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Restricted Enumerations by the Unit-Subduced-Cycle-Index (USCI) Approach. I. Factorization of Subduced Cycle Indices

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Abstract

In order to treat steric hindrance due to monodentate and bidentate ligands in isomer enumeration, the partial-cycle-index (PCI) method of the unit-subduced-cycle-index (USCI) approach is extended to enumerate derivatives by taking restricted modes of vertex and/or edge substitutions into consideration. Factorization of subduced cycle indices with chirality fittingness (SCI-CFs), which are calculated by starting from unit subduced cycle indices with chirality fittingness (USCI-CFs) assigned to respective subgroups of the group of a given skeleton, is discussed to generate restricted SCI-CFs. The restricted SCI-CF for each subgroup is effective to evaluate the numbers of fixed points (promolecules) on the action of the subgroup under the restricted conditions of enumeration. The set of the restricted SCI-CFs is multiplied by the inverse mark table to generate partial cycle indices with chirality fittingness (PCI-CFs), by which itemized enumerations for every subgroups are conducted under the restricted conditions. Several results starting from an icosahedral skeleton are discussed to examine differences between unrestricted and restricted enumerations.

1 Introduction

As found in our monographs [1, 2], we are investigating the developments and applications of the unit-subduced-cycle-index (USCI) approach, where the concepts of *subduction of coset representations* and *sphericities* are integrated to develop the concept of *unit subduced cycle indices without and with chirality fittingness* (USCIs and USCI-CFs). Thereby, the USCI approach mainly supports four methods of symmetry-itemized enumeration of chemical compounds:

1. the fixed-point matrix (FPM) method [3–5] based on generating functions derived from subduced cycle indices (SCIs) and mark tables,
2. the partial-cycle-index (PCI) method [6, 7] based on generating functions derived from partial cycle indices (PCIs),
3. the elementary superposition method [8], and
4. the partial superposition method [6, 8].

These methods regard substitution sites (positions, bonds, etc.) in a skeleton as an assembly of orbits which exhibit independent behaviors, where SCIs (or SCI-CFs) are derived to be a product of USCIs (or USCI-CFs) assigned to the respective orbits. Such independent behaviors, however, are not always assured because substitution sites can interact one another (e.g., the interaction between positions and bonds). Hence, it is desirable to develop new methodology for examining restricted cases caused by such interactions.

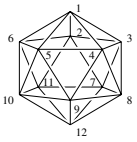
Recently, Rosenfeld and Klein have developed a versatile method for investigating such restricted cases [9], where Pólya's cycle indices [10, 11] are refined [12] and integrated with the inclusion-exclusion procedure [13]. The articles on this method [9] have prompted us to report an extended version of the USCI approach for examining restricted cases.

Hence, the purpose of the present article is to develop such an extended version of the USCI approach, where ligands and derivative are considered to have three-dimensional (3D) structures. The concepts of proligands and promolecules have been coupled with the concept of *chirality fittingness* to permit us to enumerate restricted cases of chemical compounds as 3D structures. In particular, the PCI method is extended to be applicable to such restricted cases by calculating restricted SCI-CFs.

2 Partial Cycle Indices with Chirality Fittingness

2.1 Enumeration Without Restrictions

The USCI approach precedently calculates USCI-CFs, i.e. $\mathrm{ZC}(\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j; \$_{d_{jk}}^{(i\alpha)})$, in accord with Eq. 19.4 due to Def. 9.3 of [1]. Such precalculated USCI-CFs (or USCIs) are collected in a tabular form to generate a USCI-CF table for each point group, e.g., Appendices D and E of [1]. To enumerate derivatives by starting from a given skeleton, its substitution sites (vertices, edges, etc.) to be considered are categorized into an assembly of orbits, which are assigned to coset representations $\mathbf{G}(/\mathbf{G}_i)$ distinguished by the superscript $(i\alpha)$. According to Def. 19.3 of [1], A product of USCI-CFs for each subgroup $\mathbf{G}_j$ is calculated with respect to an assembly of



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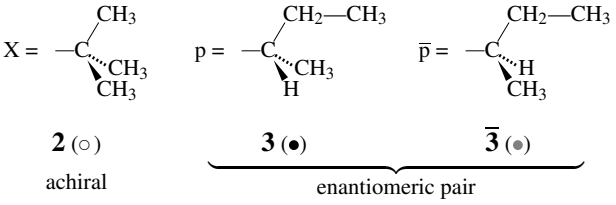


Figure 1: An icosahedral skeleton for $B_{12}H_{12}^{-2}$ and alkyl substituents

orbits, so as to generate the corresponding SCI-CF for the assembly of orbits at issue:

$$\text{SCI-CF}(\mathbf{G}_j;\$_{d_{jk}}^{(i\alpha)}) = \prod_{i=1}^{s}\prod_{\substack{\alpha=1\\ \alpha_i\neq 0}}^{\alpha_i} \text{ZC}(\mathbf{G}(/\mathbf{G}_i)\downarrow \mathbf{G}_j;\$_{d_{jk}}^{(i\alpha)}). \tag{1}$$

The PCI method of the USCI approach uses PCI-CFs for respective subgroups $\mathbf{G}_i$, which are calculated by virtue of Def. 19.6 of [1], as follows:

$$\text{PCI-CF}(\mathbf{G}_i;\$_{d_{jk}}^{(i\alpha)}) = \sum_{j=1}^{s} \overline{m}_{ji}\text{SCI-CF}(\mathbf{G}_j;\$_{d_{jk}}^{(i\alpha)}), \tag{2}$$

where the symbol $\overline{m}_{ji}$ represents the j-th element of the $\mathbf{G}_i$-column of the inverse mark table of $\mathbf{G}$ group. The symbol $\$_{d_{jk}}^{(i\alpha)}$ denotes $a_{d_{jk}}^{(i\alpha)}$ for a homospheric orbit, $c_{d_{jk}}^{(i\alpha)}$ for an enantiospheric orbit, or $b_{d_{jk}}^{(i\alpha)}$ for an hemispheric orbit, which decides a mode of substitution in terms of chirality fittingness [1].

For example, let us enumerate derivatives by starting from an icosahedral skeleton (**1**), which corresponds to a dodecahydro-*close*-dodecaborate(2-) ion ($[B_{12}H_{12}]^{-2}$). The numbering of the 12 vertices of **1** is adopted in accord with Section I-2.14 of the IUPAC Recommendations 1990 [14]. Suppose that hydrogen atoms selected from the 12 vertices are replaced by an appropriate set of ligands.

The basic data of $\mathbf{I}_h$, i.e., the mark table, its inverse, and the USCI-CF table, have already been reported in [15] for the purpose of enumerating by starting from skeletons of $\mathbf{I}_h$. Several coset representations of $\mathbf{I}_h$ have been already used for combinatorial enumeration, e.g., $\mathbf{I}_h(/\mathbf{C}_{3v})$ for the 20 vertices of dodecahedrane [15], $\mathbf{I}_h(/\mathbf{C}_s)$ for the 60 vertices [16] and for the 60 [6:5]-edges of the fullerene C_{60} (saccerane), and $\mathbf{I}_h(/\mathbf{C}_{2v})$ for the 30 [6:6]-edges of fullerene C_{60} [17].

The 12 vertices of **1** are equivalent to generate an orbit governed by the coset representation $\mathbf{I}_h(/\mathbf{C}_{5v})$, where the point group $\mathbf{I}_h$ represents the global symmetry of **1** and the subgroup $\mathbf{C}_{5v}$

Table 1: USCI-CFs and Restricted SCI-CFs for $\mathbf{I}_h(/\mathbf{C}_{5v})$

subgroup $\mathbf{G}_j$	subduction $\mathbf{I}_h(/\mathbf{C}_{5v})\downarrow\mathbf{G}_j$	SCI-CF (USCI-CF)	$\overline{\text{SCI-CF}}$
$\mathbf{C}_1$	$12\mathbf{C}_1(/\mathbf{C}_1)$	b_1^{12}	1. $12b_1$. $36b_1^2$. $20b_1^3$
$\mathbf{C}_2$	$6\mathbf{C}_2(/\mathbf{C}_1)$	b_2^6	1. $4b_2$
$\mathbf{C}_s$	$4\mathbf{C}_s(/\mathbf{C}_1)$. $4\mathbf{C}_s(/\mathbf{C}_s)$	$a_1^4c_2^4$	1. $4a_1$. $4a_1^2$. $2c_2$. $4a_1c_2$
$\mathbf{C}_i$	$6\mathbf{C}_i(/\mathbf{C}_1)$	c_2^6	1. $6c_2$
$\mathbf{C}_3$	$4\mathbf{C}_3(/\mathbf{C}_1)$	b_3^4	1. $2b_3$
$\mathbf{D}_2$	$3\mathbf{D}_2(/\mathbf{C}_1)$	b_4^3	1
$\mathbf{C}_{2v}$	$\mathbf{C}_{2v}(/\mathbf{C}_1)$. $2\mathbf{C}_{2v}(/\mathbf{C}_s)$. $2\mathbf{C}_{2v}(/\mathbf{C}'_s)$	$a_2^4c_4$	1. $2a_2$
$\mathbf{C}_{2h}$	$2\mathbf{C}_{2h}(/\mathbf{C}_1)$. $2\mathbf{C}_{2h}(/\mathbf{C}_s)$	$a_2^2c_4^2$	1. $2a_2$
$\mathbf{C}_5$	$2\mathbf{C}_5(/\mathbf{C}_1)$. $2\mathbf{C}_5(/\mathbf{C}_5)$	$b_1^2b_5^2$	1. $2b_1$. b_1^2
$\mathbf{D}_3$	$2\mathbf{D}_3(/\mathbf{C}_1)$	b_6^2	1
$\mathbf{C}_{3v}$	$4\mathbf{C}_{3v}(/\mathbf{C}_s)$	a_3^4*	1. $2a_3$
$\mathbf{C}_{3i}$	$2\mathbf{C}_{3i}(/\mathbf{C}_1)$	c_6^2	1
$\mathbf{D}_{2h}$	$\mathbf{D}_{2h}(/\mathbf{C}_s)$. $\mathbf{D}_{2h}(/\mathbf{C}'_s)$. $\mathbf{D}_{2h}(/\mathbf{C}''_s)$	a_4^3	1
$\mathbf{D}_5$	$\mathbf{D}_5(/\mathbf{C}_1)$. $\mathbf{D}_5(/\mathbf{C}_5)$	b_2b_{10}	1. b_2
$\mathbf{C}_{5v}$	$2\mathbf{C}_{5v}(/\mathbf{C}_s)$. $2\mathbf{C}_{5v}(/\mathbf{C}_{5v})$	$a_1^2a_5^2$	1. $2a_1$. a_1^2
$\mathbf{C}_{5i}$	$\mathbf{C}_{5i}(/\mathbf{C}_1)$. $\mathbf{C}_{5i}(/\mathbf{C}_5)$	c_2c_{10}	1. c_2
$\mathbf{T}$	$\mathbf{T}(/\mathbf{C}_1)$	b_{12}	1
$\mathbf{D}_{3d}$	$2\mathbf{D}_{3d}(/\mathbf{C}_s)$	a_6^2	1
$\mathbf{D}_{5d}$	$\mathbf{D}_{5d}(/\mathbf{C}_s)$. $\mathbf{D}_{5d}(/\mathbf{C}_{5v})$	a_2a_{10}*	1. a_2
$\mathbf{T}_h$	$\mathbf{T}_h(/\mathbf{C}_s)$	a_{12}	1
$\mathbf{I}$	$\mathbf{I}(/\mathbf{C}_5)$	b_{12}	1
$\mathbf{I}_h$	$\mathbf{I}_h(/\mathbf{C}_{5v})$	a_{12}	1

* Corrected data for Table 3 of [15].

represents the local symmetry of each vertex ($|\mathbf{I}_h|/|\mathbf{C}_{5v}| = 120/10 = 12$). The $\mathbf{I}_h(/\mathbf{C}_{5v})$-row of the USCI-CF table of $\mathbf{I}_h$ (Table 3 of [15]) is cited at the SCI-CF-column of Table 1, because the presence of a single orbit in **1** permits us to adopt USCI-CFs as SCI-CFs.

The $\mathbf{I}_h(/\mathbf{C}_{5v})$-row of the USCI-CF table as a hypothetical vector (i.e., a transposed vector of the SCI-CF-column of Table 1) is multiplied by each column of the inverse mark table (Table 2 of [15]). Thereby, the following PCI-CFs for every subgroups are generated as follows:

$$\begin{aligned}\text{PCI-CF}_1(\mathbf{C}_1,\$_d) &= \frac{1}{120}b_1^{12}-\frac{1}{8}b_2^6-\frac{1}{8}a_1^4c2^4-\frac{1}{120}c_2^6-\frac{1}{12}b_3^4.\ \frac{1}{12}b_4^3.\ \frac{1}{4}a_2^4c_4.\ \frac{1}{4}a_2^2c_4^2\\ &\quad -\frac{1}{20}b_1^2b_5^2.\ \frac{1}{4}b_6^2.\ \frac{1}{4}a_3^4.\ \frac{1}{12}c_6^2-\frac{1}{3}a_4^3.\ \frac{1}{4}b_2b_{10}.\ \frac{1}{4}a_1^2a_5^2.\ \frac{1}{20}c_2c_{10}\\ &\quad .\ \frac{1}{6}b_{12}-\frac{1}{2}a_6^2-\frac{1}{2}a_2a_{10}-\frac{1}{6}a_{12}-\frac{1}{2}b_{12}.\ \frac{1}{2}a_{12} \qquad (3)\\ \text{PCI-CF}_1(\mathbf{C}_2,\$_d) &= \frac{1}{4}b_2^6-\frac{1}{4}b_4^3-\frac{1}{4}a_2^4c_4-\frac{1}{4}a_2^2c_4^2-\frac{1}{2}b_6^2.\ \frac{1}{2}a_4^3-\frac{1}{2}b_2b_{10}\\ &\quad .\ \frac{1}{2}a_6^2.\ \frac{1}{2}a_2a_{10}.\ b_{12}-a_{12} \qquad (4)\\ \text{PCI-CF}_1(\mathbf{C}_s,\$_d) &= \frac{1}{4}a_1^4c2^4-\frac{1}{2}a_2^4c_4-\frac{1}{4}a_2^2c_4^2-\frac{1}{2}a_3^4.\ \frac{1}{2}a_4^3-\frac{1}{2}a_1^2a_5^2\end{aligned}$$

$$\cdot \quad \frac{1}{2}a_6^2 \cdot \quad \frac{1}{2}a_2a_{10} \tag{5}$$

$$\text{PCI-CF}_1(\mathbf{C}_i,\$_d) = \frac{1}{60}c_2^6 - \frac{1}{4}a_2^2c_4^2 - \frac{1}{6}c_{6\cdot}^2 \quad \frac{1}{6}a_4^3 - \frac{1}{10}c_2c_{10}$$
$$\cdot \quad \frac{1}{2}a_{6\cdot}^2 \quad \frac{1}{2}a_2a_{10\cdot} \quad \frac{1}{3}a_{12} - a_{12} \tag{6}$$

$$\text{PCI-CF}_1(\mathbf{C}_3,\$_d) = \frac{1}{4}b_3^4 - \frac{1}{4}b_6^2 - \frac{1}{4}a_3^4 - \frac{1}{4}c_6^2 - \frac{1}{2}b_{12\cdot} \quad \frac{1}{2}a_{6\cdot}^2 \quad \frac{1}{2}a_{12\cdot} \quad \frac{1}{2}b_{12} - \frac{1}{2}a_{12} \tag{7}$$

$$\text{PCI-CF}_1(\mathbf{D}_2,\$_d) = \frac{1}{6}b_4^3 - \frac{1}{6}a_4^3 - \frac{1}{6}b_{12\cdot} \quad \frac{1}{6}a_{12} \tag{8}$$

$$\text{PCI-CF}_1(\mathbf{C}_{2v},\$_d) = \frac{1}{2}a_2^4c_4 - \frac{1}{2}a_4^3 \tag{9}$$

$$\text{PCI-CF}_1(\mathbf{C}_{2h},\$_d) = \frac{1}{2}a_2^2c_4^2 - \frac{1}{2}a_4^3 - a_6^2 - a_2a_{10\cdot} \quad 2a_{12} \tag{10}$$

$$\text{PCI-CF}_1(\mathbf{C}_5,\$_d) = \frac{1}{4}b_1^2b_5^2 - \frac{1}{4}b_2b_{10} - \frac{1}{4}a_1^2a_5^2 - \frac{1}{4}c_2c_{10\cdot} \quad \frac{1}{2}a_2a_{10} \tag{11}$$

$$\text{PCI-CF}_1(\mathbf{D}_3,\$_d) = \frac{1}{2}b_6^2 - \frac{1}{2}a_6^2 - \frac{1}{2}b_{12\cdot} \quad \frac{1}{2}a_{12} \tag{12}$$

$$\text{PCI-CF}_1(\mathbf{C}_{3v},\$_d) = \frac{1}{2}a_3^4 - \frac{1}{2}a_6^2 \tag{13}$$

$$\text{PCI-CF}_1(\mathbf{C}_{3i},\$_d) = \frac{1}{2}c_6^2 - \frac{1}{2}a_6^2 - a_{12\cdot} \quad a_{12} = \frac{1}{2}c_6^2 - \frac{1}{2}a_6^2 \tag{14}$$

$$\text{PCI-CF}_1(\mathbf{D}_{2h},\$_d) = \frac{1}{3}a_4^3 - \frac{1}{3}a_{12} \tag{15}$$

$$\text{PCI-CF}_1(\mathbf{D}_5,\$_d) = \frac{1}{2}b_2b_{10} - \frac{1}{2}a_2a_{10} - \frac{1}{2}b_{12\cdot} \quad \frac{1}{2}a_{12} \tag{16}$$

$$\text{PCI-CF}_1(\mathbf{C}_{5v},\$_d) = \frac{1}{2}a_1^2a_5^2 - \frac{1}{2}a_2a_{10} \tag{17}$$

$$\text{PCI-CF}_1(\mathbf{C}_{5i},\$_d) = \frac{1}{2}c_2c_{10} - \frac{1}{2}a_2a_{10} \tag{18}$$

$$\text{PCI-CF}_1(\mathbf{T},\$_d) = \frac{1}{2}b_{12} - \frac{1}{2}a_{12} - \frac{1}{2}b_{12\cdot} \quad \frac{1}{2}a_{12} = 0 \tag{19}$$

$$\text{PCI-CF}_1(\mathbf{D}_{3d},\$_d) = a_6^2 - a_{12} \tag{20}$$

$$\text{PCI-CF}_1(\mathbf{D}_{5d},\$_d) = a_2a_{10} - a_{12} \tag{21}$$

$$\text{PCI-CF}_1(\mathbf{T}_h,\$_d) = a_{12} - a_{12} = 0 \tag{22}$$

$$\text{PCI-CF}_1(\mathbf{I},\$_d) = \frac{1}{2}b_{12} - \frac{1}{2}a_{12} \tag{23}$$

$$\text{PCI-CF}_1(\mathbf{I}_h,\$_d) = a_{12} \tag{24}$$

Let us now consider a ligand inventory **L**:

$$\mathbf{L} = \{\text{H}, \text{X}, \text{p}, \overline{\text{p}}\} \tag{25}$$

where the symbol X denotes a *tert*-butyl ligand (**2**) as an achiral ligand and a pair of p and $\overline{\text{p}}$ represents an enantiomeric pair of *sec*-butyl ligands (**3** and $\overline{\mathbf{3}}$). Then, suppose that these ligands can be freely attached to the 12 vertices of **1** without considering steric hindrance. The following inventory functions are derived in accord with Theorem 19.6 of [1]:

$$a_d = 1_\cdot \quad \text{X}^d \tag{26}$$

$$b_d = 1 + X^d + p^d + \overline{p}^d \tag{27}$$

$$c_d = 1 + X^d + 2p^{d/2}\overline{p}^{d/2} \tag{28}$$

Note that the designation of a hydrogen atom contained in the ligand inventory **L** (Eq. 25) is omitted according to chemical conventions, where the term (1) in the right-hand side of each inventory function corresponds to 1^d (i.e., H = 1 for H^d).

These inventory functions (Eqs. 26–28) are introduced into the PCI-CFs (Eqs. 3–24). The resulting equations are expanded to provide generating functions for giving isomer numbers of respective subgroups. Although the full list of the generation functions is omitted, only the generating functions of the point groups $\mathbf{C}_s$ (Eqs. 26–28 into Eq. 5), $\mathbf{C}_{3v}$ (Eqs. 26–28 into Eq. 13), and $\mathbf{D}_{2h}$ (Eqs. 26–28 into Eq. 15) as typical examples of such expansions are shown for the sake of below-mentioned discussions:

$$\begin{aligned} f_1(\mathbf{C}_s) = {} & 2p\overline{p} + 8Xp\overline{p} + 3X^3 + 4p^2\overline{p}^2 + 18X^2p\overline{p} + 5X^4 + 24Xp^2\overline{p}^2 + 32X^3p\overline{p} \\ & + 9X^5 + 8p^3\overline{p}^3 + 42X^2p^2\overline{p}^2 + 44X^4p\overline{p} + 2X^6 + 32Xp^3\overline{p}^3 \\ & + 72X^3p^2\overline{p}^2 + 48X^5p\overline{p} + 9X^7 + 3p^4\overline{p}^4 + 56X^2p^3\overline{p}^3 \\ & + 76X^4p^2\overline{p}^2 + 44X^6p\overline{p} + 5X^8 + 16Xp^4\overline{p}^4 + 64X^3p^3\overline{p}^3 \\ & + 72X^5p^2\overline{p}^2 + 32X^7p\overline{p} + 3X^9 + 22X^2p^4\overline{p}^4 + 56X^4p^3\overline{p}^3 \\ & + 42X^6p^2\overline{p}^2 + 18X^8p\overline{p} + 16X^3p^4\overline{p}^4 + 32X^5p^3\overline{p}^3 + 24X^7p^2\overline{p}^2 \\ & + 8X^9p\overline{p} + 3X^4p^4\overline{p}^4 + 8X^6p^3\overline{p}^3 + 4X^8p^2\overline{p}^2 + 2X^{10}p\overline{p} \end{aligned} \tag{29}$$

$$f_1(\mathbf{C}_{3v}) = 2X^3 + 2X^6 + 2X^9 \tag{30}$$

$$f_1(\mathbf{D}_{2h}) = X^4 + X^8 \tag{31}$$

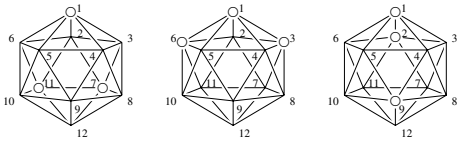
To illustrate the results shown in Eqs. 29–31, Fig. 2 shows three $\mathbf{C}_s$-derivatives (**4**–**6** for the term $3X^3$), two $\mathbf{C}_{3v}$-derivatives (**7** and **8** for the term $2X^3$), and one $\mathbf{D}_{2h}$-derivative (**9** for the term X^4), where we do not take account of steric hindrance due to branching in *tert*-butyl groups (X's represented by open circles). In other words, two *tert*-butyl groups are presumed to be able to occupy two adjacent positions of the icosahedral skeleton (**1**).

2.2 Enumeration With Restrictions

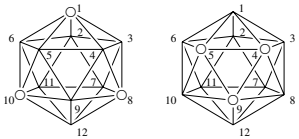
2.2.1 SCI-CFs and PCI-CFs for Restricted Cases

Let us next consider restricted cases, in which the adjacency of bulky *tert*-butyl ligands is not permitted. For example, **4**–**6** ($\mathbf{C}_s$), **8** ($\mathbf{C}_{3v}$), and **9** ($\mathbf{D}_{2h}$) are rejected, not to be counted under the condition of the restriction. To investigate such restricted cases, the SCI-CF shown by Eq. 1 should be restricted to give a restricted subduced cycle index with chirality fittingness, i.e., $\overline{\text{SCI-CF}}$. To obtain a restricted SCI-CF ($\overline{\text{SCI-CF}}$), the corresponding SCI-CF is factorized into several monomials which match the restriction to be considered. Before a general formulation for representing such factorization is shown, practical procedures are illustrated below to formulate restricted SCI-CFs concretely.

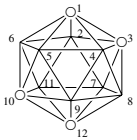
Each SCI-CF (based on USCI-CFs) for a subgroup $\mathbf{G}_i$ works as a tool to evaluate the number of fixed points (or objects, e.g., promolecules in the USCI approach) under unrestricted cases. On the same line, each restricted SCI-CF for a subgroup $\mathbf{G}_i$ can be used to evaluate the number of fixed points (or objects) under restricted cases. This means that, in a similar way to the



4 ($\mathbf{C}_s$, X^3) **5** ($\mathbf{C}_s$, X^3) **6** ($\mathbf{C}_s$, X^3)



7 ($\mathbf{C}_{3v}$, X^3) **8** ($\mathbf{C}_{3v}$, X^3)



9 ($\mathbf{D}_{2h}$, X^4)

Figure 2: Three $\mathbf{C}_s$- and two $\mathbf{C}_{3v}$-derivatives of X^3 as well as a $\mathbf{D}_{2h}$-derivative of X^4, where substitution modes of achiral ligands (X's denoted by open circles) are examined without considering steric hindrance.

PCI-CF, Eq. 2 can be rewritten to give the corresponding restricted PCI-CF ($\overline{\text{PCI-CF}}$):

$$\overline{\text{PCI-CF}}(\mathbf{G}_i;\$_{d_{jk}}^{(i\alpha)}) = \sum_{j=1}^{s} \overline{m}_{ji}\overline{\text{SCI-CF}}(\mathbf{G}_j;\$_{d_{jk}}^{(i\alpha)}) \tag{32}$$

The restricted PCI-CF (Eq. 32) can be used in place of the PCI-CF of Theorem 19.6 [1], where inventory functions for introducing into $\$_{d_{jk}}^{(i\alpha)}$ should be adopted to match such restricted cases.

2.2.2 Factorization of SCI-CFs into Restricted SCI-CFs

Let us continue the enumeration problem by starting the icosahedral skeleton (**1**). The unrestricted SCI-CFs listed in the SCI-CF-column of Table 1 are factorized into a set of monomials which match the restriction due to steric hindrance. For example, Fig. 3 illustrates the procedure for factorizing the SCI-CF of $\mathbf{C}_s$ ($a_1^4c_2^4$), where a_1^4 corresponds to four one-membered homospheric orbits, i.e., $\{1\}$, $\{2\}$, $\{9\}$, and $\{12\}$, while c_2^4 corresponds to four two-membered enantiospheric orbits, i.e., $\{3,6\}$, $\{4,5\}$, $\{7,11\}$, and $\{8,10\}$. These orbits are fixed under the action of the point group $\mathbf{C}_s$, because the mirror plane of the $\mathbf{C}_s$ is selected to contain vertices 1, 2, 9 and 12.

Let us consider the number (n) of ligands for substitution, where the remaining $12-n$ positions accommodate hydrogens to be characterized by 1. For the case of $n=0$, the factorization of $a_1^4c_2^4$ results in 1 ($=1^4\times(1^2)^4$), which corresponds to **10**. Note that **10** is fixed under $\mathbf{C}_s$.

For the case of $n = 1$, the SCI-CF $a_1^4 c_2^4$ is factorized into a monomial a_1 ($= a_1 \times 1^3 \times (1^2)^4$), which corresponds to four derivatives (**11**–**14**) fixed under $\mathbf{C}_s$. For the case of $n = 2$, the SCI-CF $a_1^4 c_2^4$ is factorized into a_1^2 ($= a_1^2 \times 1^2 \times (1^2)^4$) or c_2 (=$1^4 \times c_2 \times (1^2)^3$). The former monomial a_1^2 corresponds to four derivatives (**15**–**18**) fixed under $\mathbf{C}_s$, where the adjacency of bulky *tert*-butyl ligands or *sec*-butyl ligands is rejected because of steric hindrance. On a similar line, the latter monomial c_2 corresponds to two derivatives (**19** and **20**) fixed under $\mathbf{C}_s$. For the case of $n = 3$, the factorization of $a_1^4 c_2^4$ results in a_1^3 ($= a_1^3 \times 1^1 \times (1^2)^4$) or $a_1 c_2$ ($= a_1 \times 1^3 \times c_2 \times (1^2)^3$). The former monomial a_1^3 is rejected because of steric hindrance. The latter monomial $a_1 c_2$ corresponds to four derivatives (**21**–**24**) which are allowed and fixed under $\mathbf{C}_s$. Obviously, there are no cases of $n \geq 4$, because any derivatives of $n \geq 4$ are not free from the adjacency of bulky ligands. Finally, the sum of these monomials ($1 + 4a_1 + 4a_1^2 + 2c_2 + 4a_1 c_2$) represents the restricted SCI-CF of the subgroup $\mathbf{C}_s$.

Similar procedures for testing factorization and matching are repeated to cover all cases of respective subgroups. The resulting restricted SCI-CFs of respective subgroups are collected in the $\overline{\text{SCI-CF}}$-column of Table 1.

2.2.3 Systematic Factorization of SCI-CFs into Restricted SCI-CFs

The above-mentioned procedure for the factorization of SCI-CFs into restricted SCI-CFs is rather empirical because it is based on a trial-error inspection of fixed molecules, as exemplified by Fig. 3. To pursue a systematic method for the factorization of SCI-CFs, let us examine the unrestricted (usual) SCI of $\mathbf{C}_s$, $a_1^4 c_2^4$, from an alternative point of view by referring to Fig. 3. Each orbit characterized by a sphericity index (SI), i.e., a_1 and c_2, is linked to a set of equivalent vertices:

$$\begin{aligned} a_1^4&: \quad \text{four one-membered orbits} \quad \{1\}, \{2\}, \{9\}, \{12\} \\ c_2^4&: \quad \text{four two-membered orbits} \quad \{3,6\}, \{4,5\}, \{7,11\}, \{8,10\} \end{aligned}$$

In order to correspond the one-membered orbits (a_1) to the vertices $\{1\}$, $\{2\}$, $\{9\}$, and $\{12\}$ as substitution sites, let us introduce a dummy variable x_i for indicating the occupation of the vertex $\{i\}$. Thereby, the correspondence of the orbits to substitution sites are represented by $a_1 x_1$, $a_1 x_2$, $a_1 x_9$, and $a_1 x_{12}$. On a similar line, the two-membered orbits (c_2) are expressed by $c_2 x_3 x_6$, $c_2 x_4 x_5$, $c_2 x_7 x_{11}$, and $c_2 x_8 x_{10}$. These expressions are applied to characterize **4** (as a fixed promolecule to be rejected) and **11** (as a fixed promolecule to be accepted) as follows:

$$\begin{aligned} \mathbf{4} \quad & (a_1 x_1)(c_2 x_7 x_{11}) = a_1 c_2 \cdot x_1 x_7 x_{11} \quad \text{(to be rejected)} \\ \mathbf{11} \quad & (a_1 x_{12})(c_2 x_3 x_6) = a_1 c_2 \cdot x_3 x_6 x_{12} \quad \text{(to be accepted)} \end{aligned}$$

where the SIs and their correspondence to vertices (substitution sites) are specified. Because the parts of dummy variables, $x_1 x_7 x_{11}$ and $x_3 x_6 x_{12}$, indicate substituted vertices as territories of the remaining parts of SIs (both $a_1 c_2$), the former are called *territory indicator* (TI) and the whole are called *restricted SCI-CFs with a territory indicator*. The rejection of **4** is decided by means of the territory indicator $x_1 x_7 x_{11}$, because of the coexistence of x_7 and x_{11}, where vertices 7 and 11 are adjacent. On the other hand, the acceptance of **11** is decided by the territory indicator $x_3 x_6 x_{12}$ because vertices 3, 6, and 12 are not adjacent to one another.

Such monomials with TIs (e.g., $(a_1 x_1)(c_2 x_7 x_{11})$ and $(a_1 x_{12})(c_2 x_3 x_6)$) can be generated exhaustively by considering

$$\begin{aligned} \text{DSCI-CF}_{\mathbf{C}_s} \quad = \quad & (1 + a_1 x_1)(1 + a_1 x_2)(1 + a_1 x_9)(1 + a_1 x_{12}) \\ & \times (1 + c_2 x_3 x_6)(1 + c_2 x_4 x_5)(1 + c_2 x_7 x_{11})(1 + c_2 x_8 x_{10}), \end{aligned} \tag{33}$$

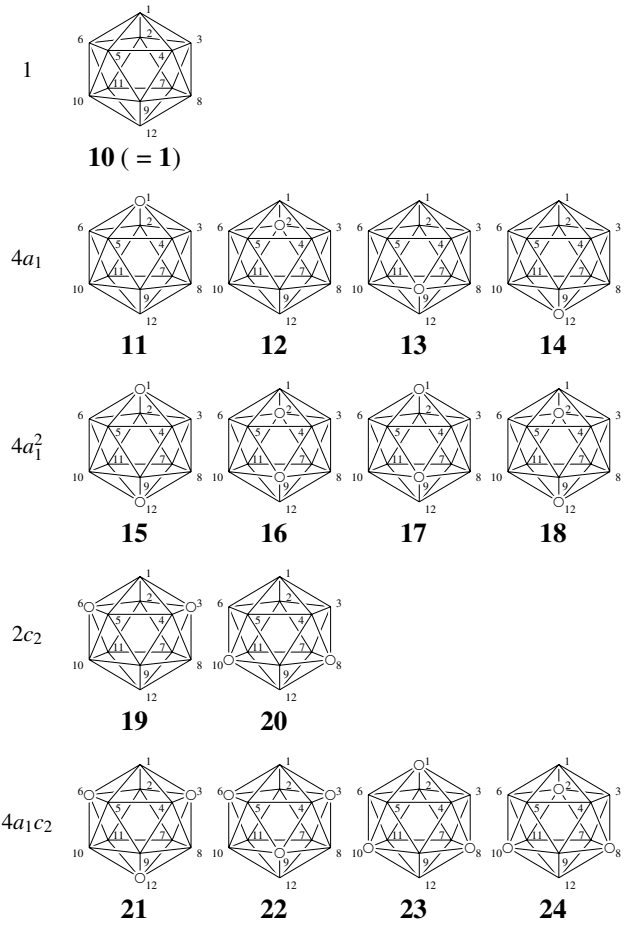


Figure 3: Fixed promolecules on the action of $\mathbf{C}_s$, the mirror plane of which contains vertices 1, 2, 9, and 12. Their restricted monomials are shown in the leftmost columns, where the sum $(1. \quad 4a_1. \quad 4a_1^2. \quad 2c_2. \quad 4a_1c_2)$ represents the restricted SCI-CF of the subgroup $\mathbf{C}_s$.

which stems from the unrestricted (usual) SCI of $\mathbf{C}_s$, $a_1^4 c_2^4$. Note that 1 in each pair of parentheses represents no selection of the SI at issue (among four a_1's and four c_2's). For example, $(a_1x_1)(c_2x_7x_{11})$ is generated by putting $1 \leftarrow a_1x_2 = 1$, $1 \leftarrow a_1x_9 = 1$, $1 \leftarrow a_1x_{12} = 1$, $1 \leftarrow c_2x_3x_6 = 1$, $1 \leftarrow c_2x_4x_5 = 1$, and $1 \leftarrow c_2x_8x_{10} = 1$, where these replacements mean that the orbits at issue are not taken into consideration. Each monomial generated by the expansion of Eq. 33 (e.g., $(a_1x_1)(c_2x_7x_{11})$ or $(a_1x_{12})(c_2x_3x_6)$) is examined whether or not its TI part exhibits the coexistence of adjacent vertices. If the coexistence of adjacent vertices is detected (e.g., $(a_1x_1)(c_2x_7x_{11})$), the monomial at issue is discarded.

The discussions in the preceding paragraphs are generalized to characterize a given suborbit $\Delta_{jk\beta}^{(i\alpha)}$, where a dummy variable is assigned to show the territory of each participating vertex, i.e., x_i for a vertex $\{i\}$. The number of the vertices at issue is presumed to be v. Then, a territory indicator for the suborbit is defined as a product of such dummy variables as follows:

$$t_{jk}^{(i\alpha)}(x_1,\ldots,x_v), \tag{34}$$

which consists of x_1, x_2, …, x_v in accord with the objects of the suborbit $\Delta_{jk\beta}^{(i\alpha)}$. We assign $\$_{d_{jk}}^{(i\alpha)} t_{jk}^{(i\alpha)}(x_1,\ldots,x_v)$ to the suborbit $\Delta_{jk\beta}^{(i\alpha)}$. For the purpose of judging whether or not the suborbit is used for enumeration, the term $1 \leftarrow \$_{d_{jk}}^{(i\alpha)} t_{jk}^{(i\alpha)}(x_1,\ldots,x_v)$ is introduced into the original $\$_{d_{jk}}^{(i\alpha)}$ of the SCI-CF (Eq. 1), where the replacement of $\$_{d_{jk}}^{(i\alpha)}$ by $1 \leftarrow \$_{d_{jk}}^{(i\alpha)} t_{jk}^{(i\alpha)}(x_1,\ldots,x_v)$ means that the corresponding suborbit $\Delta_{jk\beta}^{(i\alpha)}$ is taken into no consideration (the former term 1) or into consideration (the latter term) during the process of enumeration. Thereby, a discriminant of SCI-CF denoted by the symbol DSCI-CF is defined as follows:

Definition 1 The discriminant of the SCI-CF (Eq. 1) is defined as follows:

$$\text{DSCI-CF}(\mathbf{G}_j;\$_{d_{jk}}^{(i\alpha)},x_1,x_2,\ldots,x_v) = \prod_{i=1}^{s}\prod_{\substack{\alpha=1\\ a_i\neq 0}}^{\alpha_i} \text{ZC}(\mathbf{G}(/\mathbf{G}_i)\downarrow \mathbf{G}_j;\$_{d_{jk}}^{(i\alpha)}) \Bigg|_{\$_{d_{jk}}^{(i\alpha)}=1 \leftarrow \$_{d_{jk}}^{(i\alpha)} t_{jk}^{(i\alpha)}(x_1,\ldots,x_v)} \tag{35}$$

As an example, the discriminant of the SCI-CF for $\mathbf{C}_s$ has already shown in Eq. 33. The expansion of the right-hand side of Eq. 35 generates a polynomial, where each component monomial indicates a product of SIs ($\$_{d_{jk}}^{(i\alpha)}$) as well as the corresponding product of territory indicators. An adjacency set (AS) of vertices is defined as follows:

$$\text{AS} = \{\{k,l\} \mid \text{for all adjacent vertices } k \text{ and } l\}, \tag{36}$$

which is a set of all edges in most cases. The process described above can be conducted by the following lemma:

Lemma 1 (Restricted SCI-CFs) Among the monomials contained in the discriminant generated by Def. 1, monomials signified by a TI which contains no adjacent vertices are selected by means of the following equation:

$$\overline{\text{SCI-CF}}(\mathbf{G}_j;\$_{d_{jk}}^{(i\alpha)}) = \text{DSCI-CF}(\mathbf{G}_j;\$_{d_{jk}}^{(i\alpha)},x_1,x_2,\ldots,x_v) \Bigg|_{\substack{x_kx_l=0 \mid \forall\{k,l\}\in\text{AS}\\ \text{then } x_i=1(i=1,\ldots v)}} \tag{37}$$

where the TI part of each selected monomial is replaced by 1 (no appearance) in the last operation (i.e., "then $x_i = 1(i = 1,\ldots v)$").

The proof is obvious by the above-described example. The restricted SCI-CF (Eq. 37) is used to define the corresponding PCI-CF by virtue of Eq. 32.

As for the unrestricted (usual) SCI of $\mathbf{C}_s$, $a_1^4c_2^4$, its discriminant according to Def. 1 (Eq. 35) has been already shown in Eq. 33. The AS for the present case contains all the pairs of vertices corresponding to the 30 edges of the icosahedral skeleton (**1**):

$$\begin{aligned}\mathrm{AS} \;=\; & \{\{1,2\},\{1,3\},\{1,4\},\{1,5\},\{1,6\},\{2,3\},\{2,6\},\{2,7\},\{2,11\},\\ & \{3,4\},\{3,7\},\{3,8\},\{4,5\},\{4,8\},\{4,9\},\{5,6\},\{5,9\},\{5,10\},\\ & \{6,10\},\{6,11\},\{7,8\},\{7,11\},\{7,12\},\{8,9\},\{8,12\},\\ & \{9,10\},\{9,12\},\{10,11\},\{10,12\},\{11,12\}\}. \end{aligned} \tag{38}$$

The discriminant shown in Eq. 33 is expanded and treated by the operation represented by $x_kx_l = 0 \mid \forall\{k,l\} \in \mathrm{AS}$ in Eq. 37. For practical purposes, all of the monomials containing x_kx_l ($\forall\{k,l\} \in \mathrm{AS}$) are detected and removed from the original discriminant (cf. the Maple program shown in the Appendix), so as to leave the following polynomial:

$$\begin{aligned} & 1.\ \{a_1x_1.\ a_1x_2.\ a_1x_9.\ a_1x_{12}\}.\ \{a_1^2x_1x_{12}.\ a_1^2x_2x_9.\ a_1^2x_1x_9.\ a_1^2x_2x_{12}\}\\ & .\ \{c_2x_3x_6.\ c_2x_8x_{10}\}.\ \{a_1c_2x_{12}x_3x_6.\ a_1c_2x_9x_3x_6.\ a_1c_2x_1x_8x_{10}.\ a_1c_2x_2x_8x_{10}\}. \end{aligned} \tag{39}$$

When we examine the TI parts of Eq. 39, a set of monomials in each pair of braces of Eq. 39 corresponds to the set of fixed promolecules shown in each row of Fig. 3. Subsequently, according to Eq. 37, we place $x_i = 1 (i = 1,2,\ldots,12)$ in Eq. 39 so as to give

$$\overline{\text{SCI-CF}}(\mathbf{C}_s;\$_d) = 1.\ \ 4a_1.\ \ 4a_1^2.\ \ 2c_2.\ \ 4a_1c_2, \tag{40}$$

which is identical with the restricted SCI-CF for $\mathbf{C}_s$ listed in Table 1. Similarly, the procedure based on Lemma 1 is repeated to cover all cases of respective subgroups. The resulting restricted SCI-CFs of respective subgroups are collected in the $\overline{\text{SCI-CF}}$-column of Table 1.

The above-mentioned procedures of the systematic factorization of SCI-CFs into restricted SCI-CFs are programmed by using the Maple programming language [18]. The source list of a sample program (named "isocaResA.mpl") for obtaining the restricted SCI-CFs (the $\overline{\text{SCI-CF}}$-column of Table 1) is attached below as an Appendix.

2.2.4 Restricted PCI-CFs Derived From Restricted SCI-CFs

According to Eq. 32, restricted PCI-CFs ($\overline{\text{PCI-CF}}$) for respective subgroups are calculated by starting from the restricted SCI-CFs collected in the $\overline{\text{SCI-CF}}$-column of Table 1:

$$\begin{aligned}\overline{\text{PCI-CF}}_1(\mathbf{C}_1,\$_d) \;=\; & \frac{1}{120}(1.\ \ 12b_1.\ \ 36b_1^2.\ \ 20b_1^3) - \frac{1}{8}(1.\ \ 4b_2)\\ & - \frac{1}{8}(1.\ \ 4a_1.\ \ 4a_1^2.\ \ 2c_2.\ \ 4a_1c_2) - \frac{1}{120}(1.\ \ 6c_2) - \frac{1}{12}(1.\ \ 2b_3)\\ & .\ \ \frac{1}{12}(1).\ \ \frac{1}{4}(1.\ \ 2a_2).\ \ \frac{1}{4}(1.\ \ 2a_2) - \frac{1}{20}(1.\ \ 2b_1.\ \ b_1^2).\ \ \frac{1}{4}(1)\\ & .\ \ \frac{1}{4}(1.\ \ 2a_3).\ \ \frac{1}{12}(1) - \frac{1}{3}(1).\ \ \frac{1}{4}(1.\ \ b_2).\ \ \frac{1}{4}(1.\ \ 2a_1.\ \ a_1^2)\\ & .\ \ \frac{1}{20}(1.\ \ c_2).\ \ \frac{1}{6}(1) - \frac{1}{2}(1) - \frac{1}{2}(1.\ \ a_2) - \frac{1}{6}(1) - \frac{1}{2}(1).\ \ \frac{1}{2}(1)\end{aligned}$$

$$= \frac{1}{4}b_1^2.\quad \frac{1}{6}b_1^3-\frac{1}{2}a_1c_2-\frac{1}{4}b_2-\frac{1}{4}a_1^2-\frac{1}{4}c_2-\frac{1}{6}b_3.\quad \frac{1}{2}a_2.\quad \frac{1}{2}a_3 \tag{41}$$

$$\begin{aligned}\overline{\text{PCI-CF}}_1(\mathbf{C}_2,\$_d) &= \frac{1}{4}(1.\quad 4b_2)-\frac{1}{4}(1)-\frac{1}{4}(1.\quad 2a_2)-\frac{1}{4}(1.\quad 2a_2)-\frac{1}{2}(1).\quad \frac{1}{2}(1)\\ &\quad -\frac{1}{2}(1.\quad b_2).\quad \frac{1}{2}(1).\quad \frac{1}{2}(1.\quad a_2).\quad (1)-(1)\\ &= \frac{1}{2}b_2-\frac{1}{2}a_2 \end{aligned} \tag{42}$$

$$\begin{aligned}\overline{\text{PCI-CF}}_1(\mathbf{C}_s,\$_d) &= \frac{1}{4}(1.\quad 4a_1.\quad 4a_1^2.\quad 2c_2.\quad 4a_1c_2)-\frac{1}{2}(1.\quad 2a_2)-\frac{1}{4}(1.\quad 2a_2)\\ &\quad -\frac{1}{2}(1.\quad 2a_3).\quad \frac{1}{2}(1)-\frac{1}{2}(1.\quad 2a_1.\quad a_1^2).\quad \frac{1}{2}(1).\quad \frac{1}{2}(1.\quad a_2)\\ &= \frac{1}{2}a_1^2.\quad \frac{1}{2}c_2.\quad a_1c_2-a_2-a_3 \end{aligned} \tag{43}$$

$$\begin{aligned}\overline{\text{PCI-CF}}_1(\mathbf{C}_i,\$_d) &= \frac{1}{60}(1.\quad 6c_2)-\frac{1}{4}(1.\quad 2a_2)-\frac{1}{6}(1).\quad \frac{1}{6}(1)-\frac{1}{10}(1.\quad c_2)\\ &\quad .\quad \frac{1}{2}(1).\quad \frac{1}{2}(1.\quad a_2).\quad \frac{1}{3}(1)-1=0 \end{aligned} \tag{44}$$

$$\begin{aligned}\overline{\text{PCI-CF}}_1(\mathbf{C}_3,\$_d) &= \frac{1}{4}(1.\quad 2b_3)-\frac{1}{4}(1)-\frac{1}{4}(1.\quad 2a_3)-\frac{1}{4}(1)-\frac{1}{2}(1)\\ &\quad .\quad \frac{1}{2}(1).\quad \frac{1}{2}(1).\quad \frac{1}{2}(1)-\frac{1}{2}(1)=\frac{1}{2}b_3-\frac{1}{2}a_3 \end{aligned} \tag{45}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{D}_2,\$_d) = \frac{1}{6}(1)-\frac{1}{6}(1)-\frac{1}{6}(1).\quad \frac{1}{6}(1)=0 \tag{46}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{C}_{2v},\$_d) = \frac{1}{2}(1.\quad 2a_2)-\frac{1}{2}(1)=a_2 \tag{47}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{C}_{2h},\$_d) = \frac{1}{2}(1.\quad 2a_2)-\frac{1}{2}(1)-1-(1.\quad a_2).\quad 2(1)=0 \tag{48}$$

$$\begin{aligned}\overline{\text{PCI-CF}}_1(\mathbf{C}_5,\$_d) &= \frac{1}{4}(1.\quad 2b_1.\quad b_1^2)-\frac{1}{4}(1.\quad b_2)-\frac{1}{4}(1.\quad 2a_1.\quad a_1^2)\\ &\quad -\frac{1}{4}(1.\quad c_2).\quad \frac{1}{2}(1.\quad a_2)\\ &= \frac{1}{2}b_1.\quad \frac{1}{4}b_1^2-\frac{1}{4}b_2-\frac{1}{2}a_1-\frac{1}{4}a_1^2-\frac{1}{4}c_2.\quad \frac{1}{2}a_2 \end{aligned} \tag{49}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{D}_3,\$_d) = \frac{1}{2}(1)-\frac{1}{2}(1)-\frac{1}{2}(1).\quad \frac{1}{2}(1)=0 \tag{50}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{C}_{3v},\$_d) = \frac{1}{2}(1.\quad 2a_3)-\frac{1}{2}(1)=a_3 \tag{51}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{C}_{3i},\$_d) = \frac{1}{2}(1)-\frac{1}{2}(1)-1.\quad 1=0 \tag{52}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{D}_{2h},\$_d) = \frac{1}{3}(1)-\frac{1}{3}(1)=0 \tag{53}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{D}_5,\$_d) = \frac{1}{2}(1.\quad b_2)-\frac{1}{2}(1.\quad a_2)-\frac{1}{2}(1).\quad \frac{1}{2}(1)=\frac{1}{2}b_2-\frac{1}{2}a_2 \tag{54}$$

$$\text{PCI-CF}_1(\mathbf{C}_{5v},\$_d) = \frac{1}{2}(1.\quad 2a_1.\quad a_1^2)-\frac{1}{2}(1.\quad a_2)=a_1.\quad \frac{1}{2}a_1^2-\frac{1}{2}a_2 \tag{55}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{C}_{5i},\$_d) = \frac{1}{2}(1.\quad c_2)-\frac{1}{2}(1.\quad a_2)=\frac{1}{2}c_2-\frac{1}{2}a_2 \tag{56}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{T},\$_d) = \frac{1}{2}(1)-\frac{1}{2}(1)-\frac{1}{2}(1).\quad\frac{1}{2}(1)=0 \tag{57}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{D}_{3d},\$_d) = 1-1=0 \tag{58}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{D}_{5d},\$_d) = (1.\quad a_2)-1=a_2 \tag{59}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{T}_h,\$_d) = 1-1=0 \tag{60}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{I},\$_d) = \frac{1}{2}(1)-\frac{1}{2}(1)=0 \tag{61}$$

$$\overline{\text{PCI-CF}}_1(\mathbf{I}_h,\$_d) = 1 \tag{62}$$

2.2.5 Enumeration Results and Their Illustrations

For the purpose of conducting restricted enumeration by starting from the ligand inventory **L** (Eq. 25), the inventory functions shown in Eqs. 26–28 are modified to match the condition of restriction:

$$a_d = \mathrm{X}^d \tag{63}$$

$$b_d = \mathrm{X}^d.\ \mathrm{p}^d.\ \overline{\mathrm{p}}^d \tag{64}$$

$$c_d = \mathrm{X}^d.\ 2\mathrm{p}^{d/2}\overline{\mathrm{p}}^{d/2} \tag{65}$$

where the term (1) is omitted from the right-hand sides of Eqs. 26–28 to avoid the duplicated evaluation of hydrogens. These inventory functions are introduced into the restricted PCI-CFs shown in Eqs. 41–62. Then, the resulting equations are expanded so as to give the following generating functions for every subgroups of $\mathbf{I}_h$:

$$\overline{f_1}(\mathbf{C}_1) = \frac{1}{2}(\mathrm{Xp}.\quad \mathrm{X}\overline{\mathrm{p}}).\quad \frac{1}{2}(\mathrm{X}^2\mathrm{p}.\quad \mathrm{X}^2\overline{\mathrm{p}}).\quad \frac{1}{2}(\mathrm{Xp}^2.\quad \mathrm{X}\overline{\mathrm{p}}^2).\quad \frac{1}{2}(\mathrm{p}^2\overline{\mathrm{p}}.\quad \mathrm{Xp}\overline{\mathrm{p}}^2) \tag{66}$$

$$\overline{f_1}(\mathbf{C}_2) = \frac{1}{2}(\mathrm{p}^2.\quad \overline{\mathrm{p}}^2) \tag{67}$$

$$\overline{f_1}(\mathbf{C}_s) = \mathrm{p}\overline{\mathrm{p}}.\quad 2\mathrm{X}\mathrm{p}\overline{\mathrm{p}} \tag{68}$$

$$\overline{f_1}(\mathbf{C}_i) = 0 \tag{69}$$

$$\overline{f_1}(\mathbf{C}_3) = \frac{1}{2}(\mathrm{p}^3.\quad \overline{\mathrm{p}}^3) \tag{70}$$

$$\overline{f_1}(\mathbf{D}_2) = 0 \tag{71}$$

$$\overline{f_1}(\mathbf{C}_{2v}) = \mathrm{X}^2 \tag{72}$$

$$\overline{f_1}(\mathbf{C}_{2h}) = 0 \tag{73}$$

$$\overline{f_1}(\mathbf{C}_5) = \frac{1}{2}(\mathrm{p}.\quad \overline{\mathrm{p}}).\quad \frac{1}{2}(\mathrm{Xp}.\quad \mathrm{X}\overline{\mathrm{p}}) \tag{74}$$

$$\overline{f_1}(\mathbf{D}_3) = 0 \tag{75}$$

$$\overline{f_1}(\mathbf{C}_{3v}) = \mathrm{X}^3 \tag{76}$$

$$\overline{f_1}(\mathbf{C}_{3i}) = 0 \tag{77}$$

$$\overline{f_1}(\mathbf{D}_{2h}) = 0 \tag{78}$$

$$\overline{f_1}(\mathbf{D}_5) = \frac{1}{2}(\mathrm{p}^2.\quad \overline{\mathrm{p}}^2) \tag{79}$$

$$\overline{f_1}(\mathbf{C}_{5v}) = \mathrm{X} \tag{80}$$

$$\overline{f_1}(\mathbf{C}_{5i}) = \mathrm{p}\overline{\mathrm{p}} \tag{81}$$

$$\overline{f_1}(\mathbf{T}) = 0 \quad (82)$$
$$\overline{f_1}(\mathbf{D}_{3d}) = 0 \quad (83)$$
$$\overline{f_1}(\mathbf{D}_{5d}) = \mathrm{X}^2 \quad (84)$$
$$\overline{f_1}(\mathbf{T}_h) = 0 \quad (85)$$
$$\overline{f_1}(\mathbf{I}) = 0 \quad (86)$$
$$\overline{f_1}(\mathbf{I}_h) = 1 \quad (87)$$

It should be noted that each enantiomeric pair of chiral derivatives is counted once in the form of such a term as $\frac{1}{2}(\mathrm{p}^2 - \overline{\mathrm{p}}^2)$ (e.g., in Eq. 67). The zero values in Eq. 69 ($\mathbf{C}_i$), Eq. 71 ($\mathbf{D}_2$), Eq. 73 ($\mathbf{C}_{2h}$), Eq. 75 ($\mathbf{D}_3$), Eq. 77 ($\mathbf{C}_{3i}$), Eq. 78 ($\mathbf{D}_{2h}$), Eq. 82 ($\mathbf{T}$), Eq. 83 ($\mathbf{D}_{3d}$), Eq. 85 ($\mathbf{I}_h$), and Eq. 86 ($\mathbf{I}$) have already appeared in the level of restricted PCI-CFs (Eqs. 41–62). This means that there are no derivatives of such subsymmetries even if the ligand inventory $\mathbf{L}$ is expanded to contain other ligands.

Non-zero results shown in Eqs. 67–86 (except Eqs. 66 and 87) are illustrated in Fig. 4, where ligands are represented by the symbols shown in Fig. 1. The following comments concerning the derivatives shown in Fig. 4 should be added to examine the validity of the present restricted enumeration.

The generating function of $\mathbf{C}_s$ (Eq. 68) indicates that there are one $\mathbf{C}_s$-derivative with the formula $\mathrm{p}\overline{\mathrm{p}}$ (i.e., **26**) and two $\mathbf{C}_s$-derivatives with the formula $\mathrm{Xp}\overline{\mathrm{p}}$ (i.e., **27** and **28**). Note that the mirror plane of the $\mathbf{C}_s$ selected to draw **26**–**28** contains vertices 1, 2, 9, and 12, and that each pair of p and $\overline{\mathrm{p}}$ constructs an enantiospheric orbit.

The exchange (permutation) of p and $\overline{\mathrm{p}}$ causes an isomerization between **27** and **28**, whereas they are fixed (unchanged) under the action of the $\mathbf{C}_s$. In other words, the relationship between **27** and **28** is a diastereomeric one, which is akin to a pseudoasymmetric case of $\mathrm{CHXp}\overline{\mathrm{p}}$.

On the other hand, the $\mathbf{C}_s$-derivative **26** is fixed under an exchange (permutation) between p and $\overline{\mathrm{p}}$ as well as under the action of $\mathbf{C}_s$. Thus, the case of **26** is akin to such a degenerate case as $\mathrm{CH_2p}\overline{\mathrm{p}}$ derived from a tetrahedral skeleton (a methane skeleton). Note that the exchange (permutation) between p and $\overline{\mathrm{p}}$ in **26** is alternatively realized by a rotation around a three-fold axis which runs through the centers of two trigonal faces (vertices 1, 4, and 5; vertices 7, 9, and 11).

It should be noted that the two $\mathbf{C}_s$-derivatives (**27** and **28**) have an enantiomeric pair of bulky *sec*-butyl ligands (p and $\overline{\mathrm{p}}$ as chiral ligands in isolation). In other words, Eq. 68 (no terms concerning X, X^2, or X^3) implicitly indicates that other $\mathbf{C}_s$ derivatives only with achiral ligands (X's) do not exist under the restricted condition for rejecting the adjacency of bulky ligands. Compare this result with the corresponding unrestricted case calculated by Eq. 29, which contains the term $3X^3$ corresponding to achiral ligands. These three $\mathbf{C}_s$-derivatives have already shown in Fig. 2 (**4**, **5**, and **6**), where they suffer from steric hindrance due to the adjacency of bulky ligands.

Comparison between the term $8\mathrm{Xp}\overline{\mathrm{p}}$ in Eq. 29 (unrestricted) and the term $2\mathrm{Xp}\overline{\mathrm{p}}$ in Eq. 68 (restricted) indicates the presence of six $\mathbf{C}_s$-derivatives characterized by at least one adjacency of bulky ligands. Although their illustrations are omitted, they can be easily drawn by relating them to **4**, **5**, and **8** illustrated in Fig. 2, where an adjacent pair of X's is selected from three X's and replaced by a pair of p and $\overline{\mathrm{p}}$, so as to construct an enantiospheric orbit. Thus, the pair of X's at the positions $\{7,11\}$ of **4**, the pair of X's at the positions $\{3,6\}$ of **5**, and the pair of X's at the positions $\{4,5\}$ of **8** (the selection of $\{4,9\}$ or $\{5,9\}$ gives the same result) are selected as such an adjacent pair. Note that there are two modes of replacement by each pair of p and $\overline{\mathrm{p}}$.

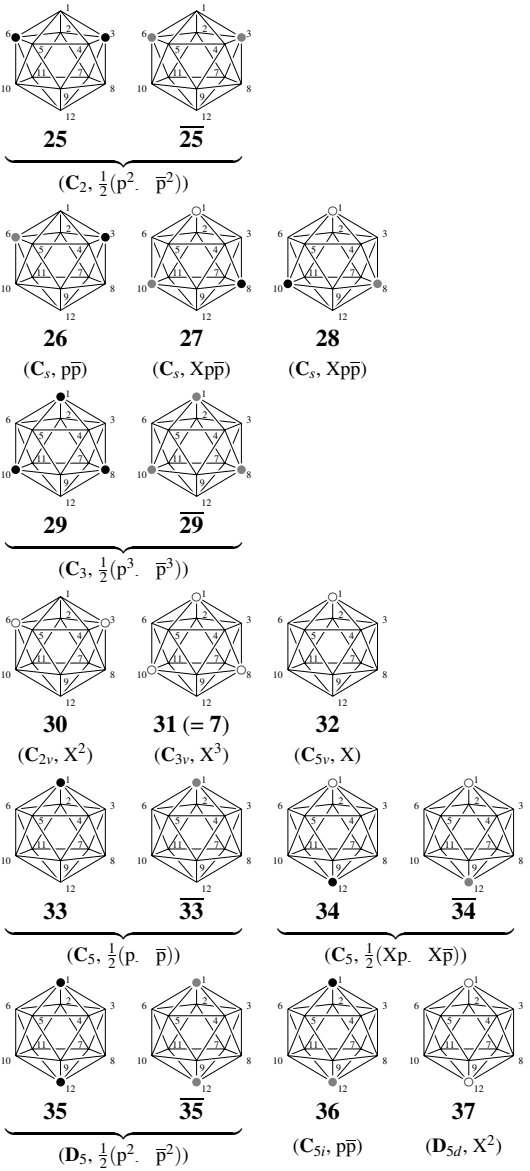


Figure 4: Icosahedral derivatives with considering steric hindrance. For the symbols of ligands, see Fig. 1.

Thereby, we have $2 \times 3 = 6$, which corresponds to $8\mathrm{Xp\overline{p}} - 2\mathrm{Xp\overline{p}} = 6\mathrm{Xp\overline{p}}$.

Among the two $\mathbf{C}_{3v}$-derivatives (**7** and **8** in Fig. 2) corresponding to the term $2\mathrm{X}^3$ of the unrestricted calculation (Eq. 30), Fig. 4 depicts only **7** (= **31**) in accord with the term X^3 of the restricted calculation (Eq. 76). Because any two X's selected from **8** occupy an adjacent pair of positions, the $\mathbf{C}_{3v}$-derivative **8** is rejected under the restriction condition.

The effect of the restriction condition is also found by comparing Eq. 78 (no term X^4) and Eq. 31 (the term X^4). Thus, the $\mathbf{D}_{2h}$-derivative (**9**) shown in Fig. 2 is rejected under the restriction condition due to steric hindrance.

3 PCI-CFs Derived From SCI-CFs for Two or More Orbits

3.1 Unrestricted Enumeration for Tow or More Orbits

Let us next consider the substitution of bulky bidentate ligands:

$$\mathbf{L}' = \{\mathrm{Z}, \mathrm{Z}', \ldots\} \tag{88}$$

in addition to such bulky monodentate ligands as shown in the ligand inventory $\mathbf{L}$ (Eq. 25). For the simplicity's sake, we here take account of achiral bidentate ligands with no directions (i.e, with symmetric constitutions such as —$\mathrm{C(CH_3)_2}$——$\mathrm{C(CH_3)_2}$—). In order that substitutions of such bidentate ligands to edges are treated properly (in addition to substitutions of monodentate ligands to the 12 vertices), the 30 edges of the icosahedral skeleton (**1**) along with the 12 vertices are taken into consideration. The edges construct a thirty-membered orbit governed by a coset representation $\mathbf{I}_h(/\mathbf{C}_{2v})$ ($|\mathbf{I}_h|/|\mathbf{C}_{2v}| = 120/4 = 30$). The corresponding USCI-CFs are cited from the $\mathbf{I}_h(/\mathbf{C}_{2v})$-row of the USCI-CF table of $\mathbf{I}_h$ (Table 3 of [15]), as collected in the SCI-CF (Edges)-column of Table 2. Table 2 also contains the USCI-CFs for $\mathbf{I}_h(/\mathbf{C}_{5v})$ for substitution of monodentate ligands to vertices in the SCI-CF (Vertices)-column. The two types of USCI-CFs for each subgroup are multiplied to give corresponding SCI-CF. For example, the USCI-CF for the 12 vertices ($\mathbf{I}_h(/\mathbf{C}_{5v})$) is $a_1^4 c_2^4$ and the USCI-CF for the 30 edges ($\mathbf{I}_h(/\mathbf{C}_{2v})$) is $a_1^4 c_2^{13}$ for the subgroup $\mathbf{C}_s$, so that the SCI-CF for the $\mathbf{C}_s$ is calculated to be $a_1^4 c_2^4 \cdot \tilde{a}_1^4 \tilde{c}_2^{13}$, where tilde accents are added to specify edge substitutions. Such SCI-CFs as obtained for every subgroups are summed up according to Eq. 2 so as to give the corresponding PCI-CFs on a similar line to the calculations of Eqs. 3–24.

The resulting PCI-CFs can be applied to unrestricted enumerations in a similar way to Section 2.1, when the bulkiness of monodentate and bidentate ligands is tentatively disregarded. Note that edge substitutions should take directions and chiralities of bidentate ligands into consideration. Because this type of consideration is difficult to be treated, we here select achiral bidentate ligands with no directions for the simplicity's sake. As a result, the ligand inventory for $\mathbf{L}'$ (Eq. 88) is obtained as follows:

$$\tilde{a}_d = \tilde{b}_d = \tilde{c}_d = \mathrm{Z}^d + \mathrm{Z}'^d + \cdots, \tag{89}$$

which is used in addition to the ligand-inventory functions for monodentate ligands (Eqs.63–65).

Table 2: SCI-CFs and Restricted SCI-CFs for Vertices ($\mathbf{I}_h(/\mathbf{C}_{5v})$) and Edges ($\mathbf{I}_h(/\mathbf{C}_{2v})$)

subgroup	SCI-CF		$\overline{\text{SCI-CF}}$
$\mathbf{G}_j$	Vertices $\times$	Edges	
$\mathbf{C}_1$	b_1^{12}	b_1^{30}	$(1.\ \ 12b_1.\ \ 36b_1^2.\ \ 20b_1^3)$ $.\ (30\tilde{b}_1.\ \ 75\tilde{b}_1^2).\ (120b_1.\ \ 30b_1^2)\tilde{b}_1$
$\mathbf{C}_2$	b_2^6	$b_1^2b_2^{14}$	$(1.\ \ 4b_2).\ (2\tilde{b}_1.\ \ \tilde{b}_1^2.\ \ 6\tilde{b}_2).\ \ 2b_2\tilde{b}_1$
$\mathbf{C}_s$	$a_1^4c_2^4$	$a_1^4c_2^{13}$	$(1.\ \ 4a_1.\ \ 4a_1^2.\ \ 2c_2.\ \ 4a_1c_2)$ $.\ (4\tilde{a}_1.\ \ 2\tilde{a}_1^2.\ \ \tilde{c}_2).\ (8a_1.\ \ 2a_1^2.\ \ 2c_2)\tilde{a}_1$
$\mathbf{C}_i$	c_2^6	c_2^{15}	$(1.\ \ 6c_2).\ \ 15\tilde{c}_2$
$\mathbf{C}_3$	b_3^4	b_3^{10}	$1.\ \ 2b_3$
$\mathbf{D}_2$	b_4^3	$b_2^3b_4^6$	$1.\ \ 3\tilde{b}_2$
$\mathbf{C}_{2v}$	$a_2^4c_4$	$a_1^2a_2^2c_4^6$	$(1.\ \ 2a_2).\ (2\tilde{a}_1.\ \ \tilde{a}_1^2.\ \ 2\tilde{c}_2).\ \ 2a_2\tilde{a}_1$
$\mathbf{C}_{2h}$	$a_2^2c_4^2$	$a_2^2c_2c_4^6$	$(1.\ \ 2a_2).\ (2\tilde{a}_2.\ \ \tilde{c}_2)$
$\mathbf{C}_5$	$b_1^2b_5^2$	b_5^6	$1.\ \ 2b_1.\ \ b_1^2$
$\mathbf{D}_3$	b_6^2	$b_3^2b_6^4$	1
$\mathbf{C}_{3v}$	a_3^4*	$a_3^4c_6^3$	$1.\ \ 2a_3$
$\mathbf{C}_{3i}$	c_6^2	c_6^5	1
$\mathbf{D}_{2h}$	a_4^3	$a_2^3c_8^3$	$1.\ \ 3\tilde{a}_2$
$\mathbf{D}_5$	b_2b_{10}	$b_5^2b_{10}^2$	$1.\ \ b_2$
$\mathbf{C}_{5v}$	$a_1^2a_5^2$	$a_5^4c_{10}$	$1.\ \ 2a_1.\ \ a_1^2$
$\mathbf{C}_{5i}$	c_2c_{10}	c_{10}^5	$1.\ \ c_2$
$\mathbf{T}$	b_{12}	$b_6b_{12}^2$	1
$\mathbf{D}_{3d}$	a_6^2	$a_6^2c_6c_{12}$	1
$\mathbf{D}_{5d}$	a_2a_{10}*	$a_{10}^2c_{10}$	$1.\ \ a_2$
$\mathbf{T}_h$	a_{12}	a_6c_{24}	1
$\mathbf{I}$	b_{12}	b_{30}	1
$\mathbf{I}_h$	a_{12}	a_{30}	1

* Corrected data for Table 3 of [15].

3.2 Restricted Enumeration for Two or More Orbits

3.2.1 Factorizations of SCI-CFs for Two or More Orbits

Suppose that bulky bidentate ligands selected from $\mathbf{L}'$ (Eq. 88) are considered to occupy an appropriate set of edges selected from **1** in addition to bulky monodentate ligands selected from **L** (Eq. 25), where the bulkiness of such monodentate and bidentate ligands is taken into explicit consideration. In other words, we consider a restriction condition that bulky bidentate ligands of any pair and/or bulky monodentate ligands of any pair are not adjacent as well as each bulky bidentate ligand is not adjacent to a ligand selected from **L**.

Let us continue and extend the restriction procedure shown in Fig. 3 for the subgroup $\mathbf{C}_s$. Because the present case is concerned both with vertices (for monodentate ligands) and edges (for bidentate ligands), the factorization of the unrestricted SCI-CF, i.e., $a_1^4c_2^4 \cdot \tilde{a}_1^4\tilde{c}_2^{13}$, should be examined by considering three types of cases, i.e., cases with vertices only, cases with edges only, and cases with interaction between vertices and edges.

First, the cases with vertices only are treated equally to Fig. 3, because the corresponding factorization of $a_1^4c_2^4 \cdot (\tilde{1}^4 \cdot (\tilde{1}^2)^{13})$ is essentially identical with that of $a_1^4c_2^4$. As found in Fig. 3, the resulting polynomial, i.e.,

$$\overline{\text{SCI-CF}}^{(\text{v})}(\mathbf{C}_s;\$_d,\tilde{\$}_d) = 1\_ \quad 4a_{1\_} \quad 4a_{1\_}^2 \quad 2c_{2\_} \quad 4a_1c_2, \tag{90}$$

is a vertex part of the restricted SCI-CF to be obtained for the subgroup $\mathbf{C}_s$, where the symbol $\$_d$ represents a_d, b_d, or c_d for vertex substitution, while the symbol $\tilde{\$}_d$ represents $\tilde{a}_d$, $\tilde{b}_d$, and $\tilde{c}_d$ for edge substitution.

The second cases with edges only are treated as shown in Fig. 5. The unrestricted SCI-CF $a_1^4c_2^4 \cdot \tilde{a}_1^4\tilde{c}_2^{13}$ is preliminarily restricted into $(1^4 \cdot (1^2)^4) \cdot \tilde{a}_1^4\tilde{c}_2^{13} = \tilde{a}_1^4\tilde{c}_2^{13}$, which is further factorized in the procedure shown in Fig. 5. Because the mirror plane of the $\mathbf{C}_s$ contains vertices 1, 2, 9, and 12, there are four edges, $\{\{1,2\}\}$, $\{\{4,5\}\}$, $\{\{7,11\}\}$, and $\{\{9,12\}\}$, each of which constructs a one-membered orbit fixed under the action of the $\mathbf{C}_s$. Hence, the factorization represented by $(\tilde{a}_1^1) \cdot \tilde{1}^3 \cdot (\tilde{1}^2)^{13} = \tilde{a}_1$ corresponds to four promolecules (**38**–**41**) so that the monomial $4\tilde{a}_1$ is assigned to them. Further the factorization represented by $(\tilde{a}_1^2) \cdot \tilde{1}^2 \cdot (\tilde{1}^2)^{13} = \tilde{a}_1^2$ corresponds to two promolecules (**42** and **43**) because of the restriction condition describe above. It follows that the monomial $2\tilde{a}_1^2$ is assigned to them.

The term $\tilde{c}_2^{13}$ (among $\tilde{a}_1^4\tilde{c}_2^{13}$) indicates that there are 13 pairs of edges, which respectively construct two-membered orbits. Among them, only the orbit $\{\{3,8\},\{6,10\}\}$ (corresponding to **44**) is fixed under the action of the $\mathbf{C}_s$ because the restriction condition describe above is taken into consideration. The selection of **44** as a fixed promolecule is characterized by the factorization $\tilde{1}^4 \cdot \tilde{c}_2 \cdot (\tilde{1}^2)^{12} = \tilde{c}_2$.

The three modes of factorization shown in Fig. 5 are summarized to give an edge part of the restricted SCI-CF to be obtained for the subgroup $\mathbf{C}_s$:

$$\overline{\text{SCI-CF}}^{(\text{e})}(\mathbf{C}_s;\$_d,\tilde{\$}_d) = 4\tilde{a}_{1\_} \quad 2\tilde{a}_{1\_}^2 \quad \tilde{c}_2, \tag{91}$$

where tilde accents characterize edge substitutions.

The third cases with interaction between vertices and edges are treated as shown in Fig. 6. For cases of substituting one vertex and one edge under the restriction condition described above, the unrestricted SCI-CF $a_1^4c_2^4 \cdot \tilde{a}_1^4\tilde{c}_2^{13}$ is factorized into $a_1^1 \cdot 1^3 \cdot (1^2)^4 \cdot \tilde{a}_1^1 \cdot \tilde{1}^3 \cdot (\tilde{1}^2)^{13} = a_1\tilde{a}_1$, which is assigned to each of eight promolecules **45**–**52**. Hence, the monomial $8a_1\tilde{a}_1$ is

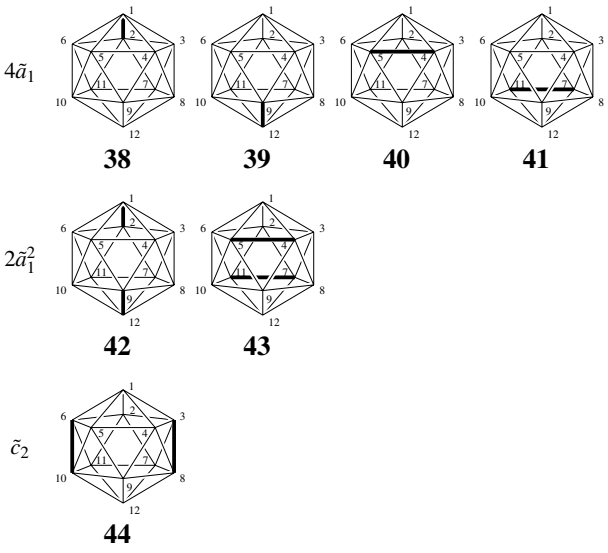


Figure 5: Promolecules with bidentate ligands, which are fixed on the action of $\mathbf{C}_s$, where the mirror plane at issue contains vertices 1, 2, 9, and 12. Their restricted monomials are shown in the leftmost columns, where the sum $(4\tilde{a}_1 + 2\tilde{a}_1^2 + \tilde{c}_2)$ represents an edge part of the restricted SCI-CF of the subgroup $\mathbf{C}_s$.

assigned to them. For cases of substituting two vertices and one edge under the restriction condition described above, the unrestricted SCI-CF $a_1^4 c_2^4 \cdot \tilde{a}_1^4 \tilde{c}_2^{13}$ is factorized into two ways, i.e., $a_1^2 \cdot 1^2 \cdot (1^2)^4 \cdot \tilde{a}_1^1 \cdot \tilde{1}^3 \cdot (\tilde{1}^2)^{13} = a_1^2 \tilde{a}_1$ and $1^4 \cdot c_2 \cdot (1^2)^3 \cdot \tilde{a}_1^1 \cdot \tilde{1}^3 \cdot (\tilde{1}^2)^{13} = c_2 \tilde{a}_1$. The former mode of factorization corresponds to **53** and **54** ($2a_1^2\tilde{a}_1$), while the latter mode of factorization corresponds to **55** and **56** ($2c_2\tilde{a}_1$).

The three modes of factorization shown in Fig. 6 are summarized to give a vertex-edge part of the restricted SCI-CF to be obtained for the subgroup $\mathbf{C}_s$:

$$\overline{\text{SCI-CF}}^{(\text{ve})}(\mathbf{C}_s; \$_d, \tilde{\$}_d) = (8a_1 + 2a_1^2 + 2c_2)\tilde{a}_1. \tag{92}$$

Because the first to third cases shown in Figs. 3, 5, and 6 cover all of the fixed promolecules under the action of $\mathbf{C}_s$, the respective polynomials (Eqs. 90, 91, and 92) are summed up to give the corresponding restricted SCI-CF as follows:

$$\begin{aligned}
&\overline{\text{SCI-CF}}(\mathbf{C}_s; \$_d, \tilde{\$}_d) \\
&\quad = \overline{\text{SCI-CF}}^{(\text{v})}(\mathbf{C}_s; \$_d, \tilde{\$}_d) + \overline{\text{SCI-CF}}^{(\text{e})}(\mathbf{C}_s; \$_d, \tilde{\$}_d) + \overline{\text{SCI-CF}}^{(\text{ve})}(\mathbf{C}_s; \$_d, \tilde{\$}_d) \\
&\quad = (1 + 4a_1 + 4a_1^2 + 2c_2 + 4a_1c_2) + (4\tilde{a}_1 + 2\tilde{a}_1^2 + \tilde{c}_2) \\
&\qquad + (8a_1 + 2a_1^2 + 2c_2)\tilde{a}_1.
\end{aligned} \tag{93}$$

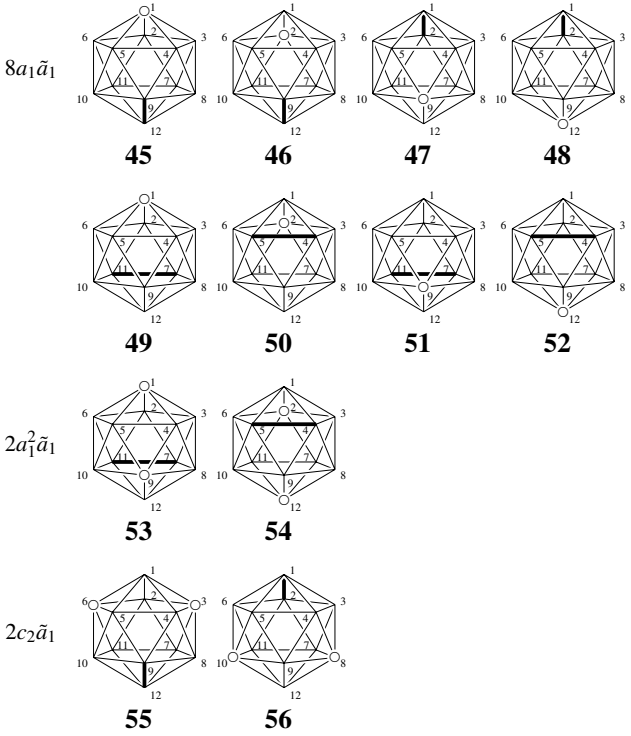


Figure 6: Promolecules with monodentate and bidentate ligands, which are fixed on the action of $\mathbf{C}_s$, where the mirror plane at issue contains vertices 1, 2, 9, and 12. Their restricted monomials are shown in the leftmost columns, where the sum $((8a_{1\cdot}\quad 2a_{1\cdot}^2\quad 2c_2)\tilde{a}_1)$ represents another part of the restricted SCI-CF of the subgroup $\mathbf{C}_s$.

Similar procedures for testing factorization and matching (cf. Figs. 3, 5, and 6) are repeated to cover all cases of respective subgroups. The resulting restricted SCI-CFs of respective subgroups are collected in the $\overline{\text{SCI-CF}}$-column of Table 2.

3.2.2 Restricted PCI-CFs for Two or More Orbits

The restricted SCI-CFs collected in the $\overline{\text{SCI-CF}}$-column of Table 2 are used to calculate restricted PCI-CFs ($\overline{\text{PCI-CF}}$) for respective subgroups according to Eq. 32, where the inverse mark table of $\mathbf{I}_h$ is used in a similar way to Eqs. 41–62.

$$\begin{aligned}\overline{\text{PCI-CF}}_2(\mathbf{C}_1,\$_d,\tilde{\$}_d) \;=\; & \frac{1}{4}b_{1\cdot}^2\quad \frac{1}{6}b_1^3-\frac{1}{4}b_2-\frac{1}{6}b_3-\frac{1}{4}a_{1\cdot}^2\quad \frac{1}{2}a_{2\cdot}\quad \frac{1}{2}a_3-\frac{1}{4}c_2-\frac{1}{2}a_1c_2\\ & -\frac{1}{2}\tilde{b}_{2\cdot}\quad \frac{1}{2}\tilde{b}_1^2-\frac{1}{2}\tilde{a}_{2\cdot}\quad \frac{1}{2}\tilde{c}_2\end{aligned}$$

$$\cdot \quad \frac{1}{2}a_2\tilde{a}_1 - a_1\tilde{a}_1 - \frac{1}{4}a_1^2\tilde{a}_1 - \frac{1}{4}c_2\tilde{a}_1 \cdot \quad b_1\tilde{b}_1 \cdot \quad \frac{1}{4}b_1^2\tilde{b}_1 - \frac{1}{4}b_2\tilde{b}_1 \tag{94}$$

$$\begin{aligned}\overline{\text{PCI-CF}}_2(\mathbf{C}_2, \$_d, \tilde{\$}_d) &= \frac{1}{2}b_2 - \frac{1}{2}a_2 \cdot \quad \frac{1}{2}\tilde{b}_1 \cdot \quad \frac{1}{4}\tilde{b}_1^2 \cdot \quad \frac{3}{4}\tilde{b}_2 - \frac{1}{4}\tilde{a}_1^2 - \frac{1}{2}\tilde{a}_1 \cdot \quad \tilde{a}_2 - \frac{3}{4}\tilde{c}_2 \\ &\quad - \frac{1}{2}a_2\tilde{a}_1 \cdot \quad \frac{1}{2}b_2\tilde{b}_1 \end{aligned} \tag{95}$$

$$\begin{aligned}\overline{\text{PCI-CF}}_2(\mathbf{C}_s, \$_d, \tilde{\$}_d) &= \frac{1}{2}a_1^2 - a_2 - a_3 \cdot \quad \frac{1}{2}c_2 \cdot \quad a_1c_2 \\ &\quad \cdot \quad \tilde{a}_2 - \tilde{c}_2 - a_2\tilde{a}_1 \cdot \quad 2a_1\tilde{a}_1 \cdot \quad \frac{1}{2}a_1^2\tilde{a}_1 \cdot \quad \frac{1}{2}c_2\tilde{a}_1 \end{aligned} \tag{96}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{C}_i, \$_d, \tilde{\$}_d) = 0 \tag{97}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{C}_3, \$_d, \tilde{\$}_d) = \frac{1}{2}b_3 - \frac{1}{2}a_3 \tag{98}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{D}_2, \$_d, \tilde{\$}_d) = \frac{1}{2}\tilde{b}_2 - \frac{1}{2}\tilde{a}_2 \tag{99}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{C}_{2v}, \$_d, \tilde{\$}_d) = a_2 \cdot \quad \tilde{a}_1 \cdot \quad \frac{1}{2}\tilde{a}_1^2 - \frac{3}{2}\tilde{a}_2 \cdot \quad \tilde{c}_2 \cdot \quad a_2\tilde{a}_1 \tag{100}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{C}_{2h}, \$_d, \tilde{\$}_d) = \frac{1}{2}\tilde{c}_2 - \frac{1}{2}\tilde{a}_2 \tag{101}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{C}_5, \$_d, \tilde{\$}_d) = \frac{1}{2}b_1 \cdot \quad \frac{1}{4}b_1^2 - \frac{1}{4}b_2 - \frac{1}{2}a_1 - \frac{1}{4}a_1^2 \cdot \quad \frac{1}{2}a_2 - \frac{1}{4}c_2 \tag{102}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{D}_3, \$_d, \tilde{\$}_d) = 0 \tag{103}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{C}_{3v}, \$_d, \tilde{\$}_d) = a_3 \tag{104}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{C}_{3i}, \$_d, \tilde{\$}_d) = 0 \tag{105}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{D}_{2h}, \$_d, \tilde{\$}_d) = \tilde{a}_2 \tag{106}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{D}_5, \$_d, \tilde{\$}_d) = \frac{1}{2}b_2 - \frac{1}{2}a_2 \tag{107}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{C}_{5v}, \$_d, \tilde{\$}_d) = a_1 \cdot \quad \frac{1}{2}a_1^2 - \frac{1}{2}a_2 \tag{108}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{C}_{5i}, \$_d, \tilde{\$}_d) = \frac{1}{2}c_2 - \frac{1}{2}a_2 \tag{109}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{T}, \$_d, \tilde{\$}_d) = 0 \tag{110}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{D}_{3d}, \$_d, \tilde{\$}_d) = 0 \tag{111}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{D}_{5d}, \$_d, \tilde{\$}_d) = a_2 \tag{112}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{T}_h, \$_d, \tilde{\$}_d) = 0 \tag{113}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{I}, \$_d, \tilde{\$}_d) = 0 \tag{114}$$

$$\overline{\text{PCI-CF}}_2(\mathbf{I}_h, \$_d, \tilde{\$}_d) = 1 \tag{115}$$

3.2.3 Enumeration Results and Their Illustrations

For the simplicity's sake, suppose that bulky bidentate ligands (Z) of one kind selected from $\mathbf{L}'$ (Eq. 88) are considered to occupy an appropriate set of edges selected from $\mathbf{1}$. It follows that Eq. 89 is simplified into the following inventory function:

$$\tilde{a}_d = \tilde{b}_d = \tilde{c}_d = \mathrm{Z}^d \tag{116}$$

The inventory functions for vertex substitution (Eqs. 63–65) and for edge substitution (Eq. 116) are introduced into the restricted PCI-CFs (Eqs. 94–115). The expansions of the resulting equations give the following generation functions:

$$\overline{f_2}(\mathbf{C}_1) = \frac{1}{2}(\mathrm{Xp}. \ \mathrm{X}\overline{\mathrm{p}}). \ \frac{1}{2}(\mathrm{X}^2\mathrm{p}. \ \mathrm{X}^2\overline{\mathrm{p}}). \ \frac{1}{2}(\mathrm{Xp}^2. \ \mathrm{X}\overline{\mathrm{p}}^2). \ \frac{1}{2}(\mathrm{p}^2\overline{\mathrm{p}}. \ \mathrm{Xp}\overline{\mathrm{p}}^2) . \ \frac{1}{2}(\mathrm{Xp}. \ \mathrm{X}\overline{\mathrm{p}})\mathrm{Z}. \ (\mathrm{p}. \ \overline{\mathrm{p}})\mathrm{Z} \quad (117)$$

$$\overline{f_2}(\mathbf{C}_2) = \frac{1}{2}(\mathrm{p}^2. \ \overline{\mathrm{p}}^2). \ \frac{1}{2}(\mathrm{p}^2. \ \overline{\mathrm{p}}^2)\mathrm{Z}. \ \mathrm{Z}^2 \quad (118)$$

$$\overline{f_2}(\mathbf{C}_s) = \mathrm{p}\overline{\mathrm{p}}. \ 2\mathrm{Xp}\overline{\mathrm{p}}. \ \mathrm{p}\overline{\mathrm{p}}\mathrm{Z}. \ 2\mathrm{XZ} \quad (119)$$

$$\overline{f_2}(\mathbf{C}_i) = 0 \quad (120)$$

$$\overline{f_2}(\mathbf{C}_3) = \frac{1}{2}(\mathrm{p}^3. \ \overline{\mathrm{p}}^3) \quad (121)$$

$$\overline{f_2}(\mathbf{D}_2) = 0 \quad (122)$$

$$\overline{f_2}(\mathbf{C}_{2v}) = \mathrm{X}^2. \ \mathrm{Z}. \ \mathrm{X}^2\mathrm{Z} \quad (123)$$

$$\overline{f_2}(\mathbf{C}_{2h}) = 0 \quad (124)$$

$$\overline{f_2}(\mathbf{C}_5) = \frac{1}{2}(\mathrm{p}. \ \overline{\mathrm{p}}). \ \frac{1}{2}(\mathrm{Xp}. \ \mathrm{X}\overline{\mathrm{p}}) \quad (125)$$

$$\overline{f_2}(\mathbf{D}_3) = 0 \quad (126)$$

$$\overline{f_2}(\mathbf{C}_{3v}) = \mathrm{X}^3 \quad (127)$$

$$\overline{f_2}(\mathbf{C}_{3i}) = 0 \quad (128)$$

$$\overline{f_2}(\mathbf{D}_{2h}) = \mathrm{Z}^2 \quad (129)$$

$$\overline{f_2}(\mathbf{D}_5) = \frac{1}{2}(\mathrm{p}^2. \ \overline{\mathrm{p}}^2) \quad (130)$$

$$\overline{f_2}(\mathbf{C}_{5v}) = \mathrm{X} \quad (131)$$

$$\overline{f_2}(\mathbf{C}_{5i}) = \mathrm{p}\overline{\mathrm{p}} \quad (132)$$

$$\overline{f_2}(\mathbf{T}) = 0 \quad (133)$$

$$\overline{f_2}(\mathbf{D}_{3d}) = 0 \quad (134)$$

$$\overline{f_2}(\mathbf{D}_{5d}) = \mathrm{X}^2 \quad (135)$$

$$\overline{f_2}(\mathbf{T}_h) = 0 \quad (136)$$

$$\overline{f_2}(\mathbf{I}) = 0 \quad (137)$$

$$\overline{f_2}(\mathbf{I}_h) = 1 \quad (138)$$

Obviously, Eqs. 117–138 involves Eqs. 66–87. The differences between them are terms containing Z's, which represent the presence of bidentate ligands on edges. Because Fig. 4 has already illustrated the derivatives calculated by Eqs. 66–87, the remaining derivatives involving Z's (calculated by Eqs. 117–138) are shown in Fig. 4.

In addition to one enantiomeric pair of $\mathbf{C}_2$-derivatives (**25**/$\overline{\mathbf{25}}$) shown in Fig. 4, Fig. 7 involves two enantiomeric pairs of $\mathbf{C}_2$-derivatives (**57**/$\overline{\mathbf{57}}$ and **58**/$\overline{\mathbf{58}}$) in accord with Eq. 118. To grasp the enantiomeric relationship for each pair, consider the mirror plane containing vertices 2, 4, 9, and 11, by which the two enantiomers of each pair can be interchanged into each other.

In accord with Eq. 119, Fig. 7 adds three $\mathbf{C}_s$-derivatives (**59**–**61**) to the listed $\mathbf{C}_s$-derivatives of Fig. 4 (**26**–**28**). The mirror plane at issue contains vertices 1, 2, 9, and 12.

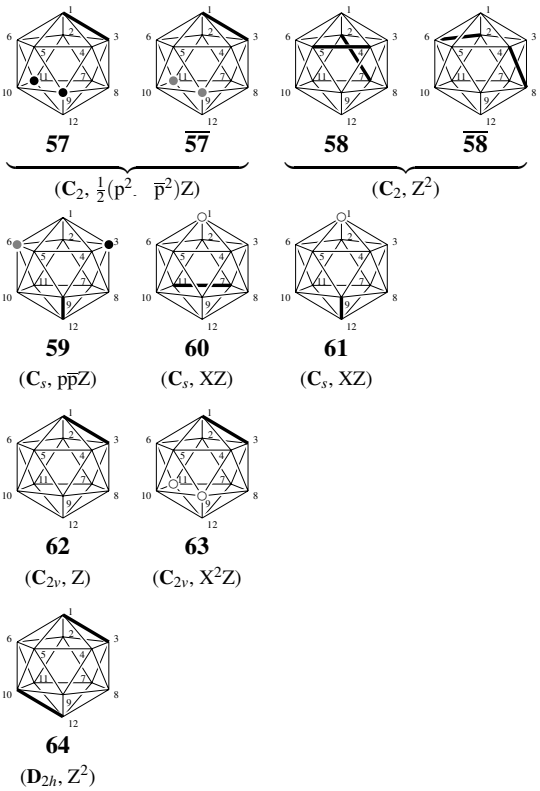


Figure 7: Icosahedral derivatives with edge substitutions in addition to vertex substitutions. For the symbols of ligands, see Fig. 1.

As for $\mathbf{C}_{2v}$, Eq. 119 indicates the presence of **62** and **63** (Fig. 7) in addition to **30** (Fig. 4). The two-fold axis of **62** (or **63**) runs through the midpoints of the edges $\{1,3\}$ and $\{10,12\}$, while the counterpart of **30** runs through the midpoints of the edges $\{1,2\}$ and $\{9,12\}$. Note that the bidentate ligand of **63** (Fig. 7) is deleted to give a homomer of **30** (Fig. 4).

It is to be noted that the $\mathbf{D}_{2h}$-derivative **64** (Fig. 7) is related to the $\mathbf{D}_{2h}$-derivative **9** (Fig. 2), which is rejected under the restriction condition due to steric hindrance. The three types of PCI-CFs for $\mathbf{D}_{2h}$, i.e, Eq. 15 (unrestricted), Eq. 53 (restricted vertices), and Eq. 106 (restricted vertices and edges) as well as the corresponding three generating functions, i.e., Eq. 31 (the term X^4), Eq. 78 (no term X^4), and Eq. 129 (the term Z^2), should be compared to verify the different behaviors with and without the restricted conditions for vertices and edges.

4 Conclusion

The PCI method of the USCI approach is extended to enumerate derivatives by taking restricted modes of vertex and/or edge substitutions into consideration. Subduced cycle indices with chirality fittingness (SCI-CFs) are calculated for respective subgroups of a given skeleton by starting from unit subduced cycle indices with chirality fittingness (USCI-CFs) and factorized into restricted SCI-CFs. The restricted SCI-CF for each subgroup contains a set of monomials, which is effective to evaluate the numbers of fixed points (promolecules) on the action of the subgroup under the restricted conditions of enumeration. The set of the restricted SCI-CFs is multiplied by the inverse mark table to generate partial cycle indices with chirality fittingness (PCI-CFs) for every subgroups, which are used to conduct enumerations itemized with respect to the subgroups under the restricted conditions. Several results starting from an icosahedral skeleton are discussed to examine differences between unrestricted and restricted enumerations.

Appendix

Maple Program for Restricted SCI-CFs of an Icosahedral Skeleton

The source list of a sample program (named "isocaResA.mpl") for obtaining the restricted SCI-CFs is attached below. The results are summarized in the $\overline{\text{SCI-CF}}$-column of Table 1.

```
#isocaResA.mpl
#read "c:/fujita0/calc/isocaResA.mpl";
# Evaluation of Restricted SCIs for an Icosahedral Skeleton
# Remove Adjacent Vertices
ResSCI := proc(SCI)
global x1,x2,x3,x4,x5,x6,x7,x8,x9,x10,x11,x12,RSCI;
local N1, N2, N3, N4, N5, N6, N7, N8, N9, N10,
N11, N12, N13, N14, N15, N16, N17, N18, N19, N20,
N21, N22, N23, N24, N25, N26, N27, N28, N29, N30,
NN1, NN2, NN3, NN4, NN5, NN6, NN7, NN8, NN9, NN10,
NN11, NN12, NN13, NN14, NN15, NN16, NN17, NN18, NN19, NN20,
NN21, NN22, NN23, NN24, NN25, NN26, NN27, NN28, NN29, NN30,
tempSCI,tempSCI1,tempSCI2,tempSCI3,tempSCI4,tempSCI5,
tempSCI6,tempSCI7,tempSCI8,tempSCI9,tempSCI10,
tempSCI11,tempSCI12,tempSCI13,tempSCI14,tempSCI15,
tempSCI16,tempSCI17,tempSCI18,tempSCI19,tempSCI20,
tempSCI21,tempSCI22,tempSCI23,tempSCI24,tempSCI25,
tempSCI26,tempSCI27,tempSCI28,tempSCI29,tempSCI30;
tempSCI := expand(SCI);
N1 := coeff(tempSCI, x1); NN1 := coeff(N1, x2);
tempSCI1 := expand(tempSCI - NN1*x1*x2);
N2 := coeff(tempSCI1, x1); NN2 := coeff(N2, x3);
tempSCI2 := expand(tempSCI1 - NN2*x1*x3);
N3 := coeff(tempSCI2, x1); NN3 := coeff(N3, x4);
tempSCI3 := expand(tempSCI2 - NN3*x1*x4);
N4 := coeff(tempSCI3, x1); NN4 := coeff(N4, x5);
tempSCI4 := expand(tempSCI3 - NN4*x1*x5);
N5 := coeff(tempSCI4, x1); NN5 := coeff(N5, x6);
tempSCI5 := expand(tempSCI4 - NN5*x1*x6);
N6 := coeff(tempSCI5, x2); NN6 := coeff(N6, x3);
tempSCI6 := expand(tempSCI5 - NN6*x2*x3);
N7 := coeff(tempSCI6, x2); NN7 := coeff(N7, x6);
tempSCI7 := expand(tempSCI6 - NN7*x2*x6);
N8 := coeff(tempSCI7, x2); NN8 := coeff(N8, x7);
```

```
tempSCI8 := expand(tempSCI7 - NN8*x2*x7);
N9 := coeff(tempSCI8, x2); NN9 := coeff(N9, x11);
tempSCI9 := expand(tempSCI8 - NN9*x2*x11);
N10 := coeff(tempSCI9, x3); NN10 := coeff(N10, x4);
tempSCI10 := expand(tempSCI9 - NN10*x3*x4);
N11 := coeff(tempSCI10, x3); NN11 := coeff(N11, x7);
tempSCI11 := expand(tempSCI10 - NN11*x3*x7);
N12 := coeff(tempSCI11, x3); NN12 := coeff(N12, x8);
tempSCI12 := expand(tempSCI11 - NN12*x3*x8);
N13 := coeff(tempSCI12, x4); NN13 := coeff(N13, x8);
tempSCI13 := expand(tempSCI12 - NN13*x4*x8);
N14 := coeff(tempSCI13, x4); NN14 := coeff(N14, x9);
tempSCI14 := expand(tempSCI13 - NN14*x4*x9);
N15 := coeff(tempSCI14, x4); NN15 := coeff(N15, x5);
tempSCI15 := expand(tempSCI14 - NN15*x4*x5);
N16 := coeff(tempSCI15, x5); NN16 := coeff(N16, x6);
tempSCI16 := expand(tempSCI15 - NN16*x5*x6);
N17 := coeff(tempSCI16, x5); NN17 := coeff(N17, x9);
tempSCI17 := expand(tempSCI16 - NN17*x5*x9);
N18 := coeff(tempSCI17, x5); NN18 := coeff(N18, x10);
tempSCI18 := expand(tempSCI17 - NN18*x5*x10);
N19 := coeff(tempSCI18, x6); NN19 := coeff(N19, x10);
tempSCI19 := expand(tempSCI18 - NN19*x6*x10);
N20 := coeff(tempSCI19, x6); NN20 := coeff(N20, x11);
tempSCI20 := expand(tempSCI19 - NN20*x6*x11);
N21 := coeff(tempSCI20, x7); NN21 := coeff(N21, x8);
tempSCI21 := expand(tempSCI20 - NN21*x7*x8);
N22 := coeff(tempSCI21, x7); NN22 := coeff(N22, x11);
tempSCI22 := expand(tempSCI21 - NN22*x7*x11);
N23 := coeff(tempSCI22, x7); NN23 := coeff(N23, x12);
tempSCI23 := expand(tempSCI22 - NN23*x7*x12);
N24 := coeff(tempSCI23, x8); NN24 := coeff(N24, x9);
tempSCI24 := expand(tempSCI23 - NN24*x8*x9);
N25 := coeff(tempSCI24, x8); NN25 := coeff(N25, x12);
tempSCI25 := expand(tempSCI24 - NN25*x8*x12);
N26 := coeff(tempSCI25, x9); NN26 := coeff(N26, x10);
tempSCI26 := expand(tempSCI25 - NN26*x9*x10);
N27 := coeff(tempSCI26, x9); NN27 := coeff(N27, x12);
tempSCI27 := expand(tempSCI26 - NN27*x9*x12);
N28 := coeff(tempSCI27, x10); NN28 := coeff(N28, x11);
tempSCI28 := expand(tempSCI27 - NN28*x10*x11);
N29 := coeff(tempSCI28, x10); NN29 := coeff(N29, x12);
tempSCI29 := expand(tempSCI28 - NN29*x10*x12);
N30 := coeff(tempSCI29, x11); NN30 := coeff(N30, x12);
tempSCI30 := expand(tempSCI29 - NN30*x11*x12);
x1 :=1: x2 :=1: x3 :=1: x4 :=1: x5 :=1: x6 :=1:
x7 :=1: x8 :=1: x9 :=1: x10 :=1: x11 :=1: x12 :=1:
RSCI := expand(tempSCI30);
end proc:

#Initialize
resetX := proc()
global x1,x2,x3,x4,x5,x6,x7,x8,x9,x10,x11,x12;
x1 :='x1'; x2 :='x2'; x3 :='x3'; x4 :='x4'; x5 :='x5';
x6 :='x6'; x7 :='x7'; x8 :='x8'; x9 :='x9'; x10 :='x10';
 x11 :='x11'; x12 :='x12';
end proc:

#Evaluation of Restricted SCIs
resetX():
DSCIC1 := (1+b1*x1)*(1+b1*x2)*(1+b1*x3)*(1+b1*x4)*(1+b1*x5)
```

```
*(1+b1*x6)*(1+b1*x7)*(1+b1*x8)*(1+b1*x9)*(1+b1*x10)*
(1+b1*x11)*(1+b1*x12);
ResSCI(DSCIC1); ResCSIC1 := RSCI;

resetX():
DSCIC2 := (1+b2*x1*x3)*(1+b2*x2*x4)*(1+b2*x5*x7)*
(1+b2*x6*x8)*(1+b2*x9*x11)*(1+b2*x10*x12);
ResSCI(DSCIC2); ResCSIC2 := RSCI;

resetX():
DSCICs := (1+a1*x1)*(1+a1*x2)*(1+a1*x9)*(1+a1*x12)*
(1+c2*x3*x6)*(1+c2*x4*x5)*(1+c2*x7*x11)*(1+c2*x8*x10);
ResSCI(DSCICs); ResCSICs := RSCI;

resetX():
DSCICi := (1+c2*x1*x12)*(1+c2*x2*x9)*(1+c2*x3*x10)*
(1+c2*x4*x11)*(1+c2*x5*x7)*(1+c2*x6*x8);
ResSCI(DSCICi); ResCSICi := RSCI;

resetX():
DSCIC3 := (1+b3*x1*x8*x10)*(1+b3*x4*x5*x9)*
(1+b3*x3*x6*x12)*(1+b3*x2*x7*x11);
ResSCI(DSCIC3); ResCSIC3 := RSCI;

resetX():
DSCID2 := (1+b4*x1*x3*x10*x12)*
(1+b4*x2*x4*x9*x11)*
(1+b4*x5*x6*x7*x8);
ResSCI(DSCID2); ResCSID2 := RSCI;

resetX():
DSCIC2v := (1+a2*x1*x3)*(1+a2*x2*x4)*(1+a2*x9*x11)*
(1+a2*x10*x12)*(1+c4*x5*x6*x7*x8);
ResSCI(DSCIC2v); ResCSIC2v := RSCI;

resetX():
DSCIC2h := (1+a2*x5*x7)*(1+a2*x6*x8)*
(1+c4*x1*x3*x10*x12)*(1+c4*x2*x4*x9*x11);
ResSCI(DSCIC2h); ResCSIC2h := RSCI;

resetX():
DSCIC5 := (1+b1*x1)*(1+b1*x12)*
(1+b5*x2*x3*x4*x5*x6)*(1+b5*x7*x8*x9*x10*x11);
ResSCI(DSCIC5); ResCSIC5 := RSCI;

resetX():
DSCID3 := (1+b6*x1*x3*x8*x12*x10*x6)*
(1+b6*x4*x5*x9*x2*x7*x11);
ResSCI(DSCID3); ResCSID3 := RSCI;

resetX():
DSCIC3v := (1+a3*x1*x8*x10)*(1+a3*x3*x12*x6)*
(1+a3*x4*x5*x9)*(1+a3*x2*x7*x11);
ResSCI(DSCIC3v); ResCSIC3v := RSCI;

resetX():
DSCIC3i := (1+c6*x1*x3*x8*x12*x10*x6)*
(1+c6*x4*x5*x9*x2*x7*x11);
ResSCI(DSCIC3i); ResCSIC3i := RSCI;
```

```
resetX():
DSCID2h := (1+a4*x1*x3*x10*x12)*
(1+a4*x2*x4*x9*x11)*(1+a4*x5*x6*x7*x8);
ResSCI(DSCID2h); ResCSID2h := RSCI;

resetX():
DSCID5 := (1+b2*x1*x12)*
(1+b10*x2*x3*x4*x5*x6*x7*x8*x9*x10*x11);
ResSCI(DSCID5); ResCSID5 := RSCI;

resetX():
DSCIC5v := (1+a1*x1)*(1+a1*x12)*
(1+a5*x2*x3*x4*x5*x6)*(1+a5*x7*x8*x9*x10*x11);
ResSCI(DSCIC5v); ResCSIC5v := RSCI;

resetX():
DSCIC5i := (1+c2*x1*x12)*
(1+c10*x2*x3*x4*x5*x6*x7*x8*x9*x10*x11);
ResSCI(DSCIC5i); ResCSIC5i := RSCI;

resetX():
DSCIT :=
(1+b12*x1*x2*x3*x4*x5*x6*x7*x8*x9*x10*x11*x12);
ResSCI(DSCIT); ResCSIT := RSCI;

resetX():
DSCID3d :=
(1+a6*x1*x3*x8*x12*x10*x6)*
(1+a6*x4*x5*x9*x2*x7*x11);
ResSCI(DSCID3d); ResCSID3d := RSCI;

resetX():
DSCID5d := (1+a2*x1*x12)*
(1+a10*x2*x3*x4*x5*x6*x7*x8*x9*x10*x11);
ResSCI(DSCID5d); ResCSID5d := RSCI;

resetX():
DSCITh :=
(1+a12*x1*x2*x3*x4*x5*x6*x7*x8*x9*x10*x11*x12);
ResSCI(DSCITh); ResCSITh := RSCI;

resetX():
DSCII :=
(1+b12*x1*x2*x3*x4*x5*x6*x7*x8*x9*x10*x11*x12);
ResSCI(DSCII); ResCSII := RSCI;

resetX():
DSCIIh :=
(1+a12*x1*x2*x3*x4*x5*x6*x7*x8*x9*x10*x11*x12);
ResSCI(DSCIIh); ResCSIIh := RSCI;
```

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