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ORIGINAL PAPER

Symmetry-itemized enumeration of quadruplets of *RS*-stereoisomers. II. The partial-cycle-index method of the USCI approach combined with the stereoisogram approach

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Abstract The symmetry-itemized enumeration of quadruplets of stereoisograms is discussed by starting from a tetrahedral skeleton, where the partial-cycle-index (PCI) method of the unit-subduced-cycle-index approach (Fujita in Symmetry and combinatorial enumeration of chemistry. Springer, Berlin, 1991) is combined with the stereoisogram approach (Fujita in J Org Chem 69:3158–3165, 2004, Tetrahedron 60:11629–11638, 2004). Such a tetrahedral skeleton as contained in the quadruplet of a stereoisogram belongs to an *RS*-stereoisomeric group denoted by $\mathbf{T}_{d\tilde{\sigma}\hat{I}}$, where the four positions of the tetrahedral skeleton accommodate achiral and chiral proligands to give quadruplets belonging to subgroups of $\mathbf{T}_{d\tilde{\sigma}\hat{I}}$ according to the stereoisogram approach. The numbers of quadruplets are calculated as generating functions by applying the PCI method. They are itemized in terms of subgroups of $\mathbf{T}_{d\tilde{\sigma}\hat{I}}$, which are further categorized into five types. Quadruples for stereoisograms of types I–V are ascribed to subgroups of $\mathbf{T}_{d\tilde{\sigma}\hat{I}}$, where their features are discussed in comparison between *RS*-stereoisomeric groups and point groups.

Keywords Stereochemistry · *RS*-stereoisomer · Combinatorial enumeration · USCI approach · Stereoisogram

1 Introduction

The unit-subduced-cycle-index (USCI) approach developed by Fujita [1] supports four methods of symmetry-itemized enumeration of chemical compounds as three-dimensional structures, i.e., the fixed-point matrix (FPM) method [2–4], the partial-cycle-index (PCI) method [5,6], the elementary superposition method [7], and the

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partial superposition method [5,7]. These methods have been applied to enumeration of chemical compounds under the action of point groups. As recent examples, symmetry-itemized enumeration of cubane derivatives have been conducted by applying the FPM method [8], the PCI method [9], and the elementary-superposition method [10] under the action of the point group $\mathbf{O}_h$.

On the other hand, the stereoisogram approach developed by Fujita [11,12] has extended point groups into *RS*-stereoisomeric groups, where the point-group theory is integrated with the permutation-group theory. By the stereoisogram approach coupled with the USCI approach, we are able to enumerate chemical compounds under the action of *RS*-stereoisomeric groups, so that type-itemized enumeration of quadruplets of *RS*-stereoisomers has been conducted under the action of *RS*-stereoisomeric groups [13].

In Part I of the present series (the accompanying paper), the subgroups of the *RS*-stereoisomeric group for characterizing stereoisograms based on a tetrahedral skeleton have been discussed by considering the isomorphism between the *RS*-stereoisomeric group and the point group $\mathbf{O}_h$. Thereby, symmetry-itemized enumeration has been conducted under the action of *RS*-stereoisomeric groups, where the FPM method of the USCI approach has been adopted. For the purpose of demonstrating the usefulness of the combination of the USCI approach and the stereoisogram approach, the present article is devoted to the PCI method of the USCI approach is adopted to enumerate quadruplets of *RS*-stereoisomers in a symmetry-itemized fashion under the action of the *RS*-stereoisomeric group on a tetrahedral skeleton.

2 Symmetry-itemized enumeration by the PCI method

2.1 Orbits and coset representations characterized by *RS*-stereoisomeric groups

A set of equivalent positions of a skeleton belongs to an orbit, which is governed by a coset representation [1]. Such a coset representation as represented by the symbol $\acute{\mathbf{G}}(/\acute{\mathbf{G}}_i)$ ($\acute{\mathbf{G}}_i \subset \acute{\mathbf{G}}$) can be considered in the case of an *RS*-stereoisomeric group $\acute{\mathbf{G}}$, which characterizes a quadruplet of *RS*-stereoisomers. The coset representation $\acute{\mathbf{G}}(/\acute{\mathbf{G}}_i)$ is based on a coset decomposition of the group $\acute{\mathbf{G}}$ by its subgroup $\acute{\mathbf{G}}_i$ ($\acute{\mathbf{G}}_i \subset \acute{\mathbf{G}}$), where the subgroup ($\acute{\mathbf{G}}_i$) is regarded as a stabilizer. The coset representation $\acute{\mathbf{G}}(/\acute{\mathbf{G}}_i)$ is characterized by a mark, which collects the numbers of fixed points on the action of each subgroup contained in a non-redundant set of subgroups (SSG).

The *RS*-stereoisomeric group for characterizing a tetrahedral skeleton is denoted by the symbol $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$, which is constructed by starting from the point group $\mathbf{T}_d$ [14]. The *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ is isomorphic to the point group $\mathbf{O}_h$, so that it has 33 subgroups up to conjugacy to provide a non-redundant SSG, as discussed in Part I of this series:

$$\begin{aligned}\mathrm{SSG}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}} = \Big\{ & \overset{1}{\mathbf{C}_1}, \overset{2}{\mathbf{C}_2}, \overset{3}{\mathbf{C}_{\widetilde{\sigma}}}, \overset{4}{\mathbf{C}_{\widehat{\sigma}}}, \overset{5}{\mathbf{C}_s}, \overset{6}{\mathbf{C}_{\widehat{I}}}, \overset{7}{\mathbf{C}_3}, \overset{8}{\mathbf{S}_{\widetilde{4}}}, \overset{9}{\mathbf{S}_4}, \overset{10}{\mathbf{D}_2}, \overset{11}{\mathbf{C}_{2\widetilde{\sigma}}}, \overset{12}{\mathbf{C}_{2\widehat{\sigma}}}, \overset{13}{\mathbf{C}_{2v}}, \overset{14}{\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}}, \overset{15}{\mathbf{C}_{2\widehat{I}}}, \\ & \overset{16}{\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}}, \overset{17}{\mathbf{C}_{3\widetilde{\sigma}}}, \overset{18}{\mathbf{C}_{3v}}, \overset{19}{\mathbf{C}_{3\widehat{I}}}, \overset{20}{\mathbf{D}_{2\widetilde{\sigma}}}, \overset{21}{\mathbf{S}_{\widetilde{4}\widehat{\sigma}}}, \overset{22}{\mathbf{S}_{\widetilde{4}\widehat{I}}}, \overset{23}{\mathbf{D}_{2d}}, \overset{24}{\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}}, \overset{25}{\mathbf{D}_{2\widehat{I}}}, \overset{26}{\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}}, \overset{27}{\mathbf{T}}, \overset{28}{\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}}, \\ & \overset{29}{\mathbf{D}_{2d\widetilde{\sigma}\widehat{I}}}, \overset{30}{\mathbf{T}_{\widetilde{\sigma}}}, \overset{31}{\mathbf{T}_{\widehat{I}}}, \overset{32}{\mathbf{T}_d}, \overset{33}{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}} \Big\}, \end{aligned} \tag{1}$$

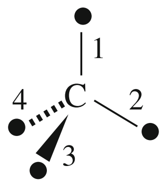

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Fig. 1 Reference tetrahedral skeleton. The orbit of the four vertices corresponds to the coset representation $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}})$ under the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ and to the coset representation $\mathbf{T}_d(/\mathbf{C}_{3v})$ under the point group $\mathbf{T}_d$

where the subgroups are aligned in the ascending order of their orders. For the convenience of cross reference, sequential numbers from 1 to 33 are attached to the respective subgroups. The mark table of $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ as a 33×33 square matrix $M_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}}$ is identical with that of $\mathbf{O}_h$ (cf. Table 1 of [15] and Table 1 of [8]), if the $\mathrm{SSG}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}}$ is constructed in accordance with $\mathrm{SSG}_{\mathbf{O}_h}$. For practices of calculations, the corresponding inverse matrix is also necessary, as reported in Table 2 of [15] and Table 2 of [8]. The 33×33 matrix form $M^{-1}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}}$ of the inverse mark table of $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ is also reported as Eq. 53 of Part I of this series.

The coset representation $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\acute{\mathbf{G}}_i)$ ($\acute{\mathbf{G}}_i \in \mathrm{SSG}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}}$) is calculated in a parallel way to the coset representation $\mathbf{O}_h(/\mathbf{G}_i)$ ($\mathbf{G}_i \in \mathrm{SSG}_{\mathbf{O}_h}$), as shown in Part I of this series. For example, the coset representation $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}})$ is calculated to have an identical set of products of cycles with the coset representation $\mathbf{O}_h(/\mathbf{D}_{3d})$, as shown in Part I of this series.

The four positions of a tetrahedral skeleton **1** construct an orbit governed by the coset representation $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}})$, the degree of which is calculated to be $|\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}|/|\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}|$ $(= 48/12 = 4)$. The *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ exhibits the global symmetry of the tetrahedral skeleton **1**, while its subgroup $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$ exhibits the local symmetry of each of the four vertices (Fig. 1).

As reported in Eq. 48 of the Part I of this series, the group $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$ consists of the following set of operations:

$$\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}} = \Big\{I, C_{3(1)}, C^2_{3(1)}, \widetilde{\sigma}_{d(1)}, \widetilde{\sigma}_{d(2)}, \widetilde{\sigma}_{d(3)}, \widehat{I}, \widehat{C}_{3(1)}, \widehat{C}^2_{3(1)}, \sigma_{d(1)}, \sigma_{d(2)}, \sigma_{d(3)}\Big\}, \qquad (\supset \mathbf{C}_{3v}) \tag{2}$$

The group $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$ as an *RS*-stereoisomeric group is constructed by extending the point group $\mathbf{C}_{3v}$:

$$\mathbf{C}_{3v} = \Big\{I, C_{3(1)}, C^2_{3(1)}, \sigma_{d(1)}, \sigma_{d(2)}, \sigma_{d(3)}\Big\} \tag{3}$$

according to a general procedure of constructing stereoisograms and *RS*-stereoisomeric groups [11,14].

It should be noted that the four positions of the tetrahedral skeleton **1** are alternatively regarded as being governed by the coset representation $\mathbf{T}_d(/\mathbf{C}_{3v})$, if the skeleton **1** is considered to belong to the point group $\mathbf{T}_d$. From this point of view, the point group $\mathbf{T}_d$ exhibits the global symmetry of the tetrahedral skeleton **1**, while its subgroup $\mathbf{C}_{3v}$ exhibits the local symmetry of each of the four vertices. Hence, it is one of the important targets of the present paper to compare between $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}})$ and $\mathbf{T}_d(/\mathbf{C}_{3v})$, which are operated onto the same skeleton **1**.

2.2 Partial cycle indices with chirality fittingness

According to the formulation of the USCI approach [1], the mark table $M_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}}$ and its inverse $M^{-1}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}}$ are further used for subductions of coset representations, i.e., $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\acute{\mathbf{G}}_i) \downarrow \acute{\mathbf{G}}_j$ (for $\acute{\mathbf{G}}_i, \acute{\mathbf{G}}_j \in \mathrm{SSG}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}}$). The results of such subductions are combined with the concept of sphericities to give unit subduced cycle indices with chirality fittingness (USCI-CFs), which are listed in a tabular form (the USCI-CF table). Because the full form of the USCI-CF table of $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ is identical with that of $\mathbf{O}_h$ (Tables 4 and 5 in [8]), its $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}})$-row (the $\mathbf{O}_h(/\mathbf{D}_{3d})$-row of Tables 4 and 5 in [8]) is cited for the purpose of applying the PCI method to the tetrahedral skeleton:

$$\begin{aligned}&\text{USCI-CF}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}})}\\ &\quad=\Big\{b_1^4, b_2^2, b_1^2b_2, c_2^2, a_1^2c_2, a_1^4, b_1b_3, b_4, c_4, b_4, b_2^2, c_4, a_2^2, a_2c_2, a_2^2, a_1^2a_2, b_1b_3,\\ &\qquad a_1a_3, a_1a_3, b_4, a_4, a_4, a_4, c_4, a_4, a_2^2, b_4, a_1a_3, a_4, b_4, a_4, a_4, a_4\Big\} \qquad (4)\end{aligned}$$

which has been also listed in Table 3 of Part I of this series. The USCI-CFs in Eq. 4 are listed in the order of $\mathrm{SSG}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}}$ (Eq. 1). Note that the symbols a_d, b_d, c_d denote sphericity indices, where a_d is assigned to a d-membered homospheric orbit of substitution positions, b_d is assigned to a d-membered hemispheric orbit, and c_d is assigned to a d-membered enantiospheric orbit.

Section 16.3 and Section 19.5 of [1] have discussed partial cycle indices without and with chirality fittingness (PCIs and PCI-CFs). According to Def. 19.6 of [1], PCI-CFs for enumerating *RS*-stereoisomers are calculated by using the $\text{USCI-CF}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}})}$ (Eq. 4), which is multiplied by the inverse mark table of $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ (Eq. 53 of Part I of this series):

$$\text{USCI-CF}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}})} \times M^{-1}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}} = (\text{PCI-CF}(\mathbf{C}_1), \ldots, \text{PCI-CF}(\acute{\mathbf{G}}_i), \ldots, \text{PCI-CF}(\mathbf{T}_{d\widetilde{\sigma}\widehat{I}})), \qquad (5)$$

where $\acute{\mathbf{G}}_i$ runs to cover the $\mathrm{SSG}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}}$ (Eq. 1). When the $\text{USCI-CF}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}})}$ (Eq. 4) is regarded as a row vector of USCI-CFs, the result of Eq. 5 is also regarded as a row vector, in which each column component, i.e., $\text{PCI-CF}(\acute{\mathbf{G}}_i)$ as a polynomial of a_d, b_d, and c_d, corresponds to the PCI-CF of a subgroup at issue, $\acute{\mathbf{G}}_i$. For example, the $\mathbf{C}_1$-column of Eq. 5 (i.e., PCI-CF($\mathbf{C}_1$)) is calculate as follows:

$$\begin{aligned}\text{PCI-CF}(\mathbf{C}_1) &= \text{USCI-CF}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}})}\\ &\quad\times {}^{T}\bigg(\frac{1}{48}, -\frac{1}{16}, -\frac{1}{8}, -\frac{1}{16}, -\frac{1}{8}, -\frac{1}{48}, -\frac{1}{12}, 0, 0, \frac{1}{24}, \frac{1}{8}, \frac{1}{8}, \frac{1}{8}, \frac{1}{4},\\ &\qquad \frac{1}{8}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{12}, 0, 0, 0, 0, 0, -\frac{1}{6}, -\frac{1}{2}, \frac{1}{12}, -\frac{1}{2}, 0, -\frac{1}{4},\\ &\qquad -\frac{1}{12}, -\frac{1}{4}, \frac{1}{2}\bigg), \qquad (6)\end{aligned}$$

where the symbol T of the last vector represents the transpose of the $\mathbf{C}_1$-column of the inverse mark table $M^{-1}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}}$. The vector calculation of Eq. 6 gives Eq. 7. Similarly, PCI-CFs for every subgroups of $\mathrm{SSG}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}}$ (Eq. 1) are obtained as follows, where the sequential numbers are shown over the respective equality symbols for the convenience of cross reference.

$$\begin{aligned}\text{PCI-CF}(\mathbf{C}_1) &\overset{1}{\underset{\text{III}}{=}} \frac{1}{48}b_1^4 - \frac{1}{48}a_1^4 - \frac{1}{8}b_1^2b_2 + \frac{1}{4}a_1^2a_2 - \frac{1}{8}a_1^2c_2 + \frac{1}{6}b_1b_3 - \frac{1}{6}a_1a_3 \\ &\quad + \frac{1}{16}b_2^2 - \frac{1}{4}a_2^2 + \frac{1}{4}a_2c_2 - \frac{1}{16}c_2^2 + \frac{1}{8}c_4 - \frac{1}{8}b_4 \end{aligned} \tag{7}$$

$$\text{PCI-CF}(\mathbf{C}_2) \overset{2}{\underset{\text{III}}{=}} 0 \tag{8}$$

$$\begin{aligned}\text{PCI-CF}(\mathbf{C}_{\widetilde{\sigma}}) &\overset{3}{\underset{\text{II}}{=}} \frac{1}{4}b_1^2b_2 - \frac{1}{4}a_1^2a_2 - \frac{1}{2}b_1b_3 + \frac{1}{2}a_1a_3 - \frac{1}{4}b_2^2 + \frac{1}{2}a_2^2 \\ &\quad - \frac{1}{4}a_2c_2 + \frac{1}{2}b_4 - \frac{1}{2}a_4 \end{aligned} \tag{9}$$

$$\text{PCI-CF}(\mathbf{C}_{\widehat{\sigma}}) \overset{4}{\underset{\text{I}}{=}} \frac{1}{8}a_2^2 - \frac{1}{4}a_2c_2 + \frac{1}{8}c_2^2 - \frac{1}{4}c_4 + \frac{1}{4}a_4 \tag{10}$$

$$\text{PCI-CF}(\mathbf{C}_s) \overset{5}{\underset{\text{V}}{=}} \frac{1}{4}a_1^2c_2 - \frac{1}{4}a_1^2a_2 + \frac{1}{4}a_2^2 - \frac{1}{4}a_2c_2 \tag{11}$$

$$\text{PCI-CF}(\mathbf{C}_{\widehat{I}}) \overset{6}{\underset{\text{I}}{=}} \frac{1}{24}a_1^4 - \frac{1}{4}a_1^2a_2 + \frac{1}{3}a_1a_3 + \frac{1}{8}a_2^2 - \frac{1}{4}a_4 \tag{12}$$

$$\text{PCI-CF}(\mathbf{C}_3) \overset{7}{\underset{\text{III}}{=}} 0 \tag{13}$$

$$\text{PCI-CF}(\mathbf{S}_{\widetilde{4}}) \overset{8}{\underset{\text{II}}{=}} 0 \tag{14}$$

$$\text{PCI-CF}(\mathbf{S}_4) \overset{9}{\underset{\text{V}}{=}} 0 \tag{15}$$

$$\text{PCI-CF}(\mathbf{D}_2) \overset{10}{\underset{\text{III}}{=}} 0 \tag{16}$$

$$\text{PCI-CF}(\mathbf{C}_{2\widetilde{\sigma}}) \overset{11}{\underset{\text{II}}{=}} \frac{1}{4}b_2^2 - \frac{1}{4}a_2^2 - \frac{1}{4}b_4 - \frac{1}{4}c_4 + \frac{1}{2}a_4 \tag{17}$$

$$\text{PCI-CF}(\mathbf{C}_{2\widehat{\sigma}}) \overset{12}{\underset{\text{I}}{=}} 0 \tag{18}$$

$$\text{PCI-CF}(\mathbf{C}_{2v}) \overset{13}{\underset{\text{V}}{=}} 0 \tag{19}$$

$$\text{PCI-CF}(\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}) \overset{14}{\underset{\text{IV}}{=}} \frac{1}{2}a_2c_2 - \frac{1}{2}a_2^2 \tag{20}$$

$$\text{PCI-CF}(\mathbf{C}_{2\widehat{I}}) \overset{15}{\underset{\text{I}}{=}} 0 \tag{21}$$

$$\text{PCI-CF}(\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}) \overset{16}{\underset{\text{IV}}{=}} \frac{1}{2}a_1^2a_2 - a_1a_3 - \frac{1}{2}a_2^2 + a_4 \tag{22}$$

$$\text{PCI-CF}(\mathbf{C}_{3\widetilde{\sigma}}) \overset{17}{\underset{\text{II}}{=}} \frac{1}{2}b_1b_3 - \frac{1}{2}a_1a_3 - \frac{1}{2}b_4 + \frac{1}{2}a_4 \tag{23}$$

$$\text{PCI-CF}(\mathbf{C}_{3v}) \overset{18}{\underset{\text{V}}{\equiv}} 0 \tag{24}$$

$$\text{PCI-CF}(\mathbf{C}_{3\widehat{I}}) \overset{19}{\underset{\text{I}}{\equiv}} 0 \tag{25}$$

$$\text{PCI-CF}(\mathbf{D}_{2\widetilde{\sigma}}) \overset{20}{\underset{\text{II}}{\equiv}} 0 \tag{26}$$

$$\text{PCI-CF}(\mathbf{S}_{\widetilde{4}\widehat{\sigma}}) \overset{21}{\underset{\text{IV}}{\equiv}} 0 \tag{27}$$

$$\text{PCI-CF}(\mathbf{S}_{\widetilde{4}\widehat{I}}) \overset{22}{\underset{\text{IV}}{\equiv}} 0 \tag{28}$$

$$\text{PCI-CF}(\mathbf{D}_{2d}) \overset{23}{\underset{\text{V}}{\equiv}} 0 \tag{29}$$

$$\text{PCI-CF}(\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}) \overset{24}{\underset{\text{IV}}{\equiv}} \frac{1}{2}c_4 - \frac{1}{2}a_4 \tag{30}$$

$$\text{PCI-CF}(\mathbf{D}_{2\widehat{I}}) \overset{25}{\underset{\text{I}}{\equiv}} 0 \tag{31}$$

$$\text{PCI-CF}(\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}) \overset{26}{\underset{\text{IV}}{\equiv}} \frac{1}{2}a_2^2 - \frac{1}{2}a_4 \tag{32}$$

$$\text{PCI-CF}(\mathbf{T}) \overset{27}{\underset{\text{III}}{\equiv}} 0 \tag{33}$$

$$\text{PCI-CF}(\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \overset{28}{\underset{\text{IV}}{\equiv}} a_1a_3 - a_4 \tag{34}$$

$$\text{PCI-CF}(\mathbf{D}_{2d\widetilde{\sigma}\widehat{I}}) \overset{29}{\underset{\text{IV}}{\equiv}} 0 \tag{35}$$

$$\text{PCI-CF}(\mathbf{T}_{\widetilde{\sigma}}) \overset{30}{\underset{\text{II}}{\equiv}} \frac{1}{2}b_4 - \frac{1}{2}a_4 \tag{36}$$

$$\text{PCI-CF}(\mathbf{T}_{\widehat{I}}) \overset{31}{\underset{\text{I}}{\equiv}} 0 \tag{37}$$

$$\text{PCI-CF}(\mathbf{T}_{d}) \overset{32}{\underset{\text{V}}{\equiv}} 0 \tag{38}$$

$$\text{PCI-CF}(\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}) \overset{33}{\underset{\text{IV}}{\equiv}} a_4 \tag{39}$$

Note that a Roman numeral below each equality symbol represents the stereoisogram type at issue (types I–V) according to Fig. 8 (and Eqs. 124–128) of Part I of this series.

2.3 Generating functions for symmetry-itemized enumeration

Suppose that substituents for the four positions of **1** are selected from an inventory of proligands:

$$\mathbf{X} = \{\text{A}, \text{B}, \text{X}, \text{Y}; \quad \text{p}, \text{q}, \text{r}, \text{s}; \quad \overline{\text{p}}, \overline{\text{q}}, \overline{\text{r}}, \overline{\text{s}}\}, \tag{40}$$

where the letters A, B, X, and Y represent achiral proligands and the pairs of p/$\overline{\text{p}}$, q/$\overline{\text{q}}$, r/$\overline{\text{r}}$, and s/$\overline{\text{s}}$ represent pairs of enantiomeric proligands in isolation. According to Theorem 19.6 (or Theorem 9.7) of [1], we use the following ligand-inventory functions:

$$a_d = \mathrm{A}^d + \mathrm{B}^d + \mathrm{X}^d + \mathrm{Y}^d \tag{41}$$

$$c_d = \mathrm{A}^d + \mathrm{B}^d + \mathrm{X}^d + \mathrm{Y}^d + 2\mathrm{p}^{d/2}\overline{\mathrm{p}}^{d/2} + 2\mathrm{q}^{d/2}\overline{\mathrm{q}}^{d/2} + 2\mathrm{r}^{d/2}\overline{\mathrm{r}}^{d/2} + 2\mathrm{s}^{d/2}\overline{\mathrm{s}}^{d/2} \tag{42}$$

$$b_d = \mathrm{A}^d + \mathrm{B}^d + \mathrm{X}^d + \mathrm{Y}^d + \mathrm{p}^d + \mathrm{q}^d + \mathrm{r}^d + \mathrm{s}^d + \overline{\mathrm{p}}^d + \overline{\mathrm{q}}^d + \overline{\mathrm{r}}^d + \overline{\mathrm{s}}^d. \tag{43}$$

It should be noted that the power $d/2$ appearing in Eq. 42 is an integer because the subscript d of c_d is always even in the light of the enantiosphericity of the corresponding orbit.

The ligand-inventory functions (Eqs. 41–43) are introduced into the PCI-CFs (Eqs. 7–39) so as to give the following generating functions:

$$\begin{aligned} f_{\mathbf{C}_1} \stackrel{1}{\underset{\mathrm{III}}{=}} & \left\{\frac{1}{2}(\mathrm{ABXp} + \mathrm{ABX}\overline{\mathrm{p}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{ABpq} + \mathrm{AB}\overline{\mathrm{pq}}) + \cdots\right\} \\ & + \left\{\frac{1}{2}(\mathrm{Ap}\overline{\mathrm{p}}\mathrm{q} + \mathrm{Ap}\overline{\mathrm{pq}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{Apqr} + \mathrm{A}\overline{\mathrm{pqr}}) + \cdots\right\} \\ & + \left\{\frac{1}{2}(\mathrm{pqrs} + \overline{\mathrm{pqrs}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{p}\overline{\mathrm{p}}\mathrm{qr} + \mathrm{p}\overline{\mathrm{pqr}}) + \cdots\right\} \end{aligned} \tag{44}$$

$$\begin{aligned} f_{\mathbf{C}_{\widetilde{\sigma}}} \stackrel{3}{\underset{\mathrm{II}}{=}} & \left\{\frac{1}{2}(\mathrm{A}^2\mathrm{Bp} + \mathrm{A}^2\mathrm{B}\overline{\mathrm{p}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{ABp}^2 + \mathrm{AB}\overline{\mathrm{p}}^2) + \cdots\right\} \\ & + \left\{\frac{1}{2}(\mathrm{A}^2\mathrm{pq} + \mathrm{A}^2\overline{\mathrm{pq}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{Ap}^2\overline{\mathrm{p}} + \mathrm{Ap}\overline{\mathrm{p}}^2) + \cdots\right\} \\ & + \left\{\frac{1}{2}(\mathrm{Ap}^2\mathrm{q} + \mathrm{A}\overline{\mathrm{p}}^2\overline{\mathrm{q}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{p}^2\overline{\mathrm{p}}\mathrm{q} + \mathrm{p}\overline{\mathrm{p}}^2\overline{\mathrm{q}}) + \cdots\right\} \\ & + \left\{\frac{1}{2}(\mathrm{p}^2\mathrm{q}\overline{\mathrm{q}} + \overline{\mathrm{p}}^2\mathrm{q}\overline{\mathrm{q}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{p}^2\mathrm{qr} + \overline{\mathrm{p}}^2\overline{\mathrm{qr}}) + \cdots\right\} \end{aligned} \tag{45}$$

$$f_{\mathbf{C}_{\widehat{\sigma}}} \stackrel{4}{\underset{\mathrm{I}}{=}} \{\mathrm{p}\overline{\mathrm{p}}\mathrm{q}\overline{\mathrm{q}} + \mathrm{p}\overline{\mathrm{p}}\mathrm{r}\overline{\mathrm{r}} + \cdots\} \tag{46}$$

$$f_{\mathbf{C}_s} \stackrel{5}{\underset{\mathrm{V}}{=}} \{\mathrm{ABp}\overline{\mathrm{p}} + \mathrm{ABq}\overline{\mathrm{q}} + \cdots\} \tag{47}$$

$$f_{\mathbf{C}_{\widehat{I}}} \stackrel{6}{\underset{\mathrm{I}}{=}} \mathrm{ABXY} \tag{48}$$

$$f_{\mathbf{C}_{2\widetilde{\sigma}}} \stackrel{11}{\underset{\mathrm{II}}{=}} \left\{\frac{1}{2}(\mathrm{A}^2\mathrm{p}^2 + \mathrm{A}^2\overline{\mathrm{p}}^2) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{p}^2\mathrm{q}^2 + \overline{\mathrm{p}}^2\overline{\mathrm{q}}^2) + \cdots\right\} \tag{49}$$

$$f_{\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}} \stackrel{14}{\underset{\mathrm{IV}}{=}} \left\{\mathrm{A}^2\mathrm{p}\overline{\mathrm{p}} + \cdots\right\} \tag{50}$$

$$f_{\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}} \stackrel{16}{\underset{\mathrm{IV}}{=}} \left\{\mathrm{A}^2\mathrm{BX} + \mathrm{A}^2\mathrm{BY} + \cdots\right\} \tag{51}$$

$$\begin{aligned} f_{\mathbf{C}_{3\widetilde{\sigma}}} \stackrel{17}{\underset{\mathrm{II}}{=}} & \left\{\frac{1}{2}(\mathrm{A}^3\mathrm{p} + \mathrm{A}^3\overline{\mathrm{p}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{Ap}^3 + \mathrm{A}\overline{\mathrm{p}}^3) + \cdots\right\} \\ & + \left\{\frac{1}{2}(\mathrm{p}^3\mathrm{q} + \overline{\mathrm{p}}^3\overline{\mathrm{q}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{p}^3\overline{\mathrm{p}} + \mathrm{p}\overline{\mathrm{p}}^3) + \cdots\right\} \end{aligned} \tag{52}$$

$$f_{\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}} \overset{24}{\underset{\mathrm{IV}}{=}} \left\{ \mathrm{p}^2\overline{\mathrm{p}}^2 + \mathrm{q}^2\overline{\mathrm{q}}^2 + \mathrm{r}^2\overline{\mathrm{r}}^2 + \mathrm{s}^2\overline{\mathrm{s}}^2 \right\} \tag{53}$$

$$f_{\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}} \overset{26}{\underset{\mathrm{IV}}{=}} \left\{ \mathrm{A}^2\mathrm{B}^2 + \mathrm{A}^2\mathrm{X}^2 + \mathrm{A}^2\mathrm{Y}^2 + \cdots \right\} \tag{54}$$

$$f_{\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}} \overset{28}{\underset{\mathrm{IV}}{=}} \left\{ \mathrm{A}^3\mathrm{B} + \mathrm{A}^3\mathrm{X} + \mathrm{A}^3\mathrm{Y} + \cdots \right\} \tag{55}$$

$$f_{\mathbf{T}_{\widetilde{\sigma}}} \overset{30}{\underset{\mathrm{II}}{=}} \left\{ \frac{1}{2}(\mathrm{p}^4 + \overline{\mathrm{p}}^4) + \cdots \right\} \tag{56}$$

$$f_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}} \overset{33}{\underset{\mathrm{IV}}{=}} \left\{ \mathrm{A}^4 + \mathrm{B}^4 + \mathrm{X}^4 + \mathrm{Y}^4 \right\} \tag{57}$$

where generating functions of zero value are omitted (cf. the sequential numbers above the equality symbols). The coefficient of the term $\mathrm{A}^a\mathrm{B}^b\mathrm{X}^x\mathrm{Y}^y\mathrm{p}^p\overline{\mathrm{p}}^{\overline{p}}\mathrm{q}^q\overline{\mathrm{q}}^{\overline{q}}\mathrm{r}^r\overline{\mathrm{q}}^{\overline{r}}\mathrm{s}^s\overline{\mathrm{q}}^{\overline{s}}$ indicates the number of fixed promolecules (quadruplets) to be counted. Because A, B, etc. appear symmetrically, each pair of braces contains at least one representative of such symmetrically appearing terms, which can be represented by the following partition:

$$[\theta] = [a, b, x, y; p, \overline{p}, q, \overline{q}, r, \overline{r}, s, \overline{s}], \tag{58}$$

where we put $a \geq b \geq x \geq y$, $p \geq \overline{p}$, $q \geq \overline{q}$, $r \geq \overline{r}$, $s \geq \overline{s}$, and $p \geq q \geq r \geq s$ without losing generality.

The results collected in Eqs. 44–57 are consistent with those of Eqs. 110 and 123 reported in Part I of this series, where the 30 pairs of braces appearing in Eqs. 44–57 corresponds the partitions $[\theta]_1$–$[\theta]_{30}$ discussed in Part I. As a result, Figs. 9 and 10 of Part I also illustrate the enumeration results collected in Eqs. 44–57.

3 Type-itemized enumeration by the PCI method

3.1 CI-CFs for characterizing five types of stereoisograms

The 33 subgroups of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ are categorized into five types represented by the following sets:

$$\text{Type I:}\mathrm{SG}^{[\mathrm{I}]}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{4}{\mathbf{C}}_{\widehat{\sigma}}, \overset{6}{\mathbf{C}}_{\widehat{I}}, \overset{12}{\mathbf{C}}_{2\widehat{\sigma}}, \overset{15}{\mathbf{C}}_{2\widehat{I}}, \overset{19}{\mathbf{C}}_{3\widehat{I}}, \overset{25}{\mathbf{D}}_{2\widehat{I}}, \overset{31}{\mathbf{T}}_{\widehat{I}} \right\} \tag{59}$$

$$\text{Type II:}\mathrm{SG}^{[\mathrm{II}]}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{3}{\mathbf{C}}_{\widetilde{\sigma}}, \overset{8}{\mathbf{S}}_{\widetilde{4}}, \overset{11}{\mathbf{C}}_{2\widetilde{\sigma}}, \overset{17}{\mathbf{C}}_{3\widetilde{\sigma}}, \overset{20}{\mathbf{D}}_{2\widetilde{\sigma}}, \overset{30}{\mathbf{T}}_{\widetilde{\sigma}} \right\} \tag{60}$$

$$\text{Type III:}\mathrm{SG}^{[\mathrm{III}]}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{1}{\mathbf{C}}_{1}, \overset{2}{\mathbf{C}}_{2}, \overset{7}{\mathbf{C}}_{3}, \overset{10}{\mathbf{D}}_{2}, \overset{27}{\mathbf{T}} \right\} \tag{61}$$

$$\text{Type IV:}\mathrm{SG}^{[\mathrm{IV}]}_{\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{14}{\mathbf{C}}_{s\widetilde{\sigma}\widehat{\sigma}}, \overset{16}{\mathbf{C}}_{s\widetilde{\sigma}\widehat{I}}, \overset{21}{\mathbf{S}}_{\widetilde{4}\widehat{\sigma}}, \overset{22}{\mathbf{S}}_{\widetilde{4}\widehat{I}\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}}, \overset{24}{\mathbf{S}}_{4\widetilde{\sigma}\widehat{\sigma}}, \overset{26}{\mathbf{C}}_{2v\widetilde{\sigma}\widehat{I}}, \overset{28}{\mathbf{C}}_{3v\widetilde{\sigma}\widehat{I}}, \overset{29}{\mathbf{D}}_{2d\widetilde{\sigma}\widehat{I}}, \overset{33}{\mathbf{T}}_{d\widetilde{\sigma}\widehat{I}} \right\} \tag{62}$$

$$\text{Type V:}\mathrm{SG}^{[\mathrm{V}]} = \left\{ \overset{5}{\mathbf{C}}_{s}, \overset{9}{\mathbf{S}}_{4}, \overset{13}{\mathbf{C}}_{2v}, \overset{18}{\mathbf{C}}_{3v}, \overset{23}{\mathbf{D}}_{2d}, \overset{32}{\mathbf{T}}_{d} \right\}. \tag{63}$$

These sets have been listed in Eqs. 124–128 of Part I of this series. These sets correspond to stereoisograms of type I–V, respectively.

According to Eqs. 59–63, cycle indices with chirality fittingness (CI-CFs) for characterizing five types are defined as follows:

$$\begin{aligned}\text{CI-CF}^{[\text{I}]} &= \text{PCI-CF}(\mathbf{C}_{\widetilde{\sigma}}) + \text{PCI-CF}(\mathbf{C}_{\widehat{I}}) + \text{PCI-CF}(\mathbf{C}_{2\widetilde{\sigma}}) \\ &\quad + \text{PCI-CF}(\mathbf{C}_{2\widehat{I}}) + \text{PCI-CF}(\mathbf{C}_{3\widehat{I}}) + \text{PCI-CF}(\mathbf{D}_{2\widehat{I}}) \\ &\quad + \text{PCI-CF}(\mathbf{T}_{\widehat{I}})\end{aligned} \tag{64}$$

$$\begin{aligned}\text{CI-CF}^{[\text{II}]} &= \text{PCI-CF}(\mathbf{C}_{\widetilde{\sigma}}) + \text{PCI-CF}(\mathbf{S}_{\widetilde{4}}) + \text{PCI-CF}(\mathbf{C}_{2\widetilde{\sigma}}) \\ &\quad + \text{PCI-CF}(\mathbf{C}_{3\widetilde{\sigma}}) + \text{PCI-CF}(\mathbf{D}_{2\widetilde{\sigma}}) + \text{PCI-CF}(\mathbf{T}_{\widetilde{\sigma}})\end{aligned} \tag{65}$$

$$\begin{aligned}\text{CI-CF}^{[\text{III}]} &= \text{PCI-CF}(\mathbf{C}_1) + \text{PCI-CF}(\mathbf{C}_2) + \text{PCI-CF}(\mathbf{C}_3) \\ &\quad + \text{PCI-CF}(\mathbf{D}_2) + \text{PCI-CF}(\mathbf{T})\end{aligned} \tag{66}$$

$$\begin{aligned}\text{CI-CF}^{[\text{IV}]} &= \text{PCI-CF}(\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}) + \text{PCI-CF}(\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}) + \text{PCI-CF}(\mathbf{S}_{\widetilde{4}\widehat{\sigma}}) \\ &\quad + \text{PCI-CF}(\mathbf{S}_{\widetilde{4}\widehat{I}}) + \text{PCI-CF}(\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}) + \text{PCI-CF}(\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}) \\ &\quad + \text{PCI-CF}(\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) + \text{PCI-CF}(\mathbf{D}_{2d\widetilde{\sigma}\widehat{I}}) + \text{PCI-CF}(\mathbf{T}_{d\widetilde{\sigma}\widehat{I}})\end{aligned} \tag{67}$$

$$\begin{aligned}\text{CI-CF}^{[\text{V}]} &= \text{PCI-CF}(\mathbf{C}_s) + \text{PCI-CF}(\mathbf{S}_4) + \text{PCI-CF}(\mathbf{C}_{2v}) \\ &\quad + \text{PCI-CF}(\mathbf{C}_{3v}) + \text{PCI-CF}(\mathbf{D}_{2d}) + \text{PCI-CF}(\mathbf{T}_d)\end{aligned} \tag{68}$$

The PCI-CFs listed in Eqs. 6–39 are added according to the definitions shown by Eqs. 64–68. Note that the symbols I–V below the equality symbols in the PCI-CFs (Eqs. 6–39) represent the categories of the five types. Thereby, we obtain the following type-itemized CI-CFs:

$$\text{CI-CF}^{[\text{I}]} = \frac{1}{24}a_1^4 - \frac{1}{4}a_1^2a_2 + \frac{1}{3}a_1a_3 + \frac{1}{4}a_2^2 - \frac{1}{4}a_2c_2 + \frac{1}{8}c_2^2 - \frac{1}{4}c_4 \tag{69}$$

$$\text{CI-CF}^{[\text{II}]} = \frac{1}{4}b_1^2b_2 - \frac{1}{4}a_1^2a_2 + \frac{1}{4}a_2^2 - \frac{1}{4}a_2c_2 + \frac{1}{4}b_4 - \frac{1}{4}c_4 \tag{70}$$

$$\begin{aligned}\text{CI-CF}^{[\text{III}]} &= \frac{1}{48}b_1^4 - \frac{1}{48}a_1^4 - \frac{1}{8}b_1^2b_2 + \frac{1}{4}a_1^2a_2 - \frac{1}{8}a_1^2c_2 + \frac{1}{6}b_1b_3 - \frac{1}{6}a_1a_3 \\ &\quad + \frac{1}{16}b_2^2 - \frac{1}{4}a_2^2 + \frac{1}{4}a_2c_2 - \frac{1}{16}c_2^2 + \frac{1}{8}c_4 - \frac{1}{8}b_4\end{aligned} \tag{71}$$

$$\text{CI-CF}^{[\text{IV}]} = \frac{1}{2}a_1^2a_2 - \frac{1}{2}a_2^2 + \frac{1}{2}a_2c_2 + \frac{1}{2}c_4 \tag{72}$$

$$\text{CI-CF}^{[\text{V}]} = \frac{1}{4}a_1^2c_2 - \frac{1}{4}a_1^2a_2 + \frac{1}{4}a_2^2 - \frac{1}{4}a_2c_2 \tag{73}$$

These CI-CFs are verified by comparison with those of [13], which have been calculated by means of an alternative method. That is to say, CI-CF$^{[\text{I}]}$ (Eq. 69) is identical with Eq. 83 of [13]; CI-CF$^{[\text{II}]}$ (Eq. 70) with Eq. 84 of [13]; CI-CF$^{[\text{III}]}$ (Eq. 71) with Eq. 85 of [13]; CI-CF$^{[\text{IV}]}$ (Eq. 72) with Eq. 81 of [13]; and CI-CF$^{[\text{V}]}$ (Eq. 69) is identical with Eq. 82 of [13].

3.2 Generating functions for type-itemized enumeration

The ligand-inventory functions (Eqs. 41–43) are introduced into the CI-CFs (Eqs. 69–73) so as to give the following generating functions:

$$f^{[\mathrm{I}]} = \mathrm{ABXY} + \{\mathrm{p\overline{p}q\overline{q}} + \mathrm{p\overline{p}r\overline{r}} + \cdots\} \tag{74}$$

$$\begin{aligned}
f^{[\mathrm{II}]} = {} & \left\{\frac{1}{2}(\mathrm{A^2Bp} + \mathrm{A^2B\overline{p}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{ABp^2} + \mathrm{AB\overline{p}^2}) + \cdots\right\} \\
& + \left\{\frac{1}{2}(\mathrm{A^2pq} + \mathrm{A^2\overline{pq}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{Ap^2\overline{p}} + \mathrm{Ap\overline{p}^2}) + \cdots\right\} \\
& + \left\{\frac{1}{2}(\mathrm{Ap^2q} + \mathrm{A\overline{p}^2\overline{q}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{p^2\overline{p}q} + \mathrm{p\overline{p}^2\overline{q}}) + \cdots\right\} \\
& + \left\{\frac{1}{2}(\mathrm{p^2q\overline{q}} + \mathrm{\overline{p}^2q\overline{q}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{p^2qr} + \mathrm{\overline{p}^2\overline{qr}}) + \cdots\right\} \\
& + \left\{\frac{1}{2}(\mathrm{A^2p^2} + \mathrm{A^2\overline{p}^2}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{p^2q^2} + \mathrm{\overline{p}^2\overline{q}^2}) + \cdots\right\} \\
& + \left\{\frac{1}{2}(\mathrm{A^3p} + \mathrm{A^3\overline{p}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{Ap^3} + \mathrm{A\overline{p}^3}) + \cdots\right\} \\
& + \left\{\frac{1}{2}(\mathrm{p^3q} + \mathrm{\overline{p}^3\overline{q}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{p^3\overline{p}} + \mathrm{p\overline{p}^3}) + \cdots\right\} \\
& + \left\{\frac{1}{2}(\mathrm{p^4} + \mathrm{\overline{p}^4}) + \cdots\right\}
\end{aligned} \tag{75}$$

$$\begin{aligned}
f^{[\mathrm{III}]} = {} & \left\{\frac{1}{2}(\mathrm{ABXp} + \mathrm{ABX\overline{p}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{ABpq} + \mathrm{AB\overline{pq}}) + \cdots\right\} \\
& + \left\{\frac{1}{2}(\mathrm{Ap\overline{p}q} + \mathrm{Ap\overline{pq}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{Apqr} + \mathrm{A\overline{pqr}}) + \cdots\right\} \\
& + \left\{\frac{1}{2}(\mathrm{pqrs} + \mathrm{\overline{pqrs}}) + \cdots\right\} + \left\{\frac{1}{2}(\mathrm{p\overline{p}qr} + \mathrm{p\overline{pqr}}) + \cdots\right\}
\end{aligned} \tag{76}$$

$$\begin{aligned}
f^{[\mathrm{IV}]} = {} & \left\{\mathrm{A^2p\overline{p}} + \cdots\right\} + \left\{\mathrm{p^2\overline{p}^2} + \mathrm{q^2\overline{q}^2} + \mathrm{r^2\overline{r}^2} + \mathrm{s^2\overline{s}^2}\right\} \\
& + \left\{\mathrm{A^2BX} + \mathrm{A^2BY} + \cdots\right\} + \left\{\mathrm{A^2B^2} + \mathrm{A^2X^2} + \mathrm{A^2Y^2} + \cdots\right\} \\
& + \left\{\mathrm{A^3B} + \mathrm{A^3X} + \mathrm{A^3Y} + \cdots\right\} + \left\{\mathrm{A^4} + \mathrm{B^4} + \mathrm{X^4} + \mathrm{Y^4}\right\}
\end{aligned} \tag{77}$$

$$f^{[\mathrm{V}]} = \{\mathrm{ABp\overline{p}} + \mathrm{ABq\overline{q}} + \cdots\} \tag{78}$$

The generating functions (Eqs. 74–78) are also obtained by starting from the generating functions for the respective subgroups (Eqs. 44–57), which are added according to the categories shown in Eqs. 59–63. The generating functions (Eqs. 74–78) are identical with Eqs. 86–90 of [13], which have been calculated by an alternative method.

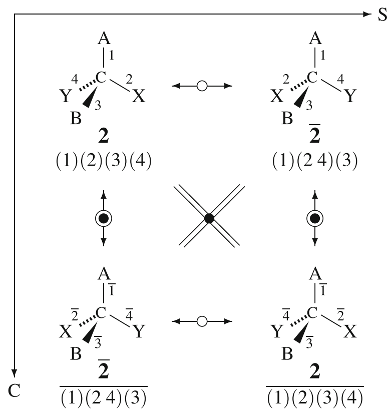


Fig. 2 Stereoisogram of type I which belongs to the *RS*-stereoisomeric group $\mathbf{C}_{\widehat{I}}$. The reference promolecule **2** belongs to the point group $\mathbf{C}_1$

4 Examination of enumeration results

4.1 *RS*-stereoisomeric groups of type I

Among the *RS*-stereoisomeric groups listed in Eq. 59, there appear a quadruplet of $\mathbf{C}_{\widehat{I}}$ having ABXY (Eq. 48) and a quadruplet of $\mathbf{C}_{\widehat{\sigma}}$ having $\mathrm{p}\overline{\mathrm{p}}\mathrm{q}\overline{\mathrm{q}}$ or a constitution of the same partition (Eq. 46). They are totally counted by Eq. 74.

4.1.1 Quadruplet of $\mathbf{C}_{\widehat{I}}$

The quadruplet of $\mathbf{C}_{\widehat{I}}$ having ABXY ($[\theta]_{10} = [1, 1, 1, 1; 0, 0, 0, 0, 0, 0, 0, 0]$. cf. Eq. 99 of Part I) is counted once (Eq. 48) and characterized by the stereoisogram of type I, as shown in Fig. 2. The diagonal equality symbol shows the equivalence based on the following *RS*-stereoisomeric group (Eq. 36 of Part I):

$$\mathbf{C}_{\widehat{I}} = \left\{I, \widehat{I}\right\} \sim \left\{(1)(2)(3)(4), \overline{(1)(2)(3)(4)}\right\}, \tag{79}$$

which is a subgroup of the following *RS*-stereoisomeric group (Eq. 43 of Part I):

$$\mathbf{C}_{s\widetilde{\sigma}\widehat{I}} = \left\{I, \widetilde{\sigma}_{d(1)}, \widehat{I}, \sigma_{d(1)}\right\} \tag{80}$$

$$\sim \left\{(1)(2)(3)(4), (1)(2\,4)(3), \overline{(1)(2)(3)(4)}, \overline{(1)(2\,4)(3)}\right\}. \tag{81}$$

It should be noted that the *RS*-stereoisomeric group $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$ (Eq. 81) is isomorphic to the Klein four group, which is in turn isomorphic to the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$. Each promolecule of the quadruplet shown in Fig. 2 is transformed into its homomeric promolecule under the action of $\mathbf{T}$ so that it is regarded as a representative of each coset appearing in the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$.

From the viewpoint of the point-group theory, the reference promolecule **2** belongs to the point group $\mathbf{C}_1$, so that a pair of **2**/$\overline{\mathbf{2}}$ is counted once under the action of the point group $\mathbf{T}_d$ [16]. From the viewpoint of the *RS*-stereoisomeric-group theory, on

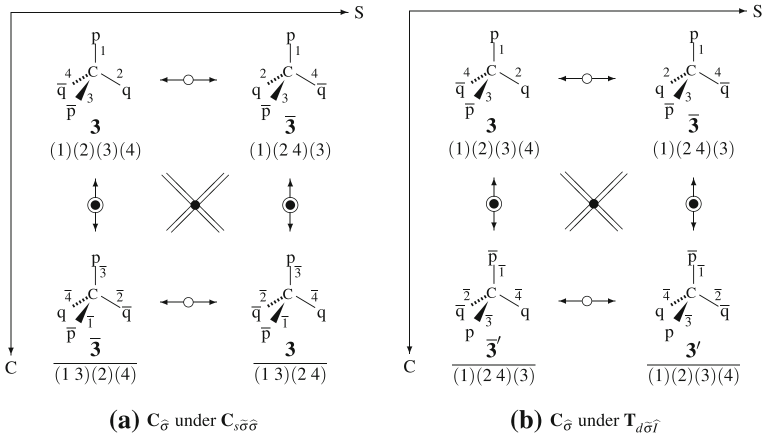


Fig. 3 Stereoisogram of type I which belongs to the *RS*-stereoisomeric group $\mathbf{C}_{\widehat{\sigma}}$. **a** The group $\mathbf{C}_{\widehat{\sigma}}$ is considered to be a subgroup of $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$, where **3** is fixed under the action of $\mathbf{C}_{\widehat{\sigma}}$. The reference promolecule **3** belongs to the point group $\mathbf{C}_1$. **b** The group $\mathbf{C}_{\widehat{I}}$ (strictly speaking, the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$) is used in place of the group $\mathbf{C}_{\widehat{\sigma}}$, where a homomer $\mathbf{3}'$ as a holantimer is drawn in place of the original holantimer $\overline{\mathbf{3}}$

the other hand, the reference promolecule **2** belongs to the *RS*-stereoisomeric group $\mathbf{C}_{\widehat{I}}$, so that a quadruplet of $\mathbf{2}/\overline{\mathbf{2}}$ (doubly contained in the stereoisogram represented by Fig. 2) is counted once under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ (Eq. 48).

4.1.2 Quadruplet of $\mathbf{C}_{\widehat{\sigma}}$

The quadruplet of $\mathbf{C}_{\widehat{\sigma}}$ having $\mathrm{p}\overline{\mathrm{p}}\mathrm{q}\overline{\mathrm{q}}$ ($[\theta]_{28} = [0, 0, 0, 0; 1, 1, 1, 1, 0, 0, 0, 0]$. cf. Eq. 119 of Part I) is counted once (Eq. 46) and characterized by the stereoisogram of type I, as shown in Fig. 3a. The diagonal equality symbol shows the equivalence based on the following *RS*-stereoisomeric group (Eq. 35 of Part I):

$$\mathbf{C}_{\widehat{\sigma}} = \left\{I, \widehat{C}_{2(3)}\right\} \sim \left\{(1)(2)(3)(4), \overline{(1\;3)(2\;4)}\right\}, \tag{82}$$

where the symbol $\widehat{\sigma}$ in the subscript is used in place of $\widehat{C}_{2(3)}$ for the sake of convenience. The group $\mathbf{C}_{\widehat{\sigma}}$ is a subgroup of the following *RS*-stereoisomeric group (Eq. 42 of Part I):

$$\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}} = \left\{I, \widetilde{\sigma}_{d(1)}, \widehat{C}_{2(3)}, \sigma_{d(6)}\right\} \tag{83}$$

$$\sim \left\{(1)(2)(3)(4), (1)(2\;4)(3), \overline{(1\;3)(2\;4)}, \overline{(1\;3)(2)(4)}\right\}. \tag{84}$$

The *RS*-stereoisomeric group $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$ (Eq. 84) is isomorphic to the Klein four group, which is in turn isomorphic to the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$. Each promolecule of the quadruplet shown in Fig. 3 is transformed into its homomeric promolecule under the action of $\mathbf{T}$ so that it is regarded as a representative of each coset appearing in the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$.

If we select the group $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$ (Eq. 81) to characterize $\mathrm{p\overline{p}q\overline{q}}$, we obtain another stereoisogram shown in Fig. 3b, where there appear promolecules $\mathbf{3}'$ (corresponding to $\overline{(1)(2)(3)(4)}$) and $\overline{\mathbf{3}}'$ (corresponding to $\overline{(1)(2\ 4)(3)}$). Under the action of $\mathbf{T}$, the promolecule $\mathbf{3}'$ is homomeric to $\mathbf{3}$, while the promolecule $\overline{\mathbf{3}}'$ is homomeric to $\overline{\mathbf{3}}$. It follows that Fig. 3b can be used in place of Fig. 3a, if we take account of the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$, which permits us to consider the homomerism due to $\mathbf{T}$.

From the viewpoint of the point-group theory, the reference promolecule **3** belongs to the point group $\mathbf{C}_1$, so that a pair of $\mathbf{3}/\overline{\mathbf{3}}$ is counted once under the action of the point group $\mathbf{T}_d$ [16]. From the viewpoint of the *RS*-stereoisomeric-group theory, on the other hand, the reference promolecule **3** belongs to the *RS*-stereoisomeric group $\mathbf{C}_{\widetilde{\sigma}}$ so that a quadruplet of $\mathbf{3}/\overline{\mathbf{3}}$ (doubly contained in the stereoisogram represented by Fig. 3a) is counted once under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ (Eq. 46).

4.2 *RS*-stereoisomeric groups of type II

Among the *RS*-stereoisomeric groups listed in Eq. 60, there appear quadruplets belonging to $\mathbf{C}_{\widetilde{\sigma}}$ ($\frac{1}{2}(\mathrm{A^2Bp} + \mathrm{A^2B\overline{p}})$, etc. in Eq. 45), $\mathbf{C}_{2\widetilde{\sigma}}$ ($\frac{1}{2}(\mathrm{A^2p^2} + \mathrm{A^2\overline{p}^2})$, etc. in Eq. 49), $\mathbf{C}_{3\widetilde{\sigma}}$ ($\frac{1}{2}(\mathrm{A^3p} + \mathrm{A^3\overline{p}})$, etc. in Eq. 52), and $\mathbf{T}_{\widetilde{\sigma}}$ ($\frac{1}{2}(\mathrm{p^4} + \mathrm{\overline{p}^4})$, etc. in Eq. 56). They are totally counted by Eq. 75.

4.2.1 Quadruplet of $\mathbf{C}_{\widetilde{\sigma}}$

The quadruplet of $\mathbf{C}_{\widetilde{\sigma}}$ having $\frac{1}{2}(\mathrm{A^2Bp}+\mathrm{A^2B\overline{p}})$ ($[\theta]_7 = [2, 1, 0, 0; 1, 0, 0, 0, 0, 0, 0, 0]$. cf. Eq. 96 of Part I) is counted once (Eq. 45) and characterized by the stereoisogram of type II, as shown in Fig. 4. The horizontal equality symbol shows the equivalence based on the following *RS*-stereoisomeric group (Eq. 29 of Part I):

$$\mathbf{C}_{\widetilde{\sigma}} = \left\{I, \widetilde{\sigma}_{d(1)}\right\} \sim \{(1)(2)(3)(4), (1)(2\ 4)(3)\}, \tag{85}$$

which is a subgroup of the *RS*-stereoisomeric group $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$ shown in Eq. 81. The $\mathbf{C}_{\widetilde{\sigma}}$-group contains no rotoreflections and no ligand reflections (with a hat accent in the present notation).

From the viewpoint of the point-group theory, the reference promolecule **4** belongs to the point group $\mathbf{C}_1$, so that a pair of $\mathbf{4}/\overline{\mathbf{4}}$ is counted once under the action of the point group $\mathbf{T}_d$ [16]. From the viewpoint of the *RS*-stereoisomeric-group theory, on the other hand, the reference promolecule **4** belongs to the *RS*-stereoisomeric group $\mathbf{C}_{\widetilde{\sigma}}$, so that a quadruplet of $\mathbf{4}/\overline{\mathbf{4}}$ (doubly contained in the stereoisogram represented by Fig. 4) is counted once under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ (Eq. 45).

4.2.2 Quadruplet of $\mathbf{C}_{2\widetilde{\sigma}}$

The quadruplet of $\mathbf{C}_{2\widetilde{\sigma}}$ having $\frac{1}{2}(\mathrm{A^2p^2}+\mathrm{A^2\overline{p}^2})$ ($[\theta]_5 = [2, 0, 0, 0; 2, 0, 0, 0, 0, 0, 0, 0]$. cf. Eq. 94 of Part I) is counted once (Eq. 49) and characterized by the stereoisogram of type II, as shown in Fig. 5. The horizontal equality symbol shows the equivalence

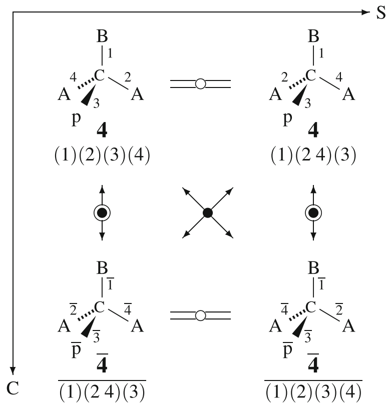


Fig. 4 Stereoisogram of type II which belongs to the *RS*-stereoisomeric group $\mathbf{C}_{\widetilde{\sigma}}$. The reference promolecule **4** belongs to the point group $\mathbf{C}_1$

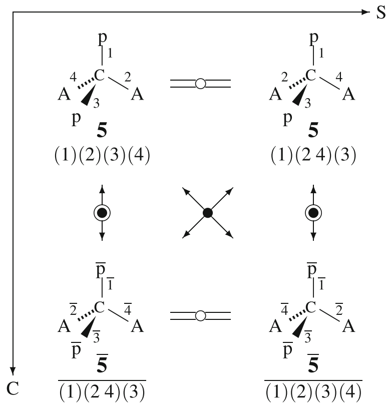


Fig. 5 Stereoisogram of type II which belongs to the *RS*-stereoisomeric group $\mathbf{C}_{2\widetilde{\sigma}}$. The reference promolecule **5** belongs to the point group $\mathbf{C}_2$

based on the following *RS*-stereoisomeric group (Eq. 31 of Part I):

$$\mathbf{C}_{2\widetilde{\sigma}} = \left\{I, C_{2(3)}, \widetilde{\sigma}_{d(1)}, \widetilde{\sigma}_{d(6)}\right\} \tag{86}$$

$$\sim \{(1)(2)(3)(4), (1\ 3)(2\ 4), (1)(2\ 4)(3), (1\ 3)(2)(4)\}, \tag{87}$$

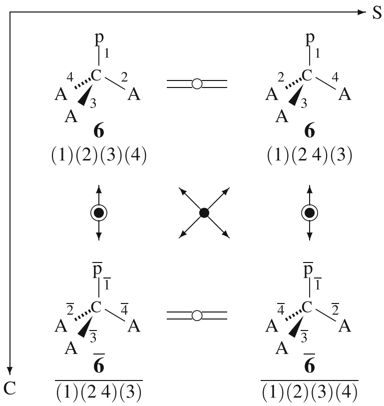
which contains no rotoreflections and no ligand reflections. The pair of homomers **5** linked with a horizontal equality symbol indicates the representatives of the following factor group:

$$\mathbf{C}_{2\widetilde{\sigma}}/\mathbf{C}_2 = \{\mathbf{C}_2, \widetilde{\sigma}_{d(1)}\mathbf{C}_2\}, \tag{88}$$

where the representatives I and $\widetilde{\sigma}_{d(1)}$ correspond to the products of cycles adopted in Fig. 5, i.e., (1)(2)(3)(4) and (1)(2 4)(3). Note that the reference promolecule **5** belongs to the point group $\mathbf{C}_2$ [16], which is regarded as an *RS*-stereoisomeric group of type II.

The *RS*-stereoisomeric group $\mathbf{C}_{2\widetilde{\sigma}}$ (Eq. 87) is a subgroup of the *RS*-stereoisomeric group $\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}$ (Eq. 47 of Part I):

Fig. 6 Stereoisogram of type II which belongs to the *RS*-stereoisomeric group $\mathbf{C}_{3\widetilde{\sigma}}$. The reference promolecule **6** belongs to the point group $\mathbf{C}_3$



$$\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}} = \left\{I, C_{2(3)}, \widetilde{\sigma}_{d(1)}, \widetilde{\sigma}_{d(6)}, \widehat{I}, \widehat{C}_{2(3)}, \sigma_{d(1)}, \sigma_{d(6)}\right\} \tag{89}$$

$$\sim \Big\{(1)(2)(3)(4), (1\ 3)(2\ 4), (1)(2\ 4)(3), (1\ 3)(2)(4)$$
$$\overline{(1)(2)(3)(4)}, \overline{(1\ 3)(2\ 4)}, \overline{(1)(2\ 4)(3)}, \overline{(1\ 3)(2)(4)}\Big\} \tag{90}$$

The type-II stereoisogram shown in Fig. 5 is drawn by considering the following factor group:

$$\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}/\mathbf{C}_2 = \{\mathbf{C}_2, \widetilde{\sigma}_{d(1)}\mathbf{C}_2, \widehat{I}\mathbf{C}_2, \sigma_{d(1)}\mathbf{C}_2\}, \tag{91}$$

which is isomorphic to the factor group the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$. Note that the factor group $\mathbf{C}_{2\widetilde{\sigma}}/\mathbf{C}_2$ (Eq. 88) is a subgroup of the factor group $\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}/\mathbf{C}_2$ (Eq. 91).

4.2.3 Quadruplet of $\mathbf{C}_{3\widetilde{\sigma}}$

The quadruplet of $\mathbf{C}_{3\widetilde{\sigma}}$ having $\frac{1}{2}(\mathrm{A}^3\mathrm{p} + \mathrm{A}^3\overline{\mathrm{p}})$ ($[\theta]_3 = [3, 0, 0, 0; 1, 0, 0, 0, 0, 0, 0, 0]$. cf. Eq. 91 of Part I) is counted once (Eq. 52) and characterized by the stereoisogram of type II, as shown in Fig. 6. The horizontal equality symbol shows the equivalence based on the following *RS*-stereoisomeric group (Eq. 32 of Part I):

$$\mathbf{C}_{3\widetilde{\sigma}} = \left\{I, C_{3(1)}, C_{3(1)}^2, \widetilde{\sigma}_{d(1)}, \widetilde{\sigma}_{d(2)}, \widetilde{\sigma}_{d(3)}\right\} \tag{92}$$

$$\sim \{(1)(2)(3)(4), (1)(2\ 3\ 4), (1)(2\ 4\ 3),$$
$$(1)(2\ 4)(3), (1)(2)(3\ 4), (1)(2\ 3)(4)\}, \tag{93}$$

where there appear no rotoreflections and no ligand reflections.

The pair of homomers **6** linked with a horizontal equality symbol indicates the representatives of the following factor group:

$$\mathbf{C}_{3\widetilde{\sigma}}/\mathbf{C}_3 = \left\{\mathbf{C}_3, \widetilde{\sigma}_{d(1)}\mathbf{C}_3\right\}, \tag{94}$$

where the representatives I and $\widetilde{\sigma}_{d(1)}$ correspond to the products of cycles adopted in Fig. 6, i.e., (1)(2)(3)(4) and (1)(2 4)(3). Note that the reference promolecule **6** belongs to the point group $\mathbf{C}_3$ [16], which is regarded as an *RS*-stereoisomeric group of type II.

The *RS*-stereoisomeric group $\mathbf{C}_{3\widetilde{\sigma}}$ (Eq. 93) is a subgroup of the *RS*-stereoisomeric group $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$ (Eq. 48 of Part I):

$$\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}} = \Big\{I, C_{3(1)}, C_{3(1)}^2, \widetilde{\sigma}_{d(1)}, \widetilde{\sigma}_{d(2)}, \widetilde{\sigma}_{d(3)}, \widehat{I}, \widehat{C}_{3(1)}, \widehat{C}_{3(1)}^2, \sigma_{d(1)}, \sigma_{d(2)}, \sigma_{d(3)}\Big\} \tag{95}$$

$$\sim \Big\{(1)(2)(3)(4), (1)(2\,3\,4), (1)(2\,4\,3), (1)(2\,4)(3), (1)(2)(3\,4), (1)(2\,3)(4), \overline{(1)(2)(3)(4)}, \overline{(1)(2\,3\,4)}, \overline{(1)(2\,4\,3)}, \overline{(1)(2\,4)(3)}, \overline{(1)(2)(3\,4)}, \overline{(1)(2\,3)(4)}\Big\} \tag{96}$$

The type-II stereoisogram shown in Fig. 6 is drawn by considering the following factor group:

$$\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}/\mathbf{C}_3 = \left\{\mathbf{C}_3, \widetilde{\sigma}_{d(1)}\mathbf{C}_3, \widehat{I}\mathbf{C}_3, \sigma_{d(1)}\mathbf{C}_3\right\}, \tag{97}$$

which is isomorphic to the factor group the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$. Note that the factor group $\mathbf{C}_{3\widetilde{\sigma}}/\mathbf{C}_3$ (Eq. 94) is a subgroup of the factor group $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}/\mathbf{C}_3$ (Eq. 97).

4.2.4 Quadruplet of $\mathbf{T}_{\widetilde{\sigma}}$

The quadruplet of $\mathbf{T}_{\widetilde{\sigma}}$ having $\frac{1}{2}(\mathrm{p}^4 + \overline{\mathrm{p}}^4)$ ($[\theta]_{20} = [0, 0, 0, 0; 4, 0, 0, 0, 0, 0, 0, 0]$. cf. Eq. 111 of Part I) is counted once (Eq. 56) and characterized by the stereoisogram of type II, as shown in Fig. 7. The horizontal equality symbol shows the equivalence based on the following *RS*-stereoisomeric group (Eqs. 3 and 34 of Part I):

$$\mathbf{T}_{\widetilde{\sigma}} = \mathbf{T} + \widetilde{\sigma}_{d(1)}\mathbf{T}, \tag{98}$$

where there appear no rotoreflections and no ligand reflections. For the concrete forms (products of cycles) of Eq. 98, see Table 1 of Part I of this series. The pair of homomers **7** linked with a horizontal equality symbol indicates the representatives of the following factor group:

$$\mathbf{T}_{\widetilde{\sigma}}/\mathbf{T} = \left\{\mathbf{T}, \widetilde{\sigma}_{d(1)}\mathbf{T}\right\}, \tag{99}$$

where the representatives I and $\widetilde{\sigma}_{d(1)}$ correspond to the products of cycles adopted in Fig. 7, i.e., (1)(2)(3)(4) and (1)(2 4)(3).

The *RS*-stereoisomeric group $\mathbf{T}_{\widetilde{\sigma}}$ (Eq. 98) is a subgroup of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ for characterizing the tetrahedral skeleton. The type-II stereoisogram shown in Fig. 7 is drawn by considering the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$.

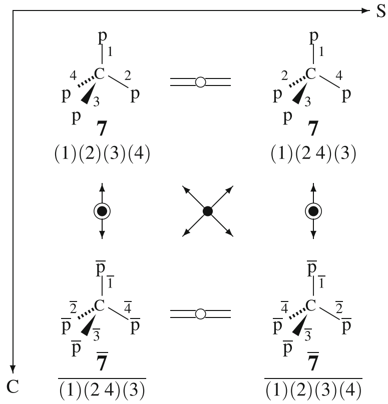


Fig. 7 Stereoisogram of type II which belongs to the *RS*-stereoisomeric group $\mathbf{T}_{\widetilde{\sigma}}$. The reference promolecule **7** belongs to the point group **T**

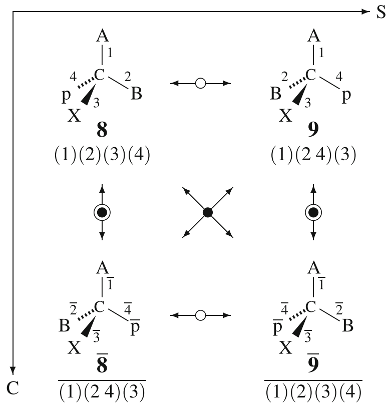


Fig. 8 Stereoisogram of type III which belongs to the *RS*-stereoisomeric group $\mathbf{C}_1$. The reference promolecule **8** belongs to the point group $\mathbf{C}_1$

From the viewpoint of the point-group theory, the reference promolecule **7** belongs to the point group **T**, so that a pair of **7**/$\overline{\mathbf{7}}$ is counted once under the action of the point group $\mathbf{T}_d$ [16]. From the viewpoint of the *RS*-stereoisomeric-group theory, on the other hand, the reference promolecule **7** belongs to the *RS*-stereoisomeric group $\mathbf{T}_{\widetilde{\sigma}}$, so that a quadruplet of **7**/$\overline{\mathbf{7}}$ (doubly contained in the stereoisogram represented by Fig. 7) is counted once under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ (Eq. 56).

4.3 *RS*-Stereoisomeric groups of type III

Among the *RS*-stereoisomeric groups listed in Eq. 61, there appear quadruplets belonging to $\mathbf{C}_1$ (e.g., $\frac{1}{2}(\mathrm{ABXp} + \mathrm{ABX}\overline{\mathrm{p}})$ etc. in Eq. 44). They are totally counted by Eq. 76.

4.3.1 Quadruplet of $\mathbf{C}_1$

The quadruplet of $\mathbf{C}_1$ having $\frac{1}{2}(\mathrm{ABXp} + \mathrm{ABX}\overline{\mathrm{p}})$ ($[\theta]_{11} = [1, 1, 1, 0; 1, 0, 0, 0, 0, 0, 0, 0]$. cf. Eq. 100 of Part I) is counted once (Eq. 44) and characterized by the stereoisogram of type III, as shown in Fig. 8.

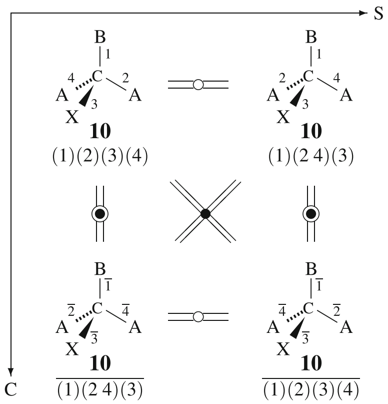


Fig. 9 Stereoisogram of type IV which belongs to the *RS*-stereoisomeric group $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$. The reference promolecule **10** belongs to the point group $\mathbf{C}_s$

The *RS*-stereoisomeric group $\mathbf{C}_1$ is a trivial subgroup of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ for characterizing the tetrahedral skeleton. The type-III stereoisogram shown in Fig. 8 is drawn by considering the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$.

From the viewpoint of the point-group theory, the reference promolecule **8** (or **9**) belongs to the point group $\mathbf{C}_1$, so that a pair of $\mathbf{8}/\overline{\mathbf{8}}$ and another pair of $\mathbf{9}/\overline{\mathbf{9}}$ are counted separately under the action of the point group $\mathbf{T}_d$ [16]. This means that the pair of $\mathbf{8}/\overline{\mathbf{8}}$ is not recognized to be equivalent (stereoisomeric) to the pair of $\mathbf{9}/\overline{\mathbf{9}}$ under the point group $\mathbf{T}_d$.

From the viewpoint of the *RS*-stereoisomeric-group theory, on the other hand, the reference promolecule **8** (or **9**) belongs to the *RS*-stereoisomeric group $\mathbf{C}_1$, so that a quadruplet of $\mathbf{8}/\overline{\mathbf{8}}$ and $\mathbf{9}/\overline{\mathbf{9}}$ (contained in the stereoisogram represented by Fig. 8) is counted once under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ (Eq. 44). This means that the pair of $\mathbf{8}/\overline{\mathbf{8}}$ is now recognized to be equivalent (*RS*-diastereomeric) to the pair of $\mathbf{9}/\overline{\mathbf{9}}$ under the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$.

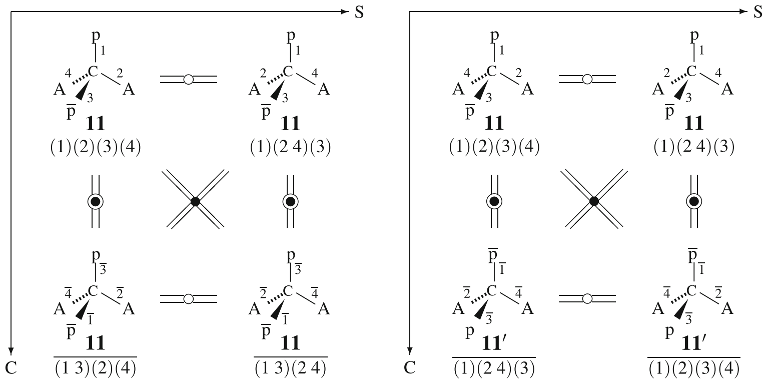
4.4 *RS*-stereoisomeric groups of type IV

Among the *RS*-stereoisomeric groups listed in Eq. 62, there appear quadruplets belonging to $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$ (A^2BX etc. in Eq. 51), $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$ ($A^2p\overline{p}$ etc. in Eq. 50), $\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}$ ($p^2\overline{p}^2$ etc. in Eq. 53), $\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}$ (A^2B^2 etc. in Eq. 54), $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$ (A^3B etc. in Eq. 55), and $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ (A^4 etc. in Eq. 57). They are totally counted by Eq. 77.

4.4.1 Quadruplet of $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$

The quadruplet of $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$ having A^2BX ($[\theta]_6 = [2, 1, 1, 0; 0, 0, 0, 0, 0, 0, 0, 0]$. cf. Eq. 95 of Part I) is counted once (Eq. 51) and characterized by the stereoisogram of type IV, as shown in Fig. 9. The *RS*-stereoisomeric group $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$ is isomorphic to the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$, where its operations are listed in Eq. 81 described above (Eq. 43 of Part I).

From the viewpoint of the point-group theory, the reference promolecule **10** belongs to the point group $\mathbf{C}_s$, so that it is counted once as an achiral promolecule under the action of the point group $\mathbf{T}_d$ [16]. From the viewpoint of the *RS*-stereoisomeric-group theory, on the other hand, the reference promolecule **10**



(a) $\mathbf{C}_{s\tilde{\sigma}\hat{\sigma}}$ by itself **(b)** $\mathbf{C}_{s\tilde{\sigma}\hat{\sigma}}$ under $\mathbf{T}_{d\tilde{\sigma}\hat{I}}$

Fig. 10 Stereoisogram of type IV which belongs to the *RS*-stereoisomeric group $\mathbf{C}_{s\tilde{\sigma}\hat{\sigma}}$. **a** The group $\mathbf{C}_{s\tilde{\sigma}\hat{\sigma}}$ is considered by itself, where **11** is fixed under the action of $\mathbf{C}_{s\tilde{\sigma}\hat{\sigma}}$. The reference promolecule **11** belongs to the point group $\mathbf{C}_s$. **b** The group $\mathbf{C}_{s\tilde{\sigma}\hat{I}}$ (strictly speaking, the factor group $\mathbf{T}_{d\tilde{\sigma}\hat{I}}/\mathbf{T}$) is used in place of the group $\mathbf{C}_{s\tilde{\sigma}\hat{\sigma}}$, where a homomer **11**′ as a holantimer is drawn in place of the original holantimer **11**

belongs to the *RS*-stereoisomeric group $\mathbf{C}_{s\tilde{\sigma}\hat{I}}$, so that a quadruplet due to **10** (contained in the stereoisogram represented by Fig. 9) is counted once under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\tilde{\sigma}\hat{I}}$ (Eq. 51).

4.4.2 Quadruplet of $\mathbf{C}_{s\tilde{\sigma}\hat{\sigma}}$

The quadruplet of $\mathbf{C}_{s\tilde{\sigma}\hat{\sigma}}$ having $\mathrm{A}^2\mathrm{p}\overline{\mathrm{p}}$ ($[\theta]_8 = [2, 0, 0, 0; 1, 1, 0, 0, 0, 0, 0, 0]$. cf. Eq. 97 of Part I) is counted once (Eq. 50) and characterized by the stereoisogram of type IV, as shown in Fig. 10a. The *RS*-stereoisomeric group $\mathbf{C}_{s\tilde{\sigma}\hat{\sigma}}$ consists of the four operations (products of cycles) listed in Eq. 84 (Eq. 42 of Part I) and is isomorphic to the factor group $\mathbf{T}_{d\tilde{\sigma}\hat{I}}/\mathbf{T}$.

If we select the group $\mathbf{C}_{s\tilde{\sigma}\hat{I}}$ (Eq. 81) to characterize $\mathrm{A}^2\mathrm{p}\overline{\mathrm{p}}$, we obtain another stereoisogram shown in Fig. 10b, where there appear a promolecule **11**′ in accord with $\overline{(1)(2)(3)(4)}$ and $\overline{(1)(2\,4)(3)}$. Under the action of **T**, the promolecule **11**′ is homomeric to **11**. It follows that Fig. 10b can be used in place of Fig. 10a, if we take account of the factor group $\mathbf{T}_{d\tilde{\sigma}\hat{I}}/\mathbf{T}$ in order to consider the homomerism due to **T**.

From the viewpoint of the point-group theory, the reference promolecule **11** belongs to the point group $\mathbf{C}_s$, so that it is counted once as an achiral promolecule under the action of the point group $\mathbf{T}_d$ [16]. From the viewpoint of the *RS*-stereoisomeric-group theory, on the other hand, the reference promolecule **11** belongs to the *RS*-stereoisomeric group $\mathbf{C}_{s\tilde{\sigma}\hat{\sigma}}$, so that a quadruplet due to **11** (contained in the stereoisogram represented by Fig. 10a) is counted once under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\tilde{\sigma}\hat{I}}$ (Eq. 50).

4.4.3 Quadruplet of $\mathbf{S}_{4\tilde{\sigma}\hat{\sigma}}$

The quadruplet of $\mathbf{S}_{4\tilde{\sigma}\hat{\sigma}}$ having $\mathrm{p}^2\overline{\mathrm{p}}^2$ ($[\theta]_{23} = [0, 0, 0, 0; 2, 2, 0, 0, 0, 0, 0, 0]$. cf. Eq. 114 of Part I) is counted once (Eq. 53) and characterized by the stereoisogram of

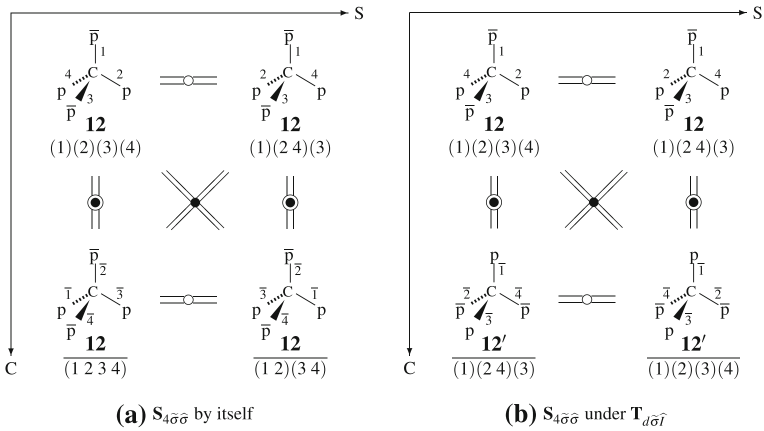


Fig. 11 Stereoisogram of type IV which belongs to the *RS*-stereoisomeric group $\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}$. **a** The group $\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}$ is considered by itself, where **12** is fixed under the action of $\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}$. The reference promolecule **11** belongs to the point group $\mathbf{S}_4$. **b** The factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$ is used in place of the group $\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}$, where a homomer **12**′ as a holantimer is drawn in place of the original holantimer **12**

type IV, as shown in Fig. 11a. The *RS*-stereoisomeric group $\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}$ consists of eight operations (Eq. 46 of Part I):

$$\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}} = \left\{I, C_{2(3)}, \widetilde{\sigma}_{d(1)}, \widetilde{\sigma}_{d(6)}, \widehat{C}_{2(1)}, \widehat{C}_{2(2)}, S_{4(3)}, S^3_{4(3)}\right\} \tag{100}$$

$$\sim \left\{(1)(2)(3)(4), (1\ 3)(2\ 4), (1)(2\ 4)(3), (1\ 3)(2\ 4)\right.$$
$$\left.\overline{(1\ 2)(3\ 4)}, \overline{(1\ 4)(2\ 3)}, \overline{(1\ 2\ 3\ 4)}, \overline{(1\ 4\ 3\ 2)}\right\} \tag{101}$$

By considering the normal subgroup $\mathbf{C}_2$, the following factor group is generated:

$$\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}/\mathbf{C}_2 = \left\{\mathbf{C}_2, \widetilde{\sigma}_{d(1)}\mathbf{C}_2, \widehat{C}_{2(1)}\mathbf{C}_2, S_{4(3)}\mathbf{C}_2\right\}. \tag{102}$$

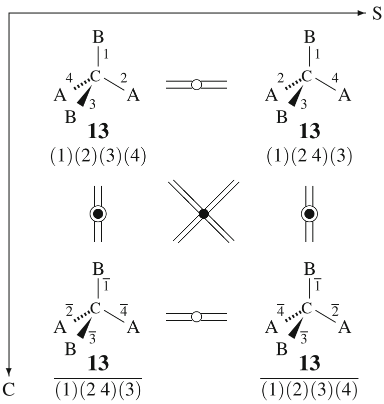
The representatives of the respective cosets are used to draw Fig. 11a.

The the factor group $\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}/\mathbf{C}_2$ is isomorphic to the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$. This isomorphism can be applied to draw another equivalent stereoisogram shown in Fig. 11b, where the homomerism between **12** and **12**′ under the **T**-group is taken into consideration.

From the viewpoint of the point-group theory, the reference promolecule **12** belongs to the point group $\mathbf{S}_4$, so that it is counted once as an achiral promolecule under the action of the point group $\mathbf{T}_d$ [16]. From the viewpoint of the *RS*-stereoisomeric-group theory, on the other hand, the reference promolecule **12** belongs to the *RS*-stereoisomeric group $\mathbf{S}_{4\widetilde{\sigma}\widehat{\sigma}}$, so that a quadruplet due to **12** (contained in the stereoisogram represented by Fig. 11a) is counted once under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ (Eq. 53).

Note that the symbol $\mathbf{S}_4$ is used to denote the cyclic group of order 4 in the present article, and not to denote the symmetric group of degree 4.

Fig. 12 Stereoisogram of type IV which belongs to the *RS*-stereoisomeric group $\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}$. The reference promolecule **13** belongs to the point group $\mathbf{C}_{2v}$



4.4.4 *Quadruplet of* $\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}$

The quadruplet of $\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}$ having A^2B^2 (Eq. 54) ($[\theta]_4 = [2, 2, 0, 0; 0, 0, 0, 0, 0, 0, 0, 0]$. cf. Eq. 93 of Part I) is counted once (Eq. 54) and characterized by the stereoisogram of type IV, as shown in Fig. 12.

The *RS*-stereoisomeric group $\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}$ shown in Eq. 90 generates the factor group $\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}/\mathbf{C}_2$ shown in Eq. 91, which is isomorphic to the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$. Thereby, we obtain the stereoisogram of type IV shown in Fig. 12.

From the viewpoint of the point-group theory, the reference promolecule **13** belongs to the point group $\mathbf{C}_{2v}$, so that it is counted once as an achiral promolecule under the action of the point group $\mathbf{T}_d$ [16]. From the viewpoint of the *RS*-stereoisomeric-group theory, on the other hand, the reference promolecule **13** belongs to the *RS*-stereoisomeric group $\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}$, so that a quadruplet due to **13** (contained in the stereoisogram represented by Fig. 12) is counted once under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ (Eq. 54).

4.4.5 *Quadruplet of* $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$

The quadruplet of $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$ having A^3B (Eq. 55) ($[\theta]_2 = [3, 1, 0, 0; 0, 0, 0, 0, 0, 0, 0, 0]$. cf. Eq. 91 of Part I) is counted once (Eq. 55) and characterized by the stereoisogram of type IV, as shown in Fig. 13. The *RS*-stereoisomeric group $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$ shown in Eq. 96 generates the factor group $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}/\mathbf{C}_3$ shown in Eq. 97, which is isomorphic to the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$. Thereby, we obtain the stereoisogram of type IV shown in Fig. 13.

From the viewpoint of the point-group theory, the reference promolecule **14** belongs to the point group $\mathbf{C}_{3v}$, so that it is counted once as an achiral promolecule under the action of the point group $\mathbf{T}_d$ [16]. From the viewpoint of the *RS*-stereoisomeric-group theory, on the other hand, the reference promolecule **14** belongs to the *RS*-stereoisomeric group $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$, so that a quadruplet due to **14** (contained in the stereoisogram represented by Fig. 13) is counted once under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ (Eq. 55).

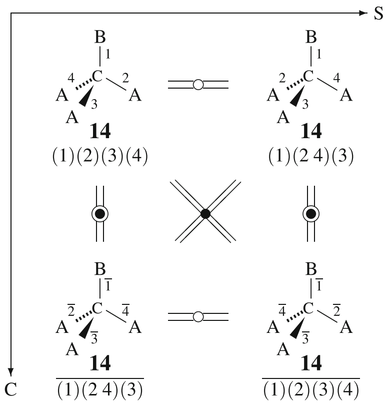


Fig. 13 Stereoisogram of type IV which belongs to the *RS*-stereoisomeric group $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$. The reference promolecule **14** belongs to the point group $\mathbf{C}_{3v}$

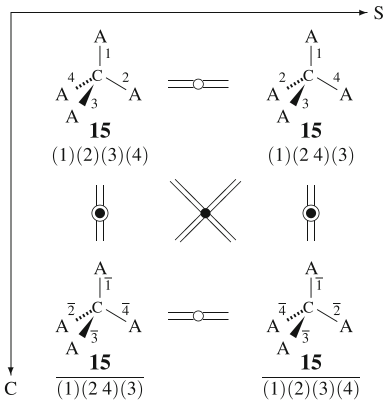


Fig. 14 Stereoisogram of type IV which belongs to the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$. The reference promolecule **15** belongs to the point group $\mathbf{T}_d$

4.4.6 *Quadruplet of* $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$

The quadruplet of $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ having A^4 ($[\theta]_1 = [4, 0, 0, 0; 0, 0, 0, 0, 0, 0, 0, 0]$. cf. Eq. 90 of Part I) is counted once (Eq. 57) and characterized by the stereoisogram of type IV, as shown in Fig. 14. The stereoisogram is based on the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$.

From the viewpoint of the point-group theory, the reference promolecule **15** belongs to the point group $\mathbf{T}_d$, so that it is counted once as an achiral promolecule under the action of the point group $\mathbf{T}_d$ [16]. From the viewpoint of the *RS*-stereoisomeric-group theory, on the other hand, the reference promolecule **15** belongs to the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$, so that a quadruplet due to **15** (contained in the stereoisogram represented by Fig. 14) is counted once under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ (Eq. 57).

4.5 *RS*-stereoisomeric groups of type V

Among the *RS*-stereoisomeric groups listed in Eq. 63, there appear quadruplets belonging to $\mathbf{C}_s$ (ABp$\overline{\text{p}}$ etc. in Eq. 47).

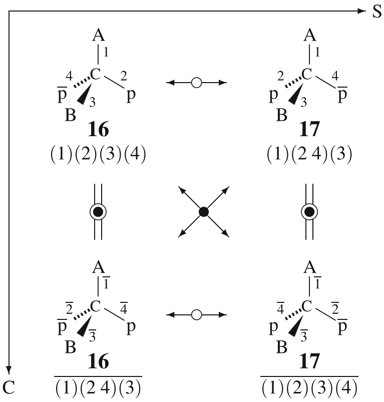


Fig. 15 Stereoisogram of type V which belongs to the *RS*-stereoisomeric group $\mathbf{C}_s$. The reference promolecule **16** belongs to the point group $\mathbf{C}_s$

4.5.1 Quadruplet of $\mathbf{C}_s$

The quadruplet of $\mathbf{C}_s$ having ABp$\overline{\text{p}}$ ($[\theta]_{13}$ = [1, 1, 0, 0; 1, 1, 0, 0, 0, 0, 0, 0]. cf. Eq. 102 of Part I) is counted once (Eq. 47) and characterized by the stereoisogram of type V, as shown in Fig. 15. The vertical equality symbol shows the equivalence based on the following *RS*-stereoisomeric group:

$$\mathbf{C}_s = \left\{I, \sigma_{d(1)}\right\} \sim \left\{(1)(2)(3)(4), \overline{(1)(2\ 4)(3)}\right\}, \tag{103}$$

which is equal to the point group $\mathbf{C}_s$. The *RS*-stereoisomeric group $\mathbf{C}_s$ is a subgroup of the *RS*-stereoisomeric group $\mathbf{C}_{s\tilde{\sigma}\widehat{I}}$ shown in Eq. 81 (Eq. 43 of Part I).

From the viewpoint of the point-group theory, the reference promolecule **16** (or **17**) belongs to the point group $\mathbf{C}_s$, so that one achiral promolecule **16** and another achiral promolecule **17** are counted separately under the action of the point group $\mathbf{T}_d$ [16]. This means that the achiral promolecules **16** and **17** are recognized to be inequivalent to each other under the point group $\mathbf{T}_d$.

From the viewpoint of the *RS*-stereoisomeric-group theory, on the other hand, the reference promolecule **16** (or **17**) belongs to the *RS*-stereoisomeric group $\mathbf{C}_s$, so that a quadruplet due to **16** and **17** (contained in the stereoisogram represented by Fig. 15) is counted once under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\tilde{\sigma}\widehat{I}}$ (Eq. 47). This means that the achiral promolecules **16** and **17** are now recognized to be equivalent (*RS*-diastereomeric) to each other under the *RS*-stereoisomeric group $\mathbf{T}_{d\tilde{\sigma}\widehat{I}}$.

5 Sphericities under point groups and under *RS*-stereoisomeric groups

5.1 Sphericities under point groups

According to the USCI approach [1,17], a coset representation $\mathbf{G}(/\mathbf{G}_i)$ based on a point group $\mathbf{G}$ is categorized as follows:

1. If both the point groups, $\mathbf{G}$ (global symmetry) and $\mathbf{G}_i$ (local symmetry), are achiral, the coset representation $\mathbf{G}(/\mathbf{G}_i)$ is defined as being homospheric and characterized by a sphericity index a_d where $d = |\mathbf{G}|/|\mathbf{G}_i|$.
2. If the global point group $\mathbf{G}$ is achiral and the local point group $\mathbf{G}_i$ is chiral, the coset representation $\mathbf{G}(/\mathbf{G}_i)$ is defined as being enantiospheric and characterized by a sphericity index c_d where $d = |\mathbf{G}|/|\mathbf{G}_i|$.
3. If both the point groups, $\mathbf{G}$ (global symmetry) and $\mathbf{G}_i$ (local symmetry), are chiral, the coset representation $\mathbf{G}(/\mathbf{G}_i)$ is defined as being hemispheric and characterized by a sphericity index b_d where $d = |\mathbf{G}|/|\mathbf{G}_i|$.

A coset representation $\mathbf{G}(/\mathbf{G}_i)$ is subduced into a subgroup $\mathbf{G}_j$. The subduction $\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j$ is represented by a sum of coset representations based on the subgroup $\mathbf{G}_j$. The sum of coset representations is characterized by a product of sphericity indices, which is called *a unit subduced cycle index with chirality fittingness* (USCI-CF). For the example date of the subduction and USCI-CFs of the coset representation $\mathbf{O}_h(/\mathbf{D}_{3d})$, see Table 2 of Part I of this series.

According to the procedure for calculating USCI-CFs [1], the subduction of $\mathbf{T}_d(/\mathbf{C}_{3v}) \downarrow \mathbf{C}_s$ is represented as follows (Table C.10 of [1]):

$$\mathbf{T}_d(/\mathbf{C}_{3v}) \downarrow \mathbf{C}_s = \mathbf{C}_s(/\mathbf{C}_1) + 2\mathbf{C}_s(/\mathbf{C}_s) \quad \cdots \left(\text{USCI-CF:} a_1^2 c_2\right), \qquad (104)$$

which corresponds to $\mathbf{O}_h(/\mathbf{D}_{3d}) \downarrow \mathbf{C}'_s$ (the 5th row of Table 2 of Part I). Because the coset representation $\mathbf{C}_s(/\mathbf{C}_1)$ is enantiospheric and $|\mathbf{C}_s|/|\mathbf{C}_1| = 2/1 = 2$, the corresponding sphericity index is obtained to be c_2. Because the coset representation $\mathbf{C}_s(/\mathbf{C}_s)$ is homospheric and $|\mathbf{C}_s|/|\mathbf{C}_s| = 2/2 = 1$, the corresponding sphericity index is obtained to be a_1. Hence, the USCI-CF for the subduction represented by Eq. 104 is obtained to be $a_1^2 c_2$, which operates under the action of the point group $\mathbf{T}_d$.

5.2 Sphericities under *RS*-stereoisomeric groups

An *RS*-stereoisomeric group and its subgroups (also *RS*-stereoisomeric groups) are categorized by means of extended chirality/achirality:

1. If an *RS*-stereoisomeric group contains a (roto)reflection operation and/or a ligand reflection operation (with a hat accent in the present notation), it is defined to be ex-achiral.
2. If an *RS*-stereoisomeric group contains no (roto)reflection operations nor ligand reflection operations, it is defined to be ex-chiral.

Note that the prefix 'ex' is an abbreviated form of 'extended'.

Among the 33 subgroups of the *RS*-stereoisomeric group $\mathbf{T}_{d\tilde{\sigma}\hat{I}}$ listed in Eqs. 59–63, for example, those listed as type II (Eq. 60) and type III (Eq. 61) are ex-chiral according to the definition described in the preceding paragraph, while those listed as type I (Eq. 59), type IV (Eq. 62), and type V (Eq. 62) are ex-achiral.

A coset representation $\acute{\mathbf{G}}(/\acute{\mathbf{G}}_i)$ based on an *RS*-stereoisomeric group $\acute{\mathbf{G}}$ is categorized as follows:

1. If both the *RS*-stereoisomeric groups, $\acute{\mathbf{G}}$ (global symmetry) and $\acute{\mathbf{G}}_i$ (local symmetry), are ex-achiral, the coset representation $\acute{\mathbf{G}}(/\acute{\mathbf{G}}_i)$ is defined as being homospheric and characterized by a sphericity index a_d where $d = |\acute{\mathbf{G}}|/|\acute{\mathbf{G}}_i|$.
2. If the global *RS*-stereoisomeric group $\acute{\mathbf{G}}$ is ex-achiral and the local *RS*-stereoisomeric group $\acute{\mathbf{G}}_i$) is ex-chiral, the coset representation $\acute{\mathbf{G}}(/\acute{\mathbf{G}}_i)$ is defined as being enantiospheric and characterized by a sphericity index c_d where $d = |\acute{\mathbf{G}}|/|\acute{\mathbf{G}}_i|$.
3. If both the *RS*-stereoisomeric groups, $\acute{\mathbf{G}}$ (global symmetry) and $\acute{\mathbf{G}}_i$) (local symmetry), are ex-chiral, the coset representation $\acute{\mathbf{G}}(/\acute{\mathbf{G}}_i)$ is defined as being hemispheric and characterized by a sphericity index b_d where $d = |\acute{\mathbf{G}}|/|\acute{\mathbf{G}}_i|$.

A coset representation $\acute{\mathbf{G}}(/\acute{\mathbf{G}}_i)$ is subduced into a subgroup $\acute{\mathbf{G}}_j$. The subduction $\acute{\mathbf{G}}(/\acute{\mathbf{G}}_i) \downarrow \acute{\mathbf{G}}_j$ is represented by a sum of coset representations based on the subgroup $\acute{\mathbf{G}}_j$. The sum of coset representations is characterized by a product of sphericity indices, which is also called *a unit subduced cycle index with chirality fittingness* (USCI-CF). For example date of the subduction and USCI-CFs of the coset representation $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}})$, see Table 3 of Part I of this series.

In a similar way to the procedure for subducing coset representations under the action of point groups [1], the subduction of $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_s$ is obtained under the action of *RS*-stereoisomeric groups as follows:

$$\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_s = \mathbf{C}_s(/\mathbf{C}_1) + 2\mathbf{C}_s(/\mathbf{C}_s) \quad \cdots (\text{USCI-CF: } a_1^2 c_2), \tag{105}$$

which has been listed in the 5th row of Table 3 of Part I. Because the coset representation $\mathbf{C}_s(/\mathbf{C}_1)$ is enantiospheric and $|\mathbf{C}_s|/|\mathbf{C}_1| = 2/1 = 2$, the corresponding sphericity index is obtained to be c_2. Because the coset representation $\mathbf{C}_s(/\mathbf{C}_s)$ is homospheric and $|\mathbf{C}_s|/|\mathbf{C}_s| = 2/2 = 1$, the corresponding sphericity index is obtained to be a_1. Hence, the USCI-CF for the subduction represented by Eq. 105 is obtained to be $a_1^2 c_2$, which operates under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$.

5.3 Chirality fittingness during proligand occupation

Let examine **16** (or **17**) shown in Fig. 15 under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$. The proligand A at the position 1 (or B at the position 3) occupies a one-membered orbit governed by the coset representation $\mathbf{C}_s(/\mathbf{C}_s)$ (Eq. 105). This occupation satisfies the chirality fittingness of the homospheric orbit. The pair of chiral proligands p/$\overline{\text{p}}$ occupies the positions 2 and 4, which construct a two-membered orbit governed by the coset representation $\mathbf{C}_s(/\mathbf{C}_1)$ (Eq. 105). This occupation satisfies the chirality fittingness of the enantiospheric orbit. Note that the $\mathbf{C}_s$ group in Eq. 105 is regarded as an *RS*-stereoisomeric group of type V.

The same promolecule **16** (or **17**) shown in Fig. 15 can be examined under the action of the point group $\mathbf{T}_d$, where the subduction represented by Eq. 104 is taken into consideration. Although the $\mathbf{C}_s$ group of Eq. 104 is regarded as a point group, the discussions described in the preceding paragraph holds true in this case. For symmetry-itemized enumeration of tetrahedral promolecules under the point group $\mathbf{T}_d$, see [16].

Let examine **11** shown in Fig. 10a under the action of the *RS*-stereoisomeric group $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$. This promolecule corresponds to the following subduction (the 14th row of

Table 3 of Part I):

$$\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}} = \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_{\widetilde{\sigma}}) + \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_{s}) \quad \cdots (\text{USCI-CF:}a_2c_2) \tag{106}$$

Because the coset representation $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_{\widetilde{\sigma}})$ is enantiospheric and $|\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}|/|\mathbf{C}_{\widetilde{\sigma}}| = 4/2 = 2$, the corresponding sphericity index is obtained to be c_2. Because the coset representation $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_{s})$ is homospheric and $|\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}|/|\mathbf{C}_{s}| = 4/2 = 2$, the corresponding sphericity index is obtained to be a_2. Hence, the USCI-CF for the subduction represented by Eq. 106 is obtained to be a_2c_2, which operates under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$.

The pair p/$\overline{\text{p}}$ occupies the positions 1 and 3 of **11**, which construct a two-membered enantiospheric orbit governed by the coset representation $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_{\widetilde{\sigma}})$. The two A's occupy the positions 2 and 4 of **11**, which construct a two-membered homospheric orbit governed by the coset representation $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_{s})$. Note that the $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$ group in Eq. 106 is regarded as an *RS*-stereoisomeric group of type IV.

The same promolecule **11** shown in Fig. 10a can be examined under the action of the point group $\mathbf{T}_d$, where the subduction represented by Eq. 104 is taken into consideration. Because **11** is regarded as belonging to the point group $\mathbf{C}_s$ group, each A at the position 2 or 4 constructs a one-membered homospheric orbit, while the pair p/$\overline{\text{p}}$ constructs a two-membered enantiospheric orbit.

It should be pointed out that, although **16** (Fig. 15) and **11** (Fig. 10a) belong to the same point group $\mathbf{C}_s$ ($\subset \mathbf{T}_d$), they belong to distinct *RS*-stereoisomeric groups, i.e., $\mathbf{C}_s$ (type V $\subset \mathbf{T}_{d\widetilde{\sigma}\widehat{\sigma}}$) and $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$ (type IV $\subset \mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$). In addition, the distinction can be diagrammatically demonstrated in terms of their stereoisograms, i.e., Fig. 15 versus Fig. 10a.

5.4 Ex-achirality versus chirality for type I

The promolecule **2** (or $\overline{\mathbf{2}}$) shown in Fig. 2 belongs to the *RS*-stereoisomeric group $\mathbf{C}_{\widehat{I}}$. This promolecule corresponds to the following subduction (the 6th row of Table 3 of Part I):

$$\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_{\widehat{I}} = 4\mathbf{C}_{\widehat{I}}(/\mathbf{C}_{\widehat{I}}) \quad \cdots (\text{USCI-CF: } a_1^4) \tag{107}$$

Because the *RS*-stereoisomeric group $\mathbf{C}_{\widehat{I}}$ is ex-achiral, the coset representation $\mathbf{C}_{\widehat{I}}(/\mathbf{C}_{\widehat{I}})$ is determined to be homospheric. As a result, the four positions of **2** accommodate different achiral proligands (ABXY) in accord with their homosphericities under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$.

Under the action of the point group $\mathbf{T}_d$, in contrast, the promolecule **2** (or $\overline{\mathbf{2}}$) should be regarded as belonging to the point group $\mathbf{C}_1$. As a result, this promolecule corresponds to the following subduction (Table C.10 of [1]):

$$\mathbf{T}_{d}(/\mathbf{C}_{3v}) \downarrow \mathbf{C}_{1} = 4\mathbf{C}_{1}(/\mathbf{C}_{1}) \quad \cdots \left(\text{USCI-CF:}b_1^4\right) \tag{108}$$

Because the point group $\mathbf{C}_1$ is chiral, the coset representation $\mathbf{C}_1(/\mathbf{C}_1)$ is determined to be hemispheric. As a result, the four positions of **2** accommodate different achiral and/or chiral proligands (involving ABXY) in accord with their hemisphericities under the action of the point group $\mathbf{T}_d$. For symmetry-itemized enumeration of tetrahedral promolecules under the point group $\mathbf{T}_d$, see [16].

The promolecule **3** (or $\overline{\mathbf{3}}$) shown in Fig. 3 belongs to the *RS*-stereoisomeric group $\mathbf{C}_{\widehat{\sigma}}$. This promolecule corresponds to the following subduction (the 4th row of Table 3 of Part I):

$$\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_{\widehat{\sigma}} = 2\mathbf{C}_{\widehat{\sigma}}(/\mathbf{C}_1) \quad \cdots (\text{USCI-CF:}c_2^2) \tag{109}$$

Because the *RS*-stereoisomeric group $\mathbf{C}_{\widehat{\sigma}}$ is ex-achiral and the *RS*-stereoisomeric group $\mathbf{C}_1$ is ex-chiral, the coset representation $\mathbf{C}_{\widehat{\sigma}}(/\mathbf{C}_1)$ is determined to be enantiospheric. As a result, each pair of positions of **3** accommodates a pair of p/$\overline{\text{p}}$ (or a pair of q/$\overline{\text{q}}$) in accord with its enantiosphericity under the action of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$.

Under the action of the point group $\mathbf{T}_d$, the promolecule **3** (or $\overline{\mathbf{3}}$) should be regarded as belonging to the point group $\mathbf{C}_1$. Hence, the subduction for characterizing **3** is equal to Eq. 108. The discussion concerning Eq. 108 is effective to explain the behavior of **3** un the action of the point group $\mathbf{T}_d$. For symmetry-itemized enumeration of tetrahedral promolecules under the point group $\mathbf{T}_d$, see [16].

One of the merits of the present enumeration under the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ is the finding that stereoisograms of type I (such as Figs. 2 and 3) are ascribed to the *RS*-stereoisomeric groups $\mathbf{C}_{\widehat{I}}$ and $\mathbf{C}_{\widehat{\sigma}}$. This provides sharp contrast to the fact that we are forced to adopt the point group $\mathbf{C}_1$ in characterizing stereoisograms of type I under the action of the point group $\mathbf{T}_d$ [16].

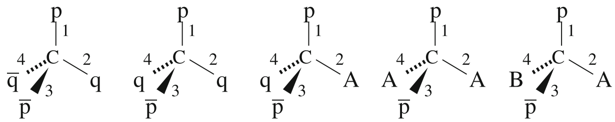
As listed in Fig. 9 of Part I, promolecules based on the tetrahedral skeleton **1** (Fig. 1) belong to the respective *RS*-stereoisomeric groups, which are categorized into five types (Eqs. 59–63). Such full categorization has been accomplished by taking account of the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$. It cannot be accomplished if we obey the point-group theory based on $\mathbf{T}_d$. Note that the $\mathbf{C}_1$-point group appears in type I, type II, and type III, whereas the $\mathbf{C}_1$-group as an *RS*-stereoisomeric group appears only in type III.

6 Subsets of *RS*-stereoisomeric groups

Each of the *RS*-stereoisomeric groups of type IV collected in Eq. 62 is capable of constructing a subset of *RS*-stereoisomeric groups, which are categorized into type I to type V. The process of constructing subsets of *RS*-Stereoisomeric groups is regarded as nested subductions for characterizing successive derivations of promolecules.

6.1 Subset concerning $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$

The *RS*-stereoisomeric group $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$ of order 4 (Eq. 84) is characterized by a subset of *RS*-stereoisomeric groups collected in Eqs. 110–114, which are constructed by selecting the subgroups of $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$ from Eqs. 59–63. The categorization to types I–V,



3	18	19	11	16′
$\mathbf{C}_{\widehat{\sigma}}$	$\mathbf{C}_{\widetilde{\sigma}}$	$\mathbf{C}_1$	$\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$	$\mathbf{C}_s$
Type I	Type II	Type III	Type IV	Type V
Fig. 3(a)			Fig. 10(a)	Fig. 15

Fig. 16 Representative promolecules for characterizing a subset of *RS*-stereoisomeric groups, which is concerned with $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$. The two A's of **11** ($\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$, type IV) are successively replaced by other proligands to give other promolecules belonging to subgroups of $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$

which originally stems from the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$ in Eqs. 59–63, turns to stem from the isomorphic factor group $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}/\mathbf{C}_1$, which is isomorphic to $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}$ itself.

$$\text{Type I:SG}^{[\mathrm{I}]}_{\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}} = \left\{\overset{4}{\mathbf{C}_{\widehat{\sigma}}}\right\} \tag{110}$$

$$\text{Type II:SG}^{[\mathrm{II}]}_{\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}} = \left\{\overset{3}{\mathbf{C}_{\widetilde{\sigma}}}\right\} \tag{111}$$

$$\text{Type III:SG}^{[\mathrm{III}]}_{\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}} = \left\{\overset{1}{\mathbf{C}_{1}}\right\}, \tag{112}$$

$$\text{Type IV:SG}^{[\mathrm{IV}]}_{\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}} = \left\{\overset{14}{\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}}\right\} \tag{113}$$

$$\text{Type V:SG}^{[\mathrm{V}]}_{\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}} = \left\{\overset{5}{\mathbf{C}_{s}}\right\} \tag{114}$$

Let us examine the reference promolecule **11** of type IV (Fig. 16), which corresponds to the stereoisogram shown in Fig. 10a. The four substitution positions of **11** are divided in accord with the subduction shown in Eq. 106. Two A's occupy a two-membered homospheric orbit governed by $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_s)$, while a pair of p/$\overline{\text{p}}$ occupies a two-membered enantiospheric orbit governed by $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_{\widetilde{\sigma}})$.

As shown in Fig. 16, an appropriate substitution of the two A's of **11** (the pair of p/$\overline{\text{p}}$ is tentatively fixed) generates a derivative promolecule. This means that we take account of further subduction of the coset representation $\mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_s)$.

When one A at the position 4 of **11** is replaced by B, there appears the promolecule **16**′ of type V, which is homomeric to **16** shown in Fig. 15. This process corresponds to symmetry reduction from Eqs. 113 to 114. Thus, the subduction of Eq. 106 is further subduced into $\mathbf{C}_s$ as follows:

$$\begin{aligned}
&\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}} \downarrow \mathbf{C}_s \\
&\quad = \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_{\widetilde{\sigma}}) \downarrow \mathbf{C}_s + \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_s) \downarrow \mathbf{C}_s \\
&\quad = \mathbf{C}_s(/\mathbf{C}_1) + 2\mathbf{C}_s(/\mathbf{C}_s),
\end{aligned} \tag{115}$$

which is identical with the direct subduction $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_s$ (Eq. 105).

When one A at the position 4 of **11** is replaced by q, there appears the promolecule **19** of type III according to symmetry reduction into Eq. 112. Thus, the subduction of Eq. 106 is further subduced into $\mathbf{C}_1$ as follows:

$$\begin{aligned}
&\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}} \downarrow \mathbf{C}_1 \\
&\quad = \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_{\widetilde{\sigma}}) \downarrow \mathbf{C}_1 + \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_s) \downarrow \mathbf{C}_1 \\
&\quad = 4\mathbf{C}_1(/\mathbf{C}_1)
\end{aligned} \tag{116}$$

which is identical with the direct subduction $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_1$ (cf. the first row of Table 3 in Part I).

When two A's at the positions 2 and 4 of **11** are replaced by two q's, there appears the promolecule **18** of type II according to symmetry reduction into Eq. 111. Thus, the subduction of Eq. 106 is further subduced into $\mathbf{C}_{\widetilde{\sigma}}$ as follows:

$$\begin{aligned}
&\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}} \downarrow \mathbf{C}_{\widetilde{\sigma}} \\
&\quad = \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_{\widetilde{\sigma}}) \downarrow \mathbf{C}_{\widetilde{\sigma}} + \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_s) \downarrow \mathbf{C}_{\widetilde{\sigma}} \\
&\quad = \mathbf{C}_{\widetilde{\sigma}}(/\mathbf{C}_1) + 2\mathbf{C}_{\widetilde{\sigma}}(/\mathbf{C}_{\widetilde{\sigma}}),
\end{aligned} \tag{117}$$

which is identical with the direct subduction $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_{\widetilde{\sigma}}$ (cf. the third row of Table 3 in Part I).

When two A's at the positions 2 and 4 of **11** are replaced by a pair of q/$\overline{\text{q}}$, there appears the promolecule **3** of type I, the stereoisogram of which is shown in Fig. 3a. This process corresponds to symmetry reduction into Eq. 110. Thus, the subduction of Eq. 106 is further subduced into $\mathbf{C}_{\widehat{\sigma}}$ as follows:

$$\begin{aligned}
&\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}} \downarrow \mathbf{C}_{\widehat{\sigma}} \\
&\quad = \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_{\widetilde{\sigma}}) \downarrow \mathbf{C}_{\widehat{\sigma}} + \mathbf{C}_{s\widetilde{\sigma}\widehat{\sigma}}(/\mathbf{C}_s) \downarrow \mathbf{C}_{\widehat{\sigma}} \\
&\quad = 2\mathbf{C}_{\widehat{\sigma}}(/\mathbf{C}_1)
\end{aligned} \tag{118}$$

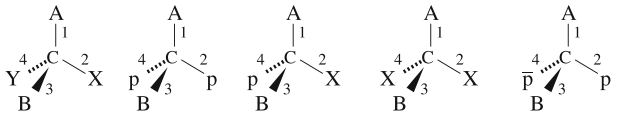
which is identical with the direct subduction $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}(/\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}) \downarrow \mathbf{C}_{\widehat{\sigma}}$ (Eq. 109).

6.2 Subset concerning $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$

The *RS*-stereoisomeric group $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$ of order 4 (Eq. 81) is characterized by a subset of *RS*-stereoisomeric groups collected in Eqs. 119–123, which are constructed by selecting the subgroups of $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$ from Eqs. 59–63. The categorization to types I–V is now considered to stem from the factor group $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}/\mathbf{C}_1$, which is isomorphic to $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$ itself.

$$\text{Type I:}\mathrm{SG}^{[\mathrm{I}]}_{\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{6}{\mathbf{C}_{\widehat{I}}} \right\} \tag{119}$$

$$\text{Type II:}\mathrm{SG}^{[\mathrm{II}]}_{\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{3}{\mathbf{C}_{\widetilde{\sigma}}} \right\} \tag{120}$$



2	**20**	**9′**	**21**	**16**
$\mathbf{C}_{\widehat{I}}$	$\mathbf{C}_{\widetilde{\sigma}}$	$\mathbf{C}_1$	$\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$	$\mathbf{C}_s$
Type I	Type II	Type III	Type IV	Type V
Fig. 2		Fig. 8	cf. **10** of Fig. 9	Fig. 15

Fig. 17 Representative promolecules for characterizing a subset of *RS*-stereoisomeric groups, which is concerned with $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$. The two X's of **21** ($\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$, type IV) are successively replaced by other proligands to give other promolecules belonging to subgroups of $\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}$

$$\text{Type III:SG}^{[\text{III}]}_{\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{1}{\mathbf{C}_1} \right\} \tag{121}$$

$$\text{Type IV:SG}^{[\text{IV}]}_{\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{16}{\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}} \right\} \tag{122}$$

$$\text{Type V:SG}^{[\text{V}]}_{\mathbf{C}_{s\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{5}{\mathbf{C}_s} \right\} \tag{123}$$

Let us examine the reference promolecule **21** of type IV (Fig. 17), which has the constitution ABX^2 in place of A^2BX of **10** (Fig. 9). Note that the constitutions ABX^2 and A^2BX are ascribed to the same partition $[\theta]_6 = [2, 1, 1, 0; 0, 0, 0, 0, 0, 0, 0, 0]$ (cf. Eq. 95 of Part I). As shown in Fig. 17, an appropriate substitution of two X's of **21** (A and B are tentatively fixed) generates a derivative promolecule.

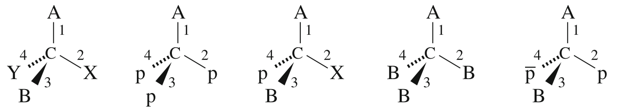
When the two X's of **21** are replaced by a pair of p/$\overline{\text{p}}$, there appears the promolecule **16** of type V, the stereoisogram of which is shown in Fig. 15. This process obeys Eq. 123. When one X at the position 4 of **21** is replaced by p, there appears the promolecule **9′** of type III, which is homomeric to **9** shown in Fig. 8. This process obeys Eq. 121. When the two X's at the positions 2 and 4 of **21** are replaced by two p's, there appears the promolecule **20** of type II according to Eq. 120. When one X at the position 4 of **21** is replaced by Y, there appears the promolecule **2** of type I, the stereoisogram of which is shown in Fig. 2. This process obeys Eq. 119.

6.3 Subset concerning $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$

The *RS*-stereoisomeric group $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$ of order 12 (Eq. 96) is characterized by a subset of *RS*-stereoisomeric groups collected in Eqs. 124–128, which are constructed by selecting the subgroups of $C_{3v\widetilde{\sigma}\widehat{I}}$ from Eqs. 59–63. The categorization to types I–V stems from the factor group $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}/\mathbf{C}_3$, which is isomorphic to the factor group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}/\mathbf{T}$.

$$\text{Type I: SG}^{[\text{I}]}_{\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{6}{\mathbf{C}_{\widehat{I}}}, \overset{19}{\mathbf{C}_{3\widehat{I}}} \right\} \tag{124}$$

$$\text{Type II: SG}^{[\text{II}]}_{\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{3}{\mathbf{C}_{\widetilde{\sigma}}}, \overset{17}{\mathbf{C}_{3\widetilde{\sigma}}} \right\} \tag{125}$$



2	**22**	**9′**	**23**	**16**
$\mathbf{C}_{\widehat{I}}$ ($\subset \mathbf{C}_{3\widehat{I}}$)	$\mathbf{C}_{3\widetilde{\sigma}}$	$\mathbf{C}_1$ ($\subset \mathbf{C}_3$)	$\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$	$\mathbf{C}_s$ ($\subset \mathbf{C}_{3v}$)
Type I	Type II	Type III	Type IV	Type V
Fig. 2	cf. **6** of Fig. 6	Fig. 8	cf. **14** of Fig. 13	Fig. 15

Fig. 18 Representative promolecules for characterizing a subset of *RS*-stereoisomeric groups, which is concerned with $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$. The three B's of **23** ($\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$, type IV) are successively replaced by other proligands to give other promolecules belonging to subgroups of $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$

$$\text{Type III: } \mathrm{SG}^{[\mathrm{III}]}_{\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{1}{\mathbf{C}}_1, \overset{7}{\mathbf{C}}_3 \right\} \tag{126}$$

$$\text{Type IV: } \mathrm{SG}^{[\mathrm{IV}]}_{\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{16}{\mathbf{C}}_{s\widetilde{\sigma}\widehat{I}}, \overset{28}{\mathbf{C}}_{3v\widetilde{\sigma}\widehat{I}} \right\} \tag{127}$$

$$\text{Type V: } \mathrm{SG}^{[\mathrm{V}]}_{\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}} = \left\{ \overset{5}{\mathbf{C}}_s, \overset{18}{\mathbf{C}}_{3v} \right\} \tag{128}$$

Note that Eqs. 124–128 cover all of the 10 subgroups contained in the non-redundant SSG of $\mathbf{C}_{3v\widetilde{\sigma}\widehat{I}}$. However, this does not always hold true. A subset of *RS*-stereoisomeric groups (e.g., for $\mathbf{C}_{2v\widetilde{\sigma}\widehat{I}}$) may not cover the corresponding SSG, because the SSG of the supergroup (e.g., $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$) may suffer from conjugacy.

Let us examine the reference promolecule **23** of type IV (Fig. 18), which has the constitution AB^3 in place of A^3B of **14** (Fig. 13). Note that the constitutions AB^3 and A^3B correspond to the same constitution $[\theta]_2 = [3, 1, 0, 0; 0, 0, 0, 0, 0, 0, 0, 0]$ (cf. Eq. 91 of Part I). As shown in Fig. 18, an appropriate substitution of three B's of **23** (A is tentatively fixed) generates a derivative promolecule.

When the two B's at the 2- and 4-positions of **23** are replaced by a pair of p/$\overline{\mathrm{p}}$, there appears the promolecule **16** of type V, the stereoisogram of which is shown in Fig. 15. This process obeys Eq. 128. When the two X's at the positions 2 and 4 of **23** are replaced by Xp, there appears the promolecule **9′** of type III, which is homomeric to **9** shown in Fig. 8. This process obeys Eq. 126, where there emerges no promolecule of the *RS*-stereoisomeric group $\mathbf{C}_3$. When the three B's at the positions 2, 3, and 4 of **23** are replaced by three p's, there appears the promolecule **22** of type II according to Eq. 125. When the two B's at the positions 2 and 4 of **23** are replaced by XY, there appears the promolecule **2** of type I, the stereoisogram of which is shown in Fig. 2. This process obeys Eq. 124, where there emerges no promolecule of the *RS*-stereoisomeric group $\mathbf{C}_{3\widehat{I}}$.

7 Conclusion

The PCI method of the USCI approach [1] is applied to the symmetry-itemized enumeration of quadruplets of stereoisograms, where the *RS*-stereoisomeric group $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$ is used to characterize the tetrahedral skeleton **1** (Fig. 1). The resulting numbers of quadruplets are itemized in terms of subgroups of $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$, which are further categorized into five types. Stereoisograms of types I–V are ascribed to subgroups of $\mathbf{T}_{d\widetilde{\sigma}\widehat{I}}$, where their features are discussed in comparison between *RS*-stereoisomeric groups and point groups.

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