_d)+\frac{1}{6}\overline{\text{SCI-CF}}(\mathbf{C}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d)\\
&= \frac{1}{12}b_1^6+\frac{1}{4}b_2^3+\frac{1}{6}b_3^2+\frac{3}{4}b_2\tilde{b}_2+\frac{3}{4}b_1^2\tilde{b}_1^2+\frac{1}{2}b_1^4\tilde{b}_1\\
&\quad+\frac{1}{4}b_1^2\hat{b}_1^2+\frac{1}{4}b_1^4\hat{b}_1+\frac{1}{4}b_2\hat{b}_2+\frac{1}{4}b_2^2\hat{b}_1\\
&\quad+\frac{1}{4}\tilde{b}_1^2\hat{b}_1+\frac{1}{4}\tilde{b}_2\hat{b}_1+\frac{1}{2}b_1^2\tilde{b}_1\hat{b}_1+\frac{1}{4}\hat{b}_1\hat{b}_2+\frac{1}{6}\hat{b}_3+\frac{1}{12}\hat{b}_1^3\\
&\quad+\frac{1}{4}a_1^2c_2^2+\frac{1}{12}c_2^3+\frac{1}{6}c_6+\frac{1}{4}a_1^2\tilde{a}_1^2+\frac{1}{2}a_1^2c_2\tilde{a}_1+\frac{1}{4}c_2\tilde{c}_2\\
&\quad+\frac{1}{4}a_1^2\hat{c}_2+\frac{1}{4}c_2\hat{a}_1^2+\frac{1}{2}c_2^2\hat{a}_1+\frac{1}{4}\tilde{a}_1^2\hat{a}_1+\frac{1}{4}\tilde{c}_2\hat{a}_1+\frac{1}{2}c_2\tilde{a}_1\hat{a}_1\\
&\quad+\frac{1}{4}\hat{a}_1\hat{c}_2+\frac{1}{6}\hat{a}_3+\frac{1}{12}\hat{a}_1^3. \qquad (54)
\end{aligned}$$

As a matter of course, Eq. 54 is alternatively obtained by summing up Eqs. 25–34, as formulated generally in Def. 3. Note that Eq. 54 contains only monomials due to cyclic subgroups because monomials for non-cyclic subgroups vanish to zero during this summation. These features of Def. 3 and Theorem 3 succeed to the general features of unrestricted enumerations [2].

The inventory functions for vertex substitution (Eqs. 35–37) as well as the inventory functions for edge substitution (Eqs. 38 and 39) are introduced to the restricted CI-CF (Eq. 54). The resulting equation is expanded to give the following generating function for obtaining the total numbers of derivatives under the restricted condition:

$$\begin{aligned}
f^{(g)} &= 1+\mathrm{X}+3\mathrm{X}^2+3\mathrm{X}^3+3\mathrm{X}^4+\mathrm{X}^5+\mathrm{X}^6+4\mathrm{p}\overline{\mathrm{p}}+11\mathrm{p}^2\overline{\mathrm{p}}^2+3\mathrm{p}^3\overline{\mathrm{p}}^3\\
&\quad+\frac{1}{2}(\mathrm{p}+\overline{\mathrm{p}})+2(\mathrm{p}^2+\overline{\mathrm{p}}^2)+2(\mathrm{p}^3+\overline{\mathrm{p}}^3)+\frac{1}{2}(\mathrm{p}^6+\overline{\mathrm{p}}^6)+5(\mathrm{X}^3\mathrm{p}^2+\mathrm{X}^3\overline{\mathrm{p}}^2)\\
&\quad+18\mathrm{X}^2\mathrm{p}\overline{\mathrm{p}}+12\mathrm{X}\mathrm{p}\overline{\mathrm{p}}+\frac{5}{2}(\mathrm{X}\mathrm{p}+\mathrm{X}\overline{\mathrm{p}})+5(\mathrm{X}^2\mathrm{p}+\mathrm{X}^2\overline{\mathrm{p}})+5(\mathrm{X}\mathrm{p}^2+\mathrm{X}\overline{\mathrm{p}}^2)\\
&\quad+5(\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{p}\overline{\mathrm{p}}^2)+15(\mathrm{X}\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{X}\mathrm{p}\overline{\mathrm{p}}^2)+12\mathrm{X}^3\mathrm{p}\overline{\mathrm{p}}+15(\mathrm{X}^2\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{X}^2\mathrm{p}\overline{\mathrm{p}}^2)\\
&\quad+17\mathrm{X}\mathrm{p}^2\overline{\mathrm{p}}^2+10(\mathrm{X}\mathrm{p}\overline{\mathrm{p}}^3+\mathrm{X}\mathrm{p}^3\overline{\mathrm{p}})+5(\mathrm{X}\mathrm{p}^3+\mathrm{X}\overline{\mathrm{p}}^3)+5(\mathrm{X}^3\mathrm{p}+\mathrm{X}^3\overline{\mathrm{p}})\\
&\quad+2(\mathrm{p}^4+\overline{\mathrm{p}}^4)+\frac{1}{2}(\mathrm{p}^5+\overline{\mathrm{p}}^5)+\frac{1}{2}(\mathrm{X}\mathrm{p}^5+\mathrm{X}\overline{\mathrm{p}}^5)+\frac{5}{2}(\mathrm{p}\overline{\mathrm{p}}^4+\mathrm{p}^4\overline{\mathrm{p}})+5(\mathrm{p}^3\overline{\mathrm{p}}^2+\mathrm{p}^2\overline{\mathrm{p}}^3)\\
&\quad+9(\mathrm{X}^2\mathrm{p}^2+\mathrm{X}^2\overline{\mathrm{p}}^2)+5(\mathrm{p}\overline{\mathrm{p}}^3+\mathrm{p}^3\overline{\mathrm{p}})+5(\mathrm{X}^2\mathrm{p}^3+\mathrm{X}^2\overline{\mathrm{p}}^3)+\frac{5}{2}(\mathrm{X}^4\mathrm{p}+\mathrm{X}^4\overline{\mathrm{p}})\\
&\quad+\frac{5}{2}(\mathrm{X}\mathrm{p}^4+\mathrm{X}\overline{\mathrm{p}}^4)+\frac{1}{2}(\mathrm{X}^5\mathrm{p}+\mathrm{X}^5\overline{\mathrm{p}})+2(\mathrm{p}^2\overline{\mathrm{p}}^4+\mathrm{p}^4\overline{\mathrm{p}}^2)+\frac{1}{2}(\mathrm{p}^5\overline{\mathrm{p}}+\mathrm{p}\overline{\mathrm{p}}^5)\\
&\quad+2(\mathrm{X}^3\mathrm{p}^3+\mathrm{X}^3\overline{\mathrm{p}}^3)+2(\mathrm{X}^2\mathrm{p}^4+\mathrm{X}^2\overline{\mathrm{p}}^4)+\frac{5}{2}(\mathrm{X}\mathrm{p}^4\overline{\mathrm{p}}+\mathrm{X}\mathrm{p}\overline{\mathrm{p}}^4)+2(\mathrm{X}^4\mathrm{p}^2+\mathrm{X}^4\overline{\mathrm{p}}^2)
\end{aligned}$$

$$
\begin{aligned}
&+4X^4 p\overline{p} + 5(X^3 p^2 \overline{p} + X^3 p\overline{p}^2) + 11X^2 p^2 \overline{p}^2 + 5(X^2 p\overline{p}^3 + X^2 p^3 \overline{p}) \\
&+5(Xp^2\overline{p}^3 + Xp^3\overline{p}^2) \\
&+\{2 + 4X + 7X^2 + 4X^3 + 2X^4 + 12p\overline{p} + 7p^2\overline{p}^2 + 3(p+\overline{p}) + 5(p^2+\overline{p}^2) \\
&+3(p^3+\overline{p}^3) + 12X^2 p\overline{p} + 20Xp\overline{p} + 9(Xp + X\overline{p}) + 9(X^2 p + X^2\overline{p}) + 9(Xp^2 + X\overline{p}^2) \\
&+9(p^2\overline{p} + p\overline{p}^2) + 9(Xp^2\overline{p} + Xp\overline{p}^2) + 3(Xp^3 + X\overline{p}^3) + 3(X^3 p + X^3\overline{p}) \\
&+(p^4+\overline{p}^4) + 5(X^2p^2 + X^2\overline{p}^2) + 3p\overline{p}^3 + 3p^3\overline{p}\}Z \\
&+\{4 + 4X + 4X^2 + 5p\overline{p} + 3(p+\overline{p}) + 3(Xp + X\overline{p}) + \frac{5}{2}(p^2+\overline{p}^2)\}Z^2 + 2Z^3. \qquad (55)
\end{aligned}
$$

Obviously, Eq. 55 is also obtained by summing up Eqs. 40–49.

3.2 Enumeration of Achiral Derivatives Under the Restricted Condition

According to Eq. 45 of Part II of this series, the number $B_\theta^{(a)}$ of achiral derivatives can be calculated by summing up $B_{\theta i}$ over all of the achiral subgroups $\mathbf{G}_{i_a}$ selected from the $\mathrm{SSG}_{\mathbf{G}}$ (Eq. 2), i.e.,

$$
B_\theta^{(a)} = \sum_{\forall i_a} B_{\theta i_a} = \sum_{\forall i_a} \sum_{j=1}^{s} \rho_{\theta j} \overline{m}_{j i_a} = \sum_{j=1}^{s} \rho_{\theta j} \left(\sum_{\forall i_a} \overline{m}_{j i_a} \right), \qquad (56)
$$

where the summation represented by $\sum_{\forall i_a}$ covers all the achiral subgroups.

On a similar line to Eq. 3, Eq. 56 can be converted into an expression for giving generating functions concerned with the weight (formula) W_θ:

$$
\begin{aligned}
\sum_{[\theta]} B_\theta^{(a)} W_\theta &= \sum_{[\theta]} \sum_{j=1}^{s} \rho_{\theta j} \left(\sum_{\forall i_a} \overline{m}_{j i_a} \right) W_\theta = \sum_{j=1}^{s} \left(\sum_{\forall i_a} \overline{m}_{j i_a} \right) \sum_{[\theta]} \rho_{\theta j} W_\theta \\
&= \sum_{j=1}^{s} \left(\sum_{\forall i_a} \overline{m}_{j i_a} \right) \overline{\text{SCI-CF}}(\mathbf{G}_j; \$_{d_{jk}}^{(i\alpha)}) \stackrel{\text{def.}}{\equiv} \overline{\text{CI-CF}}^{(a)}(\mathbf{G}; \$_{d_{jk}}^{(i\alpha)}). \qquad (57)
\end{aligned}
$$

The last part of Eq. 57 shows a definition of the restricted CI-CF for enumerating achiral derivatives. The restricted CI-CF is proved easily to be equal to the sum of the restricted PCI-CFs for achiral subgroups shown in Def. 1, because the sum concerning i and the sum concerning j are interchangeable in their order of summing up. Then, we have the following definition:

Definition 4 (Restricted CI-CF for Counting Achiral Derivative) The restricted CI-CF for counting achiral derivatives is defined as follows:

$$
\overline{\text{CI-CF}}^{(a)}(\mathbf{G}; \$_{d_{jk}}^{(i\alpha)}) = \sum_{\forall i_a} \overline{\text{PCI-CF}}(\mathbf{G}_i; \$_{d_{jk}}^{(i\alpha)}) = \sum_{j=1}^{s} \left(\sum_{\forall i_a} \overline{m}_{j i_a} \right) \overline{\text{SCI-CF}}(\mathbf{G}_j; \$_{d_{jk}}^{(i\alpha)}), \qquad (58)
$$

where the restricted SCI-CF in the right-hand side has been given in Lemma 1 of Part II of this series.

The delayed expansion described in Eq. 3 to give Theorem 1 can be also applied to Eq. 57. Thereby, we obtain a theorem for enumerating achiral derivatives by the restricted CI-CF:

Theorem 4 (Enumeration of Achiral Derivatives by the Restricted CI-CF) Generating functions for obtaining the numbers $B_\theta^{(a)}$ of achiral derivatives with weight W_θ under the restricted condition are calculated by the following equations:

$$\sum_{[\theta]} B_\theta^{(a)} W_\theta = \overline{\text{CI-CF}}^{(a)}(\mathbf{G}; \$_{d_{jk}}^{(i\alpha)}), \tag{59}$$

where the variables $\$_{d_{jk}}^{(i\alpha)}$ ($\$ = a, b, c$) are substituted by Eqs. 5–7.

The values of $\sum_{\forall i_a} \overline{m}_{ji_a}$ for the group $\mathbf{D}_{3h}$ have already been reported in the "achiral"-column of the matrix for gross enumeration (Eq. 49 of Part II of this series). According to Def. 4, the restricted SCI-CFs for achiral cyclic subgroups are selected from the restricted SCI-CFs (Eqs. 15–24) so as to give the following restricted CI-CF:

$$\begin{aligned}
\overline{\text{CI-CF}}^{(a)}(\mathbf{D}_{3h}; \$_d, \tilde{\$}_d, \hat{\$}_d) &= \frac{1}{2}\overline{\text{SCI-CF}}(\mathbf{C}_s; \$_d, \tilde{\$}_d, \hat{\$}_d) + \frac{1}{6}\overline{\text{SCI-CF}}(\mathbf{C}'_s; \$_d, \tilde{\$}_d, \hat{\$}_d) \\
&\quad + \frac{1}{3}\overline{\text{SCI-CF}}(\mathbf{C}_{3h}; \$_d, \tilde{\$}_d, \hat{\$}_d) \\
&= \frac{1}{2}a_1^2c_2^2 + \frac{1}{6}c_2^3 + \frac{1}{3}c_6 + \frac{1}{2}a_1^2\tilde{a}_1^2 + a_1^2c_2\tilde{a}_1 + \frac{1}{2}c_2\tilde{c}_2 \\
&\quad + \frac{1}{2}a_1^2\hat{c}_2 + \frac{1}{2}c_2\hat{a}_1^2 + c_2^2\hat{a}_1 + \frac{1}{2}\tilde{a}_1^2\hat{a}_1 + \frac{1}{2}\tilde{c}_2\hat{a}_1 + c_2\tilde{a}_1\hat{a}_1 \\
&\quad + \frac{1}{2}\hat{a}_1\hat{c}_2 + \frac{1}{3}\hat{a}_3 + \frac{1}{6}\hat{a}_1^3.
\end{aligned} \tag{60}$$

It is to be noted that the monomials appearing in the right-hand side of Eq. 60 contain a_d and c_d but no b_d, where their coefficients are twice of the counterparts appearing in Eq. 54.

The inventory functions for vertex substitution (Eqs. 35–37) as well as the inventory functions for edge substitution (Eqs. 38 and 39) are introduced to the restricted CI-CF (Eq. 60). The resulting equations are expanded to give the following generating function for obtaining the numbers of achiral derivatives under the restricted condition:

$$\begin{aligned}
f^{(a)} &= 1 + \mathrm{X} + 2\mathrm{X}^2 + 2\mathrm{X}^3 + 2\mathrm{X}^4 + \mathrm{X}^5 + \mathrm{X}^6 + 3\mathrm{X}^4\mathrm{p}\overline{\mathrm{p}} + 4\mathrm{X}^2\mathrm{p}^2\overline{\mathrm{p}}^2 + 3\mathrm{p}\overline{\mathrm{p}} \\
&\quad + 2\mathrm{p}^3\overline{\mathrm{p}}^3 + 4\mathrm{X}^3\mathrm{p}\overline{\mathrm{p}} + 4\mathrm{X}\mathrm{p}^2\overline{\mathrm{p}}^2 + 4\mathrm{X}\mathrm{p}\overline{\mathrm{p}} + 6\mathrm{X}^2\mathrm{p}\overline{\mathrm{p}} + 4\mathrm{p}^2\overline{\mathrm{p}}^2 \\
&\quad + (2 + 2\mathrm{X} + 4\mathrm{X}^2 + 2\mathrm{X}^3 + 2\mathrm{X}^4 + 6\mathrm{p}\overline{\mathrm{p}} + 4\mathrm{p}^2\overline{\mathrm{p}}^2 + 6\mathrm{X}^2\mathrm{p}\overline{\mathrm{p}} + 4\mathrm{X}\mathrm{p}\overline{\mathrm{p}})\mathrm{Z} \\
&\quad + (3 + 2\mathrm{X} + 3\mathrm{X}^2 + 4\mathrm{p}\overline{\mathrm{p}})\mathrm{Z}^2 + 2\mathrm{Z}^3.
\end{aligned} \tag{61}$$

Obviously, Eq. 61 is also obtained by summing up the results for achiral subgroups selected from Eqs. 40–49.

The term $4\mathrm{p}^2\overline{\mathrm{p}}^2$ in Eq. 61 shows the presence of four achiral derivatives of the formula $\mathrm{p}^2\overline{\mathrm{p}}^2$, which have been already depicted in Fig. 3, i.e., **9** ($\mathbf{C}_s$), **11** ($\mathbf{C}'_s$), **13** ($\mathbf{C}_{2v}$), and **14** ($\mathbf{C}_{2v}$). Similarly, the term $4\mathrm{p}^2\overline{\mathrm{p}}^2\mathrm{Z}$ in Eq. 61 shows the presence of four achiral derivatives of the formula $\mathrm{p}^2\overline{\mathrm{p}}^2Z$, which have been already depicted in Fig. 3, i.e., **10** ($\mathbf{C}_s$), **12** ($\mathbf{C}'_s$), **15** ($\mathbf{C}_{2v}$), and **16** ($\mathbf{C}_{2v}$).

3.3 Enumeration of Enantiomeric Pairs Under the Restricted Condition

According to Eq. 46 of Part II, the number $B_\theta^{(e)}$ of enantiomeric pairs of chiral derivatives can be calculated by summing up $B_{\theta i}$ over all of the achiral subgroups $\mathbf{G}_{i_e}$ selected from $\mathbf{G}_i$

$(i = 1, 2, \ldots, s)$:

$$B_\theta^{(e)} = \sum_{\forall i_e} B_{\theta i_e} = \sum_{\forall i_e} \sum_{j=1}^{s} \rho_{\theta j} \overline{m}_{ji_e} = \sum_{j=1}^{s} \rho_{\theta j} \left(\sum_{\forall i_e} \overline{m}_{ji_e} \right), \tag{62}$$

where the summation represented by $\sum_{\forall i_e}$ covers all the chiral subgroups.

On a similar line to Eq. 3, Eq. 62 can be converted into an expression for giving generating functions concerned with the weight (formula) W_θ:

$$\begin{aligned} \sum_{[\theta]} B_\theta^{(e)} W_\theta &= \sum_{[\theta]} \sum_{j=1}^{s} \rho_{\theta j} \left(\sum_{\forall i_e} \overline{m}_{ji_e} \right) W_\theta = \sum_{j=1}^{s} \left(\sum_{\forall i_e} \overline{m}_{ji_e} \right) \sum_{[\theta]} \rho_{\theta j} W_\theta \\ &= \sum_{j=1}^{s} \left(\sum_{\forall i_e} \overline{m}_{ji_e} \right) \overline{\text{SCI-CF}}(\mathbf{G}_j; \$_{d_{jk}}^{(i\alpha)}) \stackrel{\text{def.}}{\equiv} \overline{\text{CI-CF}}^{(e)}(\mathbf{G}; \$_{d_{jk}}^{(i\alpha)}) \end{aligned} \tag{63}$$

The last part of Eq. 63 shows a definition of the restricted CI-CF for counting enantiomeric pairs of chiral derivatives. The restricted CI-CF is proved easily to be equal to the sum of the restricted PCI-CFs for chiral subgroups shown in Def. 1, because the sum concerning i and the sum concerning j are interchangeable in their order of summing up. Then, we have the following definition:

Definition 5 (Restricted CI-CF for Counting Enantiomeric Pairs) The restricted CI-CF for counting enantiomeric pairs of chiral derivatives is defined as follows:

$$\overline{\text{CI-CF}}^{(e)}(\mathbf{G}; \$_{d_{jk}}^{(i\alpha)}) = \sum_{\forall i_e} \overline{\text{PCI-CF}}(\mathbf{G}_i; \$_{d_{jk}}^{(i\alpha)}) = \sum_{j=1}^{s} \left(\sum_{\forall i_e} \overline{m}_{ji_e} \right) \overline{\text{SCI-CF}}(\mathbf{G}_j; \$_{d_{jk}}^{(i\alpha)}), \tag{64}$$

where the restricted SCI-CF in the right-hand side has been given in Lemma 1 of Part II of this series.

The delayed expansion described in Eq. 3 to give Theorem 1 can be also applied to Eq. 63. Thereby, we obtain a theorem for enumerating enantiomeric pairs of chiral derivatives by the restricted CI-CF:

Theorem 5 (Counting Enantiomeric Pairs by the Restricted CI-CF) Generating functions for obtaining the numbers $B_\theta^{(e)}$ of enantiomeric pairs of chiral derivatives with weight W_θ under the restricted condition are calculated by the following equations:

$$\sum_{[\theta]} B_\theta^{(e)} W_\theta = \overline{\text{CI-CF}}^{(e)}(\mathbf{G}; \$_{d_{jk}}^{(i\alpha)}) \tag{65}$$

where the variables $\$_{d_{jk}}^{(i\alpha)}$ ($\$ = a, b, c$) are substituted by Eqs. 5–7.

The values of $\sum_{\forall i_e} \overline{m}_{ji_e}$ for the group $\mathbf{D}_{3h}$ have already been reported in the "chiral"-column of the matrix for gross enumeration (Eq. 49 of Part II of this series). According to Def. 4, the restricted SCI-CFs for cyclic subgroups are selected from the restricted SCI-CFs (Eqs. 15–24) so as to give the following restricted CI-CF:

$$\overline{\text{CI-CF}}^{(e)}(\mathbf{D}_{3h}; \$_d, \tilde{\$}_d, \hat{\$}_d) \;=\; \frac{1}{12}\overline{\text{SCI-CF}}(\mathbf{C}_1; \$_d, \tilde{\$}_d, \hat{\$}_d) + \frac{1}{4}\overline{\text{SCI-CF}}(\mathbf{C}_2; \$_d, \tilde{\$}_d, \hat{\$}_d)$$

$$
\begin{aligned}
& -\frac{1}{4}\overline{\text{SCI-CF}}(\mathbf{C}_s;\$_d,\tilde{\$}_d,\hat{\$}_d)-\frac{1}{12}\overline{\text{SCI-CF}}(\mathbf{C}'_s;\$_d,\tilde{\$}_d,\hat{\$}_d) \\
& +\frac{1}{6}\overline{\text{SCI-CF}}(\mathbf{C}_3;\$_d,\tilde{\$}_d,\hat{\$}_d)-\frac{1}{6}\overline{\text{SCI-CF}}(\mathbf{C}_{3h};\$_d,\tilde{\$}_d,\hat{\$}_d) \\
= \quad & \frac{1}{12}b_1^6+\frac{1}{4}b_2^3+\frac{1}{6}b_3^2+\frac{3}{4}b_2\tilde{b}_2+\frac{3}{4}b_1^2\tilde{b}_1^2+\frac{1}{2}b_1^4\tilde{b}_1 \\
& +\frac{1}{4}b_1^2\hat{b}_1^2+\frac{1}{4}b_1^4\hat{b}_1+\frac{1}{4}b_2\hat{b}_2+\frac{1}{4}b_2^2\hat{b}_1 \\
& +\frac{1}{4}\tilde{b}_1^2\hat{b}_1+\frac{1}{4}\tilde{b}_2\hat{b}_1+\frac{1}{2}b_1^2\tilde{b}_1\hat{b}_1+\frac{1}{4}\hat{b}_1\hat{b}_2+\frac{1}{6}\hat{b}_3+\frac{1}{12}\hat{b}_1^3 \\
& -\frac{1}{4}a_1^2c_2^2-\frac{1}{12}c_2^3-\frac{1}{6}c_6-\frac{1}{4}a_1^2\tilde{a}_1^2-\frac{1}{2}a_1^2c_2\tilde{a}_1-\frac{1}{4}c_2\tilde{c}_2 \\
& -\frac{1}{4}a_1^2\hat{c}_2-\frac{1}{4}c_2\hat{a}_1^2-\frac{1}{2}c_2^2\hat{a}_1-\frac{1}{4}\tilde{a}_1^2\hat{a}_1-\frac{1}{4}\tilde{c}_2\hat{a}_1-\frac{1}{2}c_2\tilde{a}_1\hat{a}_1 \\
& -\frac{1}{4}\hat{a}_1\hat{c}_2-\frac{1}{6}\hat{a}_3-\frac{1}{12}\hat{a}_1^3
\end{aligned} \tag{66}
$$

It is to be noted that the monomials contained in Eq. 66 are the same as those of Eq. 54 although plus signs are changed into minus for the monomials containing a_d and c_d. Obviously, the sum of Eq. 60 and Eq. 66 provides Eq. 54.

The inventory functions for vertex substitution (Eqs. 35–37) as well as the inventory functions for edge substitution (Eqs. 38 and 39) are introduced into the restricted CI-CF (Eq. 66). The resulting equations are expanded to give the following generating function for obtaining the numbers of enantiomeric pairs of chiral derivatives under the restricted condition:

$$
\begin{aligned}
f^{(e)} \quad = \quad & \mathrm{X}^2+\mathrm{X}^3+\mathrm{X}^4+\mathrm{p}\overline{\mathrm{p}}+7\mathrm{p}^2\overline{\mathrm{p}}^2+\mathrm{p}^3\overline{\mathrm{p}}^3+\frac{1}{2}(\mathrm{p}+\overline{\mathrm{p}})+2(\mathrm{p}^2+\overline{\mathrm{p}}^2)+2(\mathrm{p}^3+\overline{\mathrm{p}}^3) \\
& +\frac{1}{2}(\mathrm{p}^6+\overline{\mathrm{p}}^6)+12\mathrm{X}^2\mathrm{p}\overline{\mathrm{p}}+8\mathrm{X}\mathrm{p}\overline{\mathrm{p}}+\frac{5}{2}(\mathrm{X}\mathrm{p}+\mathrm{X}\overline{\mathrm{p}})+5(\mathrm{X}^2\mathrm{p}+\mathrm{X}^2\overline{\mathrm{p}})+5(\mathrm{X}\mathrm{p}^2+\mathrm{X}\overline{\mathrm{p}}^2) \\
& +5(\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{p}\overline{\mathrm{p}}^2)+15(\mathrm{X}\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{X}\mathrm{p}\overline{\mathrm{p}}^2)+8\mathrm{X}^3\mathrm{p}\overline{\mathrm{p}}+15(\mathrm{X}^2\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{X}^2\mathrm{p}\overline{\mathrm{p}}^2)+13\mathrm{X}\mathrm{p}^2\overline{\mathrm{p}}^2 \\
& +10(\mathrm{X}\mathrm{p}\overline{\mathrm{p}}^3+\mathrm{X}\mathrm{p}^3\overline{\mathrm{p}})+5(\mathrm{X}\mathrm{p}^3+\mathrm{X}\overline{\mathrm{p}}^3)+5(\mathrm{X}^3\mathrm{p}+\mathrm{X}^3\overline{\mathrm{p}})+2(\mathrm{p}^4+\overline{\mathrm{p}}^4)+\frac{1}{2}(\mathrm{p}^5+\overline{\mathrm{p}}^5) \\
& +\frac{5}{2}(\mathrm{p}\overline{\mathrm{p}}^4+\mathrm{p}^4\overline{\mathrm{p}})+5(\mathrm{p}^2\overline{\mathrm{p}}^3+\mathrm{p}^3\overline{\mathrm{p}}^2)+9(\mathrm{X}^2\mathrm{p}^2+\mathrm{X}^2\overline{\mathrm{p}}^2)+5(\mathrm{p}\overline{\mathrm{p}}^3+\mathrm{p}^3\overline{\mathrm{p}}) \\
& +5(\mathrm{X}^2\mathrm{p}^3+\mathrm{X}^2\overline{\mathrm{p}}^3)+\frac{5}{2}(\mathrm{X}^4\mathrm{p}+\mathrm{X}^4\overline{\mathrm{p}})+\frac{5}{2}(\mathrm{X}\mathrm{p}^4+\mathrm{X}\overline{\mathrm{p}}^4)+5(\mathrm{X}^3\mathrm{p}^2+\mathrm{X}^3\overline{\mathrm{p}}^2) \\
& +2(\mathrm{p}^2\overline{\mathrm{p}}^4+\mathrm{p}^4\overline{\mathrm{p}}^2)+\frac{1}{2}(\mathrm{p}^5\overline{\mathrm{p}}+\mathrm{p}\overline{\mathrm{p}}^5)+\frac{1}{2}(\mathrm{X}\mathrm{p}^5+\mathrm{X}\overline{\mathrm{p}}^5)+2(\mathrm{X}^3\mathrm{p}^3+\mathrm{X}^3\overline{\mathrm{p}}^3) \\
& +\frac{1}{2}(\mathrm{X}^5\mathrm{p}+\mathrm{X}^5\overline{\mathrm{p}})+2(\mathrm{X}^2\mathrm{p}^4+\mathrm{X}^2\overline{\mathrm{p}}^4)+2(\mathrm{X}^4\mathrm{p}^2+\mathrm{X}^4\overline{\mathrm{p}}^2)+\mathrm{X}^4\mathrm{p}\overline{\mathrm{p}} \\
& +5(\mathrm{X}^3\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{X}^3\mathrm{p}\overline{\mathrm{p}}^2)+7\mathrm{X}^2\mathrm{p}^2\overline{\mathrm{p}}^2+5(\mathrm{X}^2\mathrm{p}\overline{\mathrm{p}}^3+\mathrm{X}^2\mathrm{p}^3\overline{\mathrm{p}}) \\
& +\frac{5}{2}(\mathrm{X}\mathrm{p}\overline{\mathrm{p}}^4+\mathrm{X}\mathrm{p}^4\overline{\mathrm{p}})+5(\mathrm{X}\mathrm{p}^2\overline{\mathrm{p}}^3+\mathrm{X}\mathrm{p}^3\overline{\mathrm{p}}^2) \\
& +\{2\mathrm{X}+3\mathrm{X}^2+2\mathrm{X}^3+6\mathrm{p}\overline{\mathrm{p}}+3\mathrm{p}^2\overline{\mathrm{p}}^2+3(\mathrm{p}+\overline{\mathrm{p}})+5(\mathrm{p}^2+\overline{\mathrm{p}}^2)+3(\mathrm{p}^3+\overline{\mathrm{p}}^3) \\
& +6\mathrm{X}^2\mathrm{p}\overline{\mathrm{p}}+16\mathrm{X}\mathrm{p}\overline{\mathrm{p}}+9(\mathrm{X}\mathrm{p}+\mathrm{X}\overline{\mathrm{p}})+9(\mathrm{X}^2\mathrm{p}+\mathrm{X}^2\overline{\mathrm{p}})+9(\mathrm{X}\mathrm{p}^2+\mathrm{X}\overline{\mathrm{p}}^2) \\
& +9(\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{p}\overline{\mathrm{p}}^2)+9(\mathrm{X}\mathrm{p}^2\overline{\mathrm{p}}+\mathrm{X}\mathrm{p}\overline{\mathrm{p}}^2)+3(\mathrm{X}\mathrm{p}^3+\mathrm{X}\overline{\mathrm{p}}^3)+3(\mathrm{X}^3\mathrm{p}+\mathrm{X}^3\overline{\mathrm{p}}) \\
& +(\mathrm{p}^4+\overline{\mathrm{p}}^4)+5(\mathrm{X}^2\mathrm{p}^2+\mathrm{X}^2\overline{\mathrm{p}}^2)+3(\mathrm{p}\overline{\mathrm{p}}^3+\mathrm{p}^3\overline{\mathrm{p}})\}\mathrm{Z}
\end{aligned}
$$

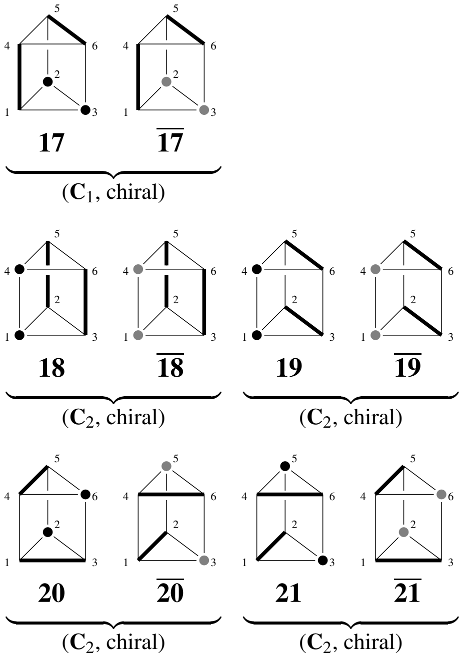


Figure 4: Enantiomeric pairs of chiral derivatives, each corresponding to $\frac{1}{2}(\mathrm{p}^2+\overline{\mathrm{p}}^2)\mathrm{Z}^2$, where a chiral ligand p is represented by a black solid circle and its enantiomeric ligand $\overline{\mathrm{p}}$ is represented by a gray solid circle.

$$+\{1+2\mathrm{X}+\mathrm{X}^2+3(\mathrm{p}+\overline{\mathrm{p}})+3(\mathrm{Xp}+\mathrm{X}\overline{\mathrm{p}})+\frac{5}{2}(\mathrm{p}^2+\overline{\mathrm{p}}^2)+\mathrm{p}\overline{\mathrm{p}}\}\mathrm{Z}^2 \tag{67}$$

Obviously, Eq. 67 is also obtained by summing up the results for chiral subgroups selected from Eqs. 40–49.

To exemplify the validity of the results shown in Eq. 67, Fig. 4 shows five enantiomeric pairs corresponding to the term $\frac{5}{2}(\mathrm{p}^2+\overline{\mathrm{p}}^2)Z^2$, which is interpreted to be $5\times\frac{1}{2}(\mathrm{p}^2+\overline{\mathrm{p}}^2)\mathrm{Z}^2$. Among them, the pair of **17**/$\overline{\mathbf{17}}$ belongs to $\mathbf{C}_1$, which corresponds to the term $\frac{1}{2}(\mathrm{p}^2+\overline{\mathrm{p}}^2)\mathrm{Z}^2$ appearing in Eq. 40. On the other hand, the four pairs of **18**/$\overline{\mathbf{18}}$, **19**/$\overline{\mathbf{19}}$, **20**/$\overline{\mathbf{20}}$, and **21**/$\overline{\mathbf{21}}$ belong to $\mathbf{C}_2$, which corresponds to the term $2(\mathrm{p}^2+\overline{\mathrm{p}}^2)\mathrm{Z}^2$ (= $4\times\frac{1}{2}(\mathrm{p}^2+\overline{\mathrm{p}}^2)\mathrm{Z}^2$) appearing in Eq. 41.

3.4 Restricted CIs for Degenerate Cases

On a similar line to the derivation of Def. 2 from Def. 1, restricted CIs (without chirality fittingness) are derived from the corresponding CI-CFs (Defs. 3, 4, and 5). The derivation simply stems from the replacement of $\$_{d_{jk}}^{(i\alpha)}$ by $s_{d_{jk}}^{(i\alpha)}$.

Definition 6 (Restricted CIs for Gross Enumerations) Three definitions for gross enumerations of degenerate cases (without considering the chirality/achirality of substituents) are itemized below, where the restricted SCI in each right-hand side, i.e., $\overline{\mathrm{SCI}}(\mathbf{G}_j; s_{d_{jk}}^{(i\alpha)})$, is derived from the restricted SCI-CF given in Lemma 1 of Part II of this series by putting $\$_{d_{jk}}^{(i\alpha)} = s_{d_{jk}}^{(i\alpha)}$.

1. The restricted CI for counting total derivatives is defined as follows:

$$\overline{\mathrm{CI}}(\mathbf{G}; s_{d_{jk}}^{(i\alpha)}) = \sum_{i=1}^{s} \overline{\mathrm{PCI}}(\mathbf{G}_i; s_{d_{jk}}^{(i\alpha)}) = \sum_{j=1}^{s} \left(\sum_{i=1}^{s} \overline{m}_{ji} \right) \overline{\mathrm{SCI}}(\mathbf{G}_j; s_{d_{jk}}^{(i\alpha)}). \tag{68}$$

2. The restricted CI for counting achiral derivatives is defined as follows:

$$\overline{\mathrm{CI}}^{(a)}(\mathbf{G}; s_{d_{jk}}^{(i\alpha)}) = \sum_{\forall i_a} \overline{\mathrm{PCI}}(\mathbf{G}_i; s_{d_{jk}}^{(i\alpha)}) = \sum_{j=1}^{s} \left(\sum_{\forall i_a} \overline{m}_{ji_a} \right) \overline{\mathrm{SCI}}(\mathbf{G}_j; s_{d_{jk}}^{(i\alpha)}). \tag{69}$$

3. The restricted CI for counting enantiomeric pairs of chiral derivatives is defined as follows:

$$\overline{\mathrm{CI}}^{(e)}(\mathbf{G}; s_{d_{jk}}^{(i\alpha)}) = \sum_{\forall i_e} \overline{\mathrm{PCI}}(\mathbf{G}_i; s_{d_{jk}}^{(i\alpha)}) = \sum_{j=1}^{s} \left(\sum_{\forall i_e} \overline{m}_{ji_e} \right) \overline{\mathrm{SCI}}(\mathbf{G}_j; s_{d_{jk}}^{(i\alpha)}). \tag{70}$$

Theorems 3, 4, 5 are degenerated into the following set of theorems by using the definitions collected in Def. 6.

Theorem 6 (Gross Enumeration by the Restricted CIs) Three theorems for gross enumerations of degenerate cases (without considering the chirality/achirality of substituents) are itemized below, where the variables $s_{d_{jk}}^{(i\alpha)}$ are substituted by Eq. 13.

1. Generating functions for obtaining the total numbers B_θ of derivatives with weight W_θ under the restricted condition are calculated by the following equations:

$$\sum_{[\theta]} B_\theta W_\theta = \overline{\mathrm{CI}}(\mathbf{G}; s_{d_{jk}}^{(i\alpha)}). \tag{71}$$

2. Generating functions for obtaining the numbers $B_\theta^{(a)}$ of achiral derivatives with weight W_θ under the restricted condition are calculated by the following equations:

$$\sum_{[\theta]} B_\theta^{(a)} W_\theta = \overline{\mathrm{CI}}^{(a)}(\mathbf{G}; s_{d_{jk}}^{(i\alpha)}). \tag{72}$$

3. Generating functions for obtaining the numbers $B_\theta^{(e)}$ of enantiomeric pairs of chiral derivatives with weight W_θ under the restricted condition are calculated by the following equations:

$$\sum_{[\theta]} B_\theta^{(e)} W_\theta = \overline{\mathrm{CI}}^{(e)}(\mathbf{G}; s_{d_{jk}}^{(i\alpha)}), \tag{73}$$

To exemplify enumerations of degenerate cases, let us consider achiral monodentate ligands of a single kind (X) and bidentate ligand of a single kind (Z) as a continuation of the enumeration of trigonal prismatic derivatives. According to Eq. 68 of Def. 6, Eq. 54 is degenerated into the following CI by placing $a_d = b_d = c_d = s_d$, $\tilde{a}_d = \tilde{b}_d = \tilde{c}_d = \tilde{s}_d$, and $\hat{a}_d = \hat{b}_d = \hat{c}_d = \hat{s}_d$.

$$\begin{aligned}
\overline{\mathrm{CI}}(\mathbf{D}_{3h}; s_d, \tilde{s}_d, \hat{s}_d) &= \frac{1}{12}\overline{\mathrm{SCI}}(\mathbf{C}_1; s_d, \tilde{s}_d, \hat{s}_d) + \frac{1}{4}\overline{\mathrm{SCI}}(\mathbf{C}_2; s_d, \tilde{s}_d, \hat{s}_d) \\
&\quad + \frac{1}{4}\overline{\mathrm{SCI}}(\mathbf{C}_s; s_d, \tilde{s}_d, \hat{s}_d) + \frac{1}{12}\overline{\mathrm{SCI}}(\mathbf{C}'_s; s_d, \tilde{s}_d, \hat{s}_d) \\
&\quad + \frac{1}{6}\overline{\mathrm{SCI}}(\mathbf{C}_3; s_d, \tilde{s}_d, \hat{s}_d) + \frac{1}{6}\overline{\mathrm{SCI}}(\mathbf{C}_{3h}; s_d, \tilde{s}_d, \hat{s}_d) \\
&= \frac{1}{12}s_1^6 + \frac{1}{3}s_2^3 + \frac{1}{6}s_3^2 + \frac{1}{4}s_1^2 s_2^2 + \frac{1}{6}s_6 + s_2\tilde{s}_2 + s_1^2\tilde{s}_1^2 + \frac{1}{2}s_1^4\tilde{s}_1 \\
&\quad + \frac{1}{4}s_1^2\hat{s}_1^2 + \frac{1}{4}s_1^4\hat{s}_1 + \frac{1}{4}s_2\hat{s}_2 + \frac{3}{4}s_2^2\hat{s}_1 + \frac{1}{4}s_1^2\hat{s}_2 + \frac{1}{4}s_2\hat{s}_1^2 \\
&\quad + \frac{1}{2}\tilde{s}_1^2\hat{s}_1 + \frac{1}{2}\tilde{s}_2\hat{s}_1 + \frac{1}{2}s_1^2\tilde{s}_1\hat{s}_1 + \frac{1}{2}\hat{s}_1\hat{s}_2 + \frac{1}{3}\hat{s}_3 + \frac{1}{6}\hat{s}_1^3 \\
&\quad + \frac{1}{2}s_1^2 s_2\tilde{s}_1 + \frac{1}{2}s_2\tilde{s}_1\hat{s}_1. \qquad (74)
\end{aligned}$$

The inventory functions of this degenerate case is obtained as follows:

$$s_d = 1 + \mathrm{X}^d \qquad (75)$$

$$\tilde{s}_d = \hat{s}_d = \mathrm{Z}. \qquad (76)$$

These are introduced into Eq. 74. The resulting equation is expanded to give the following generating function:

$$\begin{aligned}
f^{(g)'} &= 1 + \mathrm{X} + 3\mathrm{X}^2 + 3\mathrm{X}^3 + 3\mathrm{X}^4 + \mathrm{X}^5 + \mathrm{X}^6 \\
&\quad + (2 + 4\mathrm{X} + 7\mathrm{X}^2 + 4\mathrm{X}^3 + 2\mathrm{X}^4)\mathrm{Z} + (4 + 4\mathrm{X} + 4\mathrm{X}^2)\mathrm{Z}^2 + 2\mathrm{Z}^3. \qquad (77)
\end{aligned}$$

As a matter of course, Eq. 77 is contained in Eq. 55, where all of the terms containing p and/or $\overline{\mathrm{p}}$ are deleted to give Eq. 77. The same result is alternatively obtained by introducing degenerate inventory functions, i.e., $a_d = b_d = c_d = 1 + \mathrm{X}^d$, $\tilde{a}_d = \tilde{b}_d = \tilde{c}_d = \mathrm{Z}^d$, and $\hat{a}_d = \hat{b}_d = \hat{c}_d = \mathrm{Z}^d$, into the restricted CI-CF (Eq. 54).

4 Conclusion

The restricted partial-cycle-index (PCI) method is proposed to enumerate derivatives by means of vertex substitution (monodentate ligands) and/or edge substitution (bidentate ligands) under a restriction condition that occupation of a common vertex (or occupation of adjacent edges) is avoided. Restricted subduced cycle indices without and with chirality fittingness (SCIs and SCI-CFs) are derived from unit subduced cycle indices without and with chirality fittingness (USCIs and USCI-CFs). The restricted SCI-CFs (and also the restricted SCIs as degenerate cases) are transformed into restricted PCI-CFs, which enable us to enumerate derivatives under the restricted condition in a symmetry-itemized fashion. The restricted PCI-CFs are further transformed into restricted cycle indices with chirality fittingness (restricted CI-CFs) for gross enumerations of total, achiral, chiral derivatives.

Appendix

Maple Program for Calculation by the Restricted PCI Method

The following program is based on the restricted SCI-CFs shown in Eqs. 15–24, where the symbol a_1, b_1, c_2, etc. are replaced by a1, b1, c2, etc.; the symbol $\tilde{a}_1$, $\tilde{b}_1$, $\tilde{c}_2$, etc. are replaced by A1, B1, C2, etc.; and the symbol $\hat{a}_1$, $\hat{b}_1$, $\hat{c}_2$, etc. are replaced by AA1, BB1, CC2, and so on. The restricted PCI-CFs (Eqs. 25–34) are calculated by using the restricted SCI-CFs. Then, the inventory functions for vertex substitution (Eqs. 35–37) and the inventory functions for edge substitution (Eqs. 38 and 39) are introduced into the resulting restricted PCI-CFs to give generating functions.

```
#prismPCI2-2-1BR.mpl for Trigonal Prisms
restart;
#read "c:/fujita0/calc3/prismPCI2-2-1BR.mpl";

#Restricted SCI-CFs
MC1:= 6*b1^2*B1*BB1 +3*b1^2*BB1^2 + 9*b1^2*B1^2  + 3*b1^4 *BB1
+ 6*b1^4*B1 + b1^6 + 3*B1^2*BB1 + BB1^3;
MC2:= b2^3+b2^2*BB1+3*b2*B2+B2*BB1+b2*BB2+BB1*BB2;
MCs:= 2*c2*A1*AA1+2*a1^2*c2*A1+a1^2*c2^2+a1^2*A1^2+c2^2*AA1
+A1^2*AA1+a1^2*CC2+AA1*CC2;
MCsp:= c2^3+AA1^3+3*C2*AA1+3*c2*C2+3*c2^2*AA1+3*c2*AA1^2;
MC3 := BB3+b3^2;
MC2v := a2*AA2+a2*c4+a2*A2+AA1*AA2+A2*AA1+c4*AA1;
MC3v := AA3+a3^2;
MC3h := AA3+c6;
MD3 := BB3+b6;
MD3h := AA3+a6;

#Resricted PCI-CFs
MFMC1 := (1/12)*MC1-(1/4)*MC2-(1/4)*MCs-(1/12)*MCsp-(1/12)*MC3
+(1/2)*MC2v+(1/4)*MC3v+(1/12)*MC3h+(1/4)*MD3-(1/2)*MD3h;
MFMC2 := (1/2)*MC2-(1/2)*MC2v-(1/2)*MD3+(1/2)*MD3h;
MFMCs := (1/2)*MCs-(1/2)*MC2v-(1/2)*MC3v+(1/2)*MD3h;
MFMCsp := (1/6)*MCsp-(1/2)*MC2v-(1/6)*MC3h+(1/2)*MD3h;
MFMC3 := (1/4)*MC3-(1/4)*MC3v-(1/4)*MC3h-(1/4)*MD3+(1/2)*MD3h;
MFMC2v := MC2v-MD3h;
MFMC3v := (1/2)*MC3v-(1/2)*MD3h;
MFMC3h := (1/2)*MC3h-(1/2)*MD3h;
MFMD3 := (1/2)*MD3-(1/2)*MD3h;
MFMD3h := MD3h;

#Inventory Functions for Vertex Substitution
a1 := 1+X; a2 := 1+X^2; a3 := 1+X^3; a6 := 1+X^6;
b1 := 1+X + p + P; b2 := 1+X^2 + p^2 + P^2;
b3 := 1+X^3 + p^3 + P^3; b6 := 1+X^6 + p^6 + P^6;
c2 := 1+X^2 + 2*p*P; c4 := 1+X^4 + 2*p^2*P^2;
c6 := 1+X^6 + 2*p^3*P^3;

#Inventory Functions for Edge Substitution
A1 := Z; A2 := Z^2; A3 := Z^3; A6 := Z^6;
B1 := Z; B2 := Z^2; B3 := Z^3; B6 := Z^6;
C2 := Z^2; C4 := Z^4; C6 := Z^6;

AA1 := Z; AA2 := Z^2; AA3 := Z^3;
BB1 := Z; BB2 := Z^2; BB3 := Z^3;
CC2 := Z^2;
```

```
#Expansion into Generating Functions
GFC1 := collect(expand(MFMC1),Z);
GFC2 := collect(expand(MFMC2),Z);
GFCs := collect(expand(MFMCs),Z);
GFCsp := collect(expand(MFMCsp),Z);
GFC3 := collect(expand(MFMC3),Z);
GFC2v := collect(expand(MFMC2v),Z);
GFC3v := collect(expand(MFMC3v),Z);
GFC3h := collect(expand(MFMC3h),Z);
GFD3 := collect(expand(MFMD3),Z);
GFD3h := collect(expand(MFMD3h),Z);
```

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