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SUBDUCTION OF COSET REPRESENTATIONS. AN APPLICATION TO ENUMERATION OF CHEMICAL STRUCTURES WITH ACHIRAL AND CHIRAL LIGANDS

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Abstract

Molecules derived from a parent skeleton are enumerated where both achiral ligands as well as chiral ligands are allowed. Chirality fittingness of an orbit is proposed in order to permit chiral ligands. The enumeration is conducted with and without consideration of obligatory minimum valency (OMV). The effect of the OMV is formulated by assigning different weights to the respective orbits of the parent skeleton. The importance of coset representations and their subduction by subgroups is discussed. The subduced representations are classified into three classes through their chirality fittingness, which determines the mode of substitution with chiral and achiral ligands. Several novel concepts such as a unit subduced cycle index and a subduced cycle index are given in general forms.

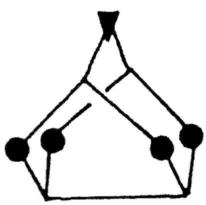
1. Introduction

Enumerations of chemical structures have long been studied by using Pólya's theorem, which dates back to the 1930s [1]. In the early 1970s, Ruch [2] pointed out that double cosets are useful in enumeration problems. More recently, Hässelbarth [3] reported an excellent method that utilizes a table of marks. Brocas [4] dealt with such problems by using another formulation which is related to double cosets and framework groups [5]. Mead [6] discussed the relationship between these methods, and pointed out the merits of Hässelbarth's approach.

In a previous paper [7], we discussed subduction of coset representations (SCR) and presented the SCR notation for a systematic classification of molecular symmetry. In addition, we pointed out that several related concepts, e.g. unit subduced cycle indices (USCIs) and the USCIs with chirality fittingness (USCI-CFs), are useful for *qualitative* discussions on molecular symmetry. In continuation of the work, this paper clarifies their meanings (especially that of chirality fittingness) and deals with a *quantitative* application of the USCI(-CF)s to enumeration problems.

2. Orbits specified by coset representations and obligatory minimum valencies

If a skeleton of a given symmetry is considered to be a chemical objective, the positions of the skeleton are classified into several sets (orbits) of equivalent positions. For example, noradamantane (**1**) has four orbits when we consider the carbon skeleton only. Similarly, both adamantane (**2**) and iceane (**3**) have two orbits. For the purpose of enumerating chemical structures, it is necessary to clarify the symmetrical behavior of such orbits.



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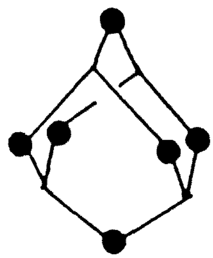

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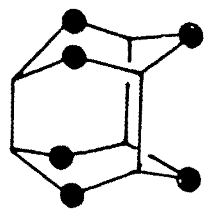

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This task is accomplished by considering a coset representation (appendix A). We use the symbol $G(/G_i)$ to denote a coset representation (CR) of G by a subgroup G_i. The following theorem has already been proved in Burnside's excellent book [8].

THEOREM 1

Any permutation representation P_G of a finite group G acting on $\Delta = \{\delta_1, \delta_2, \ldots, \delta_{|\Delta|}\}$ can be reduced into transitive CRs in accord with the following equation:

$$P_G = \sum_{i=1}^{s} \alpha_i G(/G_i). \tag{1}$$

The multiplicities (α_i) are non-negative integers, which are obtained as solutions of the following equation:

$$\mu_j = \sum_{i=1}^{s} \alpha_i m_{ij}, \quad j = 1, 2, \ldots, s, \tag{2}$$

where μ_j is the mark (the number of fixed points) of G_j in P_G. The symbol m_{ij} denotes the mark of G_j in $G(/G_i)$.

In chemical applications, the G-set (Δ) is regarded as a set of positions contained in a skeleton. Equation (1) divides the set into orbits in the manner that a transitive

$G(/G_i)$ acts on each of the α_i orbits, $\Delta_{i1}, \Delta_{i2}, \ldots$, and $\Delta_{i\alpha_i}$ $(i = 1, 2, \ldots, s)$, the respective length of which is equal to $|G|/|G_i|$. The total number of such orbits is

$$\sum_{i=1}^{s} \alpha_i .$$

For an illustration of theorem 1, appendix B deals with a trigonal pyramid of C_{3v} symmetry. This calculation requires a table of marks such as that listed in table 1. The concrete forms of coset representations for the C_{3v} group are found in table 2.

Table 1

Mark table of C_{3v}

	C_1	C_s	C_3	C_{3v}
$C_{3v}(/C_1)$	6	0	0	0
$C_{3v}(/C_s)$	3	1	0	0
$C_{3v}(/C_3)$	2	0	2	0
$C_{3v}(/C_{3v})$	1	1	1	1

Table 2

Coset representations of C_{3v}

C_{3v}	$C_{3v}(/C_1)$	$C_{3v}(/C_s)$	$C_{3v}(/C_3)$	$C_{3v}(/C_{3v})$
I	(1) (2) (3) (4) (5) (6)	(1) (2) (3)	(1) (2)	(1)
C_3	(1 2 3) (4 5 6)	(1 2 3)	(1) (2)	(1)
C_3^2	(1 3 2) (4 6 5)	(1 3 2)	(1) (2)	(1)
$\sigma_{v(1)}$	(1 4) (2 6) (3 5)	(1) (2 3)	(1 2)	(1)
$\sigma_{v(2)}$	(1 5) (2 4) (3 6)	(1 2) (3)	(1 2)	(1)
$\sigma_{v(3)}$	(1 6) (2 5) (3 4)	(1 3) (2)	(1 2)	(1)

In the present enumeration of chemical structures, a molecule is considered to be a derivative of a given skeleton with appropriate ligands (or atoms) on its positions (vertices). From this point of view, it is necessary to consider an obligatory minimum valency (OMV) inherent in each position of the skeleton. The OMV is the degree of the position in a graph-theoretical sense [9,10]. For example, in the noradamantane skeleton (**1**), two orbits (methylene bridges marked by heavy dots and by a small triangle) have an OMV = 2, which indicates the capability of taking C, N, and O from a set of C, N, and O atoms. The bridgehead positions of **1** construct two orbits, which have an OMV = 3. This means that these positions take C and N but no O.

Thus, the OMV restricts the mode of substitution at a position, in which the position is incapable of taking an atom or a ligand that has a valency less than its OMV. Hence, we should take the OMV into account in enumerations of molecules. Since positions of an orbit have the same OMV, the effect of the OMV can be formulated by assigning a different (or, more strictly, an independent) weight to every orbit of a parent skeleton.

3. Chirality fittingness of an orbit

This section discusses another chemical explanation of coset representations (CRs) and affords a foundation to the concept of chirality fittingness. The discussion stems from the relationship between a regular representation (RR) and other CRs.

A regular representation $G(/G_1)$ on $\Delta = \{\delta_1, \delta_2, \ldots, \delta_{|\Delta|}\}$, where $G_1 = C_1$ and $|\Delta| = |G|$, is a faithful representation of G acting on Δ. Let G_j be a subgroup of G. We then define a subduced representation of the RR, $G(/G_1)$, by G_j as a representation in which elements associated only with G_j are selected from $G(/G_1)$. Let the symbol $G(/G_1)\downarrow G_j$ denote the subduced representation. Since the regular representation $G(/G_1)$ is transitive, the domain (Δ) contains only one orbit. However, the subduced representation $G(/G_1)\downarrow G_j$ acting on Δ is generally intransitive and hence can be reduced by the following set of equations,

$$G(/G_1)\downarrow G_j = (|G|/|G_j|)G_j(/H_1^{(j)}) \quad \text{for } j = 1, 2, \ldots, s, \tag{3}$$

where $H_1^{(j)}$ is an identity representation (appendix C). Equation (3) indicates that the domain Δ is partitioned into $|G|/|G_j|$ sub-orbits, $\omega_1, \omega_2, \ldots, \omega_r$, on each of which $G_j(/H_1^{(j)})$ act. Since $r = |G|/|G_j|$, the length of each orbit is equal to $|G_j|$. If we take $\Omega_1 = \omega_1$, we can construct a system of imprimitive blocks, $\Gamma = \{\Omega_1, \Omega_2, \ldots, \Omega_r\}$, where $t_\tau\Omega_1 = \Omega_\tau$ for $\exists t_\tau \in G$ (appendices D and E).

As an illustration, let us examine a coset representation $C_{3v}(/C_s)$, which is shown explicitly in table 2. First, the corresponding regular representation $C_{3v}(/C_1)$ is subduced with respect to C_s. Thus, the subduced representation $C_{3v}(/C_1)\downarrow C_s = \{(1)(2)(3)(4)(5)(6), (1\ 4)(2\ 6)(3\ 5)\}$ creates a partition of the domain $\Delta = \{1, 2, 3, 3, 5, 6\}$ into three orbits, i.e. $\Delta_1 = \{1, 4\}$, $\Delta_2 = \{2, 6\}$, $\Delta_3 = \{3, 5\}$. This can be done by using eqs. (1) and (2), but it is easy to obtain the result directly in the present case. If we select $\Omega_1 = \Delta_1 = \{1, 4\}$ and the stabilizer C_s, the corresponding coset partition is $C_{3v} = C_s + C_sC_3 + C_sC_3^2$. This equation affords a system of imprimitive blocks, $\Gamma = \{\Omega_1, \Omega_2, \Omega_3\}$, where $\Omega_2 = C_3\Omega_1 = \{2, 5\}$ and $\Omega_3 = C_3^2\Omega = \{3, 6\}$ (appendix E). The representation $C_{3v}(/C_s)$ can be considered to act on Γ. If we select orbits other than Ω_1, other systems of imprimitive blocks are obtained. These results are illustrated in fig. 1, in which benzene is regarded as cyclohexa-1,3,5-triene with two different faces (i.e. so-called polarized cyclohexa-1,3,5-triene) which has C_{3v} symmetry. The relationship between G and G_j that appears in a CR ($G/(G_j)$) controls the mode of substitution on the corresponding

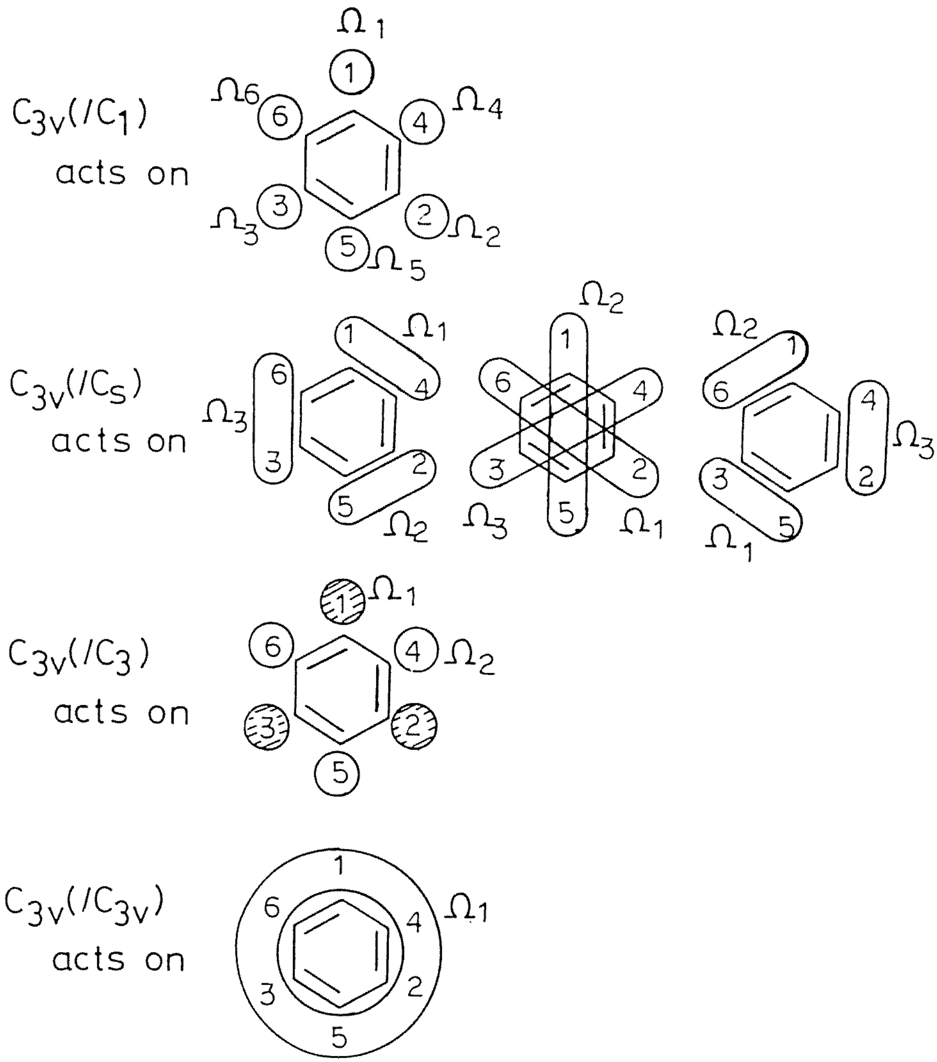

Fig. 1. Action of coset representations on blocks in a $C_{3v}(/C_1)$ set.

orbit. this mode is clarified by examining the action of $G(/G_j)$ on $\Gamma = \{\Omega_1, \Omega_2, \ldots, \Omega_r\}$. Thus, the discussions shown in appendix F afford the following theorem concerned with chirality fittingness.

THEOREM 2

A coset representation $G(/G_j)$ can act on:

(a) a domain that takes only achiral ligands, if both G and $G_j \leq G$ contain improper rotations (an achiral part);

(b) a domain that takes achiral as well as chiral ligands, if both $\boldsymbol{G}$ and $\boldsymbol{G}_j \leq \boldsymbol{G}$ contain only proper rotations (a neutral part); and

(c) a domain that takes achiral as well as chiral ligands, if $\boldsymbol{G}$ contains improper rotations and $\boldsymbol{G}_j$ contains only proper rotations (a chiral part).

4. Subduced representations of a coset representation

Let us consider a subduced representation (SR), $\boldsymbol{G}(/\boldsymbol{G}_i)\downarrow\boldsymbol{G}_j$, where $\boldsymbol{G}_i \leq \boldsymbol{G}$ and $\boldsymbol{G}_j \leq \boldsymbol{G}$. This SR is a permutation representation of $\boldsymbol{G}_j$ and acts on each orbit $\Delta_{i\alpha}$ ($\alpha = 1, 2, \ldots, \alpha_i$) in an intransitive fashion. Hence, the orbit ($\Delta_{i\alpha}$) is subdivided into the corresponding sub-orbits on the action of $\boldsymbol{G}(/\boldsymbol{G}_i)\downarrow\boldsymbol{G}_j$ on $\Delta_{i\alpha}$ in the same manner as discussed for theorem 1 (eqs. (1) and (2)). Thus, we end up with:

COROLLARY 1-1

$$\boldsymbol{G}(/\boldsymbol{G}_i)\downarrow\boldsymbol{G}_j = \sum_{k=1}^{\upsilon_j} \beta_k^{(ij)} 2\boldsymbol{G}_j(/\boldsymbol{H}_k^{(j)}) \quad \text{for } i = 1, 2, \ldots, s \text{ and } j = 1, 2, \ldots, s, \tag{4}$$

where $\boldsymbol{H}_k^{(j)}$ denotes a subgroup of a conjugacy class of $\boldsymbol{G}_j$; $\boldsymbol{G}_j(/\boldsymbol{H}_k^{(j)})$ is the CR of $\boldsymbol{G}_j$ by $\boldsymbol{H}_k^{(j)}$; $\beta_k^{(ij)}$ are non-negative integers; and υ_j is the number of conjugacy classes of subgroups. The multiplicities $\beta_k^{(ij)}$ are calculated by the equation

$$v_l = \sum_{k=1}^{\upsilon_j} \beta_k^{(ij)} m_{kl}^{(j)}, \qquad l = 1, 2, \ldots, \upsilon_j, \tag{5}$$

where v_l is the mark of $\boldsymbol{H}_l^{(j)}$ in $\boldsymbol{G}(/\boldsymbol{G}_i)\downarrow\boldsymbol{G}_j$.

Figure 2 shows a division and subdivision during the actions of $\boldsymbol{G}$ and $\boldsymbol{G}(/\boldsymbol{G}_i)\downarrow\boldsymbol{G}_j$. The division of Δ by $\boldsymbol{G}$ affords orbits $\Delta_{i\alpha}$ ($i = 1, 2, \ldots, s$ and $\alpha = 1, 2, \ldots, \alpha_i$) in the light of eq. (1). The subdivision of $\Delta_{i\alpha}$ into the corresponding sub-orbits is accomplished in terms of eq. (4). Table 3 summarizes the subductions of CRs for $\boldsymbol{C}_{3v}$.

When we apply theorem 2 to $\boldsymbol{G}_j(/\boldsymbol{H}_k^{(j)})$, we obtain the following corollary concerned with chirality fittingness.

COROLLARY 2.1

A coset representation $\boldsymbol{G}_j(/\boldsymbol{H}_k^{(j)})$ can act on:

(a) a sub-orbit that takes only achiral ligands, if both $\boldsymbol{G}_j$ and $\boldsymbol{H}_k^{(j)} \leq \boldsymbol{G}_j$ contain improper rotations (an achiral part);

(b) a sub-orbit that takes achiral as well as chiral ligands, if both $\boldsymbol{G}_j$ and $\boldsymbol{H}_k^{(j)} \leq \boldsymbol{G}_j$ contain only proper rotations (a neutral part); and

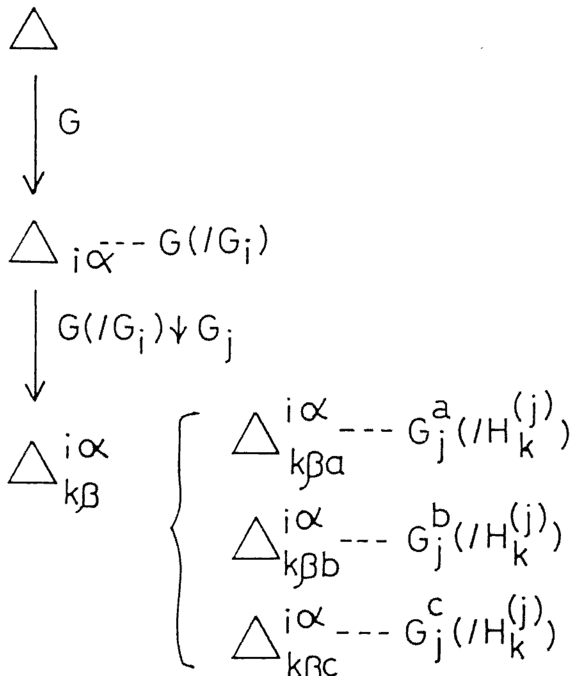

Fig. 2. Orbits and sub-orbits in subduction of coset representation.

Table 3

The subduction of $C_{3v}(/G_i)\downarrow G_j$

i \ j	C_1	C_s	C_3	C_{3v}
$C_{3v}(/C_1)$	$6C_1(/C_1)$	$3C_s(/C_1)$	$2C_3(/C_1)$	$C_{3v}(/C_1)$
$C_{3v}(/C_s)$	$3C_1(/C_1)$	$C_s(/C_1) + C_s(/C_s)$	$C_3(/C_1)$	$C_{3v}(/C_s)$
$C_{3v}(/C_3)$	$2C_1(/C_1)$	$C_s(/C_1)$	$2C_3(/C_3)$	$C_{3v}(/C_3)$
$C_{3v}(/C_{3v})$	$C_1(/C_1)$	$C_s(/C_s)$	$C_3(/C_3)$	$C_{3v}(/C_{3v})$

(c) a sub-orbit that takes achiral as well as chiral ligands, if G_j contains improper rotations and $H_k^{(j)} \leq G_j$ contains only proper rotations (a chiral part).

In order to simplify notations, we use the following formal expression containing achiral, neutral, and chiral parts:

$$G_j(/H_k^{(j)}) = \chi_{ak}^{(j)} G_j^{(a)}(H_k^{(j)}) + \chi_{bk}^{(j)} G_j^{(b)}(/H_k^{(j)}) + \chi_{ck}^{(j)} G_j^{(c)}(/H_k^{(j)}), \quad (6)$$

where $\chi_{ak}^{(j)} + \chi_{bk}^{(j)} + \chi_{ck}^{(j)} = 1$ and $\chi_{ak}^{(j)}$, $\chi_{bk}^{(j)}$, and $\chi_{ck}^{(j)}$ are all non-negative integers. The superscripts (a, b, and c) denote achiral, neutral, and chiral parts. The right-hand side of this equation indicates that only one of the three parts is effective.

In the light of this notation, eq. (4) is replaced by eq. (7), which affords a decomposition into achiral, neutral, and chiral parts:

$$G(/G_i) \downarrow G_j = \sum_{k=1}^{v_j} \chi_{ak}^{(j)} \beta_k^{(ij)} G_j^{(a)}(/H_k^{(j)}) + \sum_{k=1}^{v_j} \chi_{bk}^{(j)} \beta_k^{(ij)} G_j^{(b)}(/H_k^{(j)}) + \sum_{k=1}^{v_j} \chi_{ck}^{(j)} \beta_k^{(ij)} G_j^{(c)}(/H_k^{(j)}), \quad \text{for } i = 1, 2, \ldots, s \text{ and } j = 1, 2, \ldots, s. \tag{7}$$

The resulting sub-orbits are classified into three categories, i.e. $\Delta_{k\beta a}^{i\alpha}$, $\Delta_{k\beta b}^{i\alpha}$, and $\Delta_{k\beta c}^{i\alpha}$, which are acted on by $G_j^{(a)}(/H_k^{(j)})$, $G_j^{(b)}(/H_k^{(i)})$ and $G_j^{(c)}(/H_k^{(j)})$, respectively. We call the sub-orbits G_j- achiral, G_j-neutral, and G_j-chiral sub-orbits, respectively.

The degree of $G_j^{(\$)}(/H_k^{(j)})$ is $d_{jk} = |G_j|/|H_k^{(j)}|$, in which $\$$ denotes a, b, or c for achiral, neutral, or chiral, respectively. This is equal to the length of each subdivided orbit $\Delta_{k\beta\$}^{i\alpha}$ ($\beta = 1, 2, \ldots, \beta_k^{(ij)}$). We then assign a variable $\$_{d_{jk}}$ to the sub-orbit $\Delta_{k\beta\$}^{i\alpha}$ on which $G_j^{(\$)}(/H_k^{(j)})$ acts. Since the multiplicity of this orbit is $\beta_k^{(ij)}$, a variable for the sub-orbit $\Delta_{k\beta}^{i\alpha}$ is represented by

$$\left(a_{d_{jk}}^{(\alpha)}\right)^{\chi_{ak}^{(j)}\beta_k^{(ij)}} \left(b_{d_{jk}}^{(\alpha)}\right)^{\chi_{bk}^{(j)}\beta_k^{(ij)}} \left(c_{d_{jk}}^{(\alpha)}\right)^{\chi_{ck}^{(j)}\beta_k^{(ij)}}. \tag{8}$$

It should be noted that only one of the three terms is effective in the light of $\chi_{ak}^{(j)}$, $\chi_{bk}^{(j)}$, and $\chi_{ck}^{(j)}$.

By using the variables represented by eq. (8), we arrive at:

DEFINITION 1

(Unit subduced cycle index with chirality fittingness (USCI-CF).)

$$Z(G(/G_i) \downarrow G_j;\ a, b, c) = \prod_{k=1}^{v_j} \left[\left(a_{d_{jk}}^{(\alpha)}\right)^{\chi_{ak}^{(j)}\beta_k^{(ij)}} \left(b_{d_{jk}}^{(\alpha)}\right)^{\chi_{bk}^{(j)}\beta_k^{(ij)}} \left(c_{d_{jk}}^{(\alpha)}\right)^{\chi_{ck}^{(j)}\beta_k^{(ij)}} \right]. \tag{9}$$

The sum of the powers in each of the parts of eq. (9) is also useful to enumerate organic structures. We define

$$\beta_{ij}^{(a)} = \sum_{k=1}^{v_j} \chi_{ak}^{(j)} \beta_k^{(ij)}, \tag{10}$$

$$\beta_{ij}^{(b)} = \sum_{k=1}^{v_j} \chi_{bk}^{(j)} \beta_k^{(ij)}, \tag{11}$$

and

$$\beta_{ij}^{(c)} = \sum_{k=1}^{v_j} \chi_{ck}^{(j)} \beta_k^{(ij)}, \tag{12}$$

which are the numbers of sub-orbits of the respective chiralities. These are summarized in the form of

$$\left(\beta_{ij}^{(a)}, \beta_{ij}^{(b)}, \beta_{ij}^{(c)}\right).$$

We call this term the *orbit index* for the SCR. The data of table 3 provide tables 4 and 5 for the C_{3v} group by this procedure.

Table 4

Unit subduced cycle index for $C_{3v}(/G_i)\downarrow G_j$

$i \backslash j$	C_1	C_s	C_3	C_{3v}
$C_{3v}(/C_1)$	b_1^6	c_2^3	b_3^2	c_6
$C_{3v}(/C_s)$	b_1^3	a_1c_2	b_3	a_3
$C_{3v}(/C_3)$	b_1^2	c_2	b_1^2	c_2
$C_{3v}(/C_{3v})$	b_1	a_1	b_1	c_1

Table 5

$(\beta_{ij}^{(a)}, \beta_{ij}^{(b)}, \beta_{ij}^{(c)})$ for $C_{3v}(/G_i)\downarrow G_j$

$i \backslash j$	C_1	C_s	C_3	C_{3v}
$C_{3v}(/C_1)$	(0,6,0)	(0,0,3)	(0,2,0)	(0,0,1)
$C_{3v}(/C_s)$	(0,3,0)	(1,0,1)	(0,1,0)	(1,0,0)
$C_{3v}(/C_3)$	(0,2,0)	(0,0,1)	(0,2,0)	(0,0,1)
$C_{3v}(/C_{3v})$	(0,1,0)	(1,0,0)	(0,1,0)	(1,0,0)

5. Orbits of configuration and their symmetries

Let $\Delta = \{\delta_1, \delta_2, \ldots, \delta_{|\Delta|}\}$ be a domain which consists of $|\Delta|$ elements called *positions*. Let $\boldsymbol{X} = \{X_1, X_2, \ldots, X_{|X|}\}$ be a co-domain which contains $|\boldsymbol{X}|$ elements called *figures*. In chemistry, the figures may be ligands or atoms. Suppose that f is a function (called a *configuration*), i.e. $f:\Delta \rightarrow X$. The mode of this mapping is restricted by the following weights:

$$w_{i\alpha}(X_r) \tag{13}$$

for $i = 1, 2, \ldots, s$, $\alpha = 1, 2, \ldots, \alpha_i$ and $r = 1, 2, \ldots, |X|$, which is assigned to each element X_r of the co-domain X in agreement with the behavior of each orbit $\Delta_{i\alpha}$. We then define a weight $W(f)$ for each function f.

DEFINITION 2

The weight of a function is represented by

$$W(f) = \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \prod_{\delta \in \Delta_{i\alpha}} w_{i\alpha}(f(\delta))$$

$$= \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \left[\prod_{\delta \in \Delta^{i\alpha}_{k\beta a}} w_{i\alpha}(f(\delta)) \prod_{\delta \in \Delta^{i\alpha}_{k\beta b}} w_{i\alpha}(f(\delta)) \prod_{\delta \in \Delta^{i\alpha}_{k\beta c}} w_{i\alpha}(f(\delta)) \right]. \tag{14}$$

The products in the parentheses of eq. (14) are monomials of total powers of $d_{jk}\beta_{ij}^{(a)}$, $d_{jk}\beta_{ij}^{(b)}$, and $d_{jk}\beta_{ij}^{(c)}$, respectively.

A set of all functions ($f: \Delta \rightarrow X$) is defined as

$$F = \{f_1, f_2, \ldots, f_\gamma, \ldots, f_\varepsilon, \ldots, f_{|F|}\}.$$

Suppose that a group G acts on domain $\Delta = \{\delta_1, \delta_2, \ldots, \delta_{|\Delta|}\}$ in the form of the corresponding permutation representation P_G on Δ and that the group G acts simultaneously on a co-domain $X = \{X_1, X_2, \ldots, X_{|X|}\}$ via a permutation group Q_G on X. For $P_g \in P_G$ and $Q_g \in Q_G$, a binary relation between f_γ ($\in F$) and f_ε ($\in F$) is defined as

$$Q_g f_\gamma(\delta) = f_\varepsilon(P_g(\delta)) \qquad \text{for } \forall\, \delta \in \Delta, \tag{15}$$

which holds for $\exists\, g \in G$. This binary relation is an equivalence relation. Hence, this affords a partition of the set (F) into equivalence classes. This type of action was discussed in detail by Hässelbarth [3]. In order to simplify our discussion, $Q_g(X_r)$ is an operation that keeps X_r invariant for a proper rotation $g \in G$, but gives its antipode ($X_r^{\#}$) for an improper rotation $g \in G$.

Let $\lambda_g : f_\varepsilon \rightarrow f_\gamma$ be a mapping corresponding to $g \in G$ and let Λ_G be a set containing all λ_g. Then, Λ_G is proved to be a permutation representation of G (appendix G). Hence, theorem 1 (eqs. (1) and (2)) also holds for this case.

THEOREM 3

Suppose that a group $\boldsymbol{G}$ acts on $\boldsymbol{F}$ by the simultaneous actions of $\boldsymbol{G}$ on Δ and $\boldsymbol{X}$. The action constructs a permutation representation Λ_G on $\boldsymbol{F}$. The multiplicity of each transitive coset representation $\boldsymbol{G}(/\boldsymbol{G}_i)$ in Λ_G is determined by

$$\Lambda_G = \sum_{i=1}^{s} B_i \boldsymbol{G}(/\boldsymbol{G}_i), \tag{16}$$

wherein B_i's are non-negative integers. The multiplicities B_i are obtained by solving the following equations:

$$\rho_j = \sum_{i=1}^{s} B_i m_{ij}, \quad \text{for } j = 1, 2, \ldots, s, \tag{17}$$

where ρ_j is the mark of $\boldsymbol{G}_j$ in Λ_G.

Each orbit corresponding to a transitive $\boldsymbol{G}(/\boldsymbol{G}_i)$ contains functions (configurations) of symmetry $\boldsymbol{G}_i$. Hence, B_i is the number of different configurations of symmetry $\boldsymbol{G}_i$.

The mark ρ_j is the number of fixed functions (configurations) of $\boldsymbol{F}$ with respect to $\boldsymbol{G}_j$. Suppose that an appropriate configuration $f^{(j)} \in \boldsymbol{F}$ is fixed to all the elements $g \in \boldsymbol{G}_j$. This requires

$$Q_g f^{(j)}(\delta) = f^{(j)}(P_g(\delta)), \quad \text{for } \forall\, \delta \in \Delta \quad \text{and} \quad \forall\, g \in \boldsymbol{G}_j. \tag{18}$$

Let us now go back to the division into orbits and the further subdivision into sub-orbits shown in fig. 2. Then, in order for $f^{(j)}$ ($\in \boldsymbol{F}$) to be constant with respect to eq. (18), all the positions of each sub-orbit have to take the same figure (or ligand) of suitable chirality. If the sub-orbit is an achiral part, there are $|X_{i\alpha}^{(a)}|$ ways of substitution for each sub-orbit $\Delta_{k\beta a}^{i\alpha}$, where $|X_{i\alpha}^{(a)}|$ is the number of non-zero $w_{i\alpha}(X_r)$ with achiral X_r for each sub-orbit $\Delta_{k\beta a}^{i\alpha}$. Since the number of sub-orbits is $\beta_{ij}^{(a)}$, the number of fixed configurations for chiral parts contained in $\Delta_{i\alpha}$ is represented by

$$\prod_{\alpha=0}^{\alpha_i} |X_{i\alpha}^{(a)}|^{\beta_{ij}^{(a)}}, \tag{19}$$

where $|X_{i0}^{(a)}| = 1$.

Similarly, the number of fixed configurations for a neutral part is obtained as follows:

$$\prod_{\alpha=0}^{\alpha_i} |X_{i\alpha}^{(b)}|^{\beta_{ij}^{(b)}}, \tag{20}$$

where $|X^{(b)}_{i0}| = 1$ and

$|X^{(b)}_{i\alpha}|$ = the number of non-zero $w_{i\alpha}(X_r)$ for each sub-orbit $\Delta^{i\alpha}_{k\beta b} = |X_{i\alpha}|$.

For counting the number of fixed configurations in a chiral part, a saturation of each orbit with chiral ligands is accomplished in either of the following two ways, due to its chirality fittingness:

c	c	. . .	c	c
c#	c#		c#	c#

or

c#	c#	. . .	c#	c#
c	c		c	c

Thus, we obtain

$$\prod_{\alpha=0}^{\alpha_i} |X^{(c)}_{i\alpha}|^{\beta^{(c)}_{ij}}, \tag{21}$$

where $|X^{(c)}_{i0}| = 1$ and

$|X^{(c)}_{i\alpha}|$ = the number of non-zero $w_{i\alpha}(X_r)$ with achiral X_r plus twice the number of non-zero $w_{i\alpha}(X_r)$ with chiral X_r (one of the antipodes) for each sub-orbit $\Delta^{i\alpha}_{k\beta c}$

= the number of non-zero $w_{i\alpha}(X_r)$ with achiral X_r and chiral X_r

= $|X_{i\alpha}|$.

The product of eqs. (19), (20) and (21) provides the number of fixed configurations for each orbit $\Delta_{i\alpha}$. A further multiplication of the products over all s is equal to ρ_j. Hence, the following corollary is derived from eq. (17):

COROLLARY 3-1

$$\prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \left[|X^{(a)}_{i\alpha}|^{\beta^{(a)}_{ij}} |X^{(b)}_{i\alpha}|^{\beta^{(b)}_{ij}} |X^{(c)}_{i\alpha}|^{\beta^{(c)}_{ij}} \right] = \sum_{i=1}^{s} B_i m_{ij}, \quad j = 1, 2, \ldots, s. \tag{22}$$

Since $|X^{(b)}_{i\alpha}| = |X^{(c)}_{i\alpha}| = |X_{i\alpha}|$, a simpler expression can be derived:

$$\prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \left[|X^{(a)}_{i\alpha}|^{\beta^{(a)}_{ij}} |X_{i\alpha}|^{\beta^{(b)}_{ij} + \beta^{(c)}_{ij}} \right] = \sum_{i=1}^{s} B_i m_{ij}, \quad j = 1, 2, \ldots, s. \tag{23}$$

Example 1. In appendix B, we have shown that the vertices {1, 2, 3, 4} of a trigonal pyramid (C_{3v}) are partitioned into two orbits, i.e. $\Delta_1 = \{4\}$ on which $\boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v})$ acts and $\Delta_2 = \{1, 2, 3\}$ on which $\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)$ acts (fig. 3).

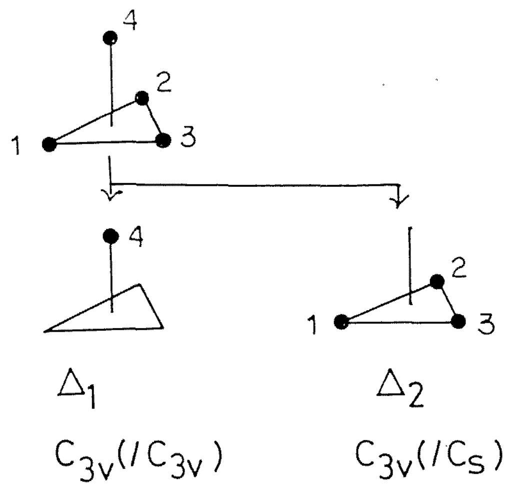

Fig. 3. Orbits of a trigonal pyramid.

Suppose that the orbit Δ_1 takes A, B, C and $C^{\#}$ and that the orbit Δ_2 can take A, C and $C^{\#}$, where C and $C^{\#}$ are antipodes to each other. For this purpose, we choose $\boldsymbol{X} = \{A, B, C, C^{\#}\}$ as a co-domain and determine the following weights:

$$w_1(A) = A,\ \ w_1(B) = B,\ \ w_1(C) = C,\ \ w_1(C^{\#}) = C^{\#}\ \text{ for }\ \Delta_1,\ \ \text{and}$$
$$w_2(A) = A,\ \ w_2(B) = 0,\ \ w_2(C) = C,\ \ w_2(C^{\#}) = C^{\#}\ \text{ for }\ \Delta_2.$$

In terms of these weights, the number of allowed ligands are obtained as follows:

$$|\boldsymbol{X}_1^{(a)}| = 2,\ \ |\boldsymbol{X}_1^{(b)}| = 4,\ \ \text{and}\ \ |\boldsymbol{X}_1^{(c)}| = 4\ \text{ for }\ \Delta_1,\ \ \text{and}$$
$$|\boldsymbol{X}_2^{(a)}| = 1,\ \ |\boldsymbol{X}_2^{(b)}| = 3,\ \ \text{and}\ \ |\boldsymbol{X}_2^{(c)}| = 3\ \text{ for }\ \Delta_2.$$

From table 5, we pick up the rows of $\boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v})$ and $\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)$. For example, (0,1,0) and (0,3,0) for the $\boldsymbol{C}_1$ column afford $\rho_{C_1} = 2^0 4^1 4^0 1^0 3^3 3^0 = 108$ by using the left-hand side of eq. (22). Similarly, we obtain

$$\rho_{C_s} = 2^1 1^1 3^1 = 6,\ \rho_{C_3} = 4^1 3^1 = 12\ \text{ and }\ \rho_{C_{3v}} = 2^1 1^1 = 2.$$

We then find eq. (22) for this case:

$$(108\ 6\ 12\ 2) = (B_{C_1}\ B_{C_s}\ B_{C_3}\ B_{C_{3v}}) \begin{bmatrix} 6 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 \\ 2 & 0 & 2 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}.$$

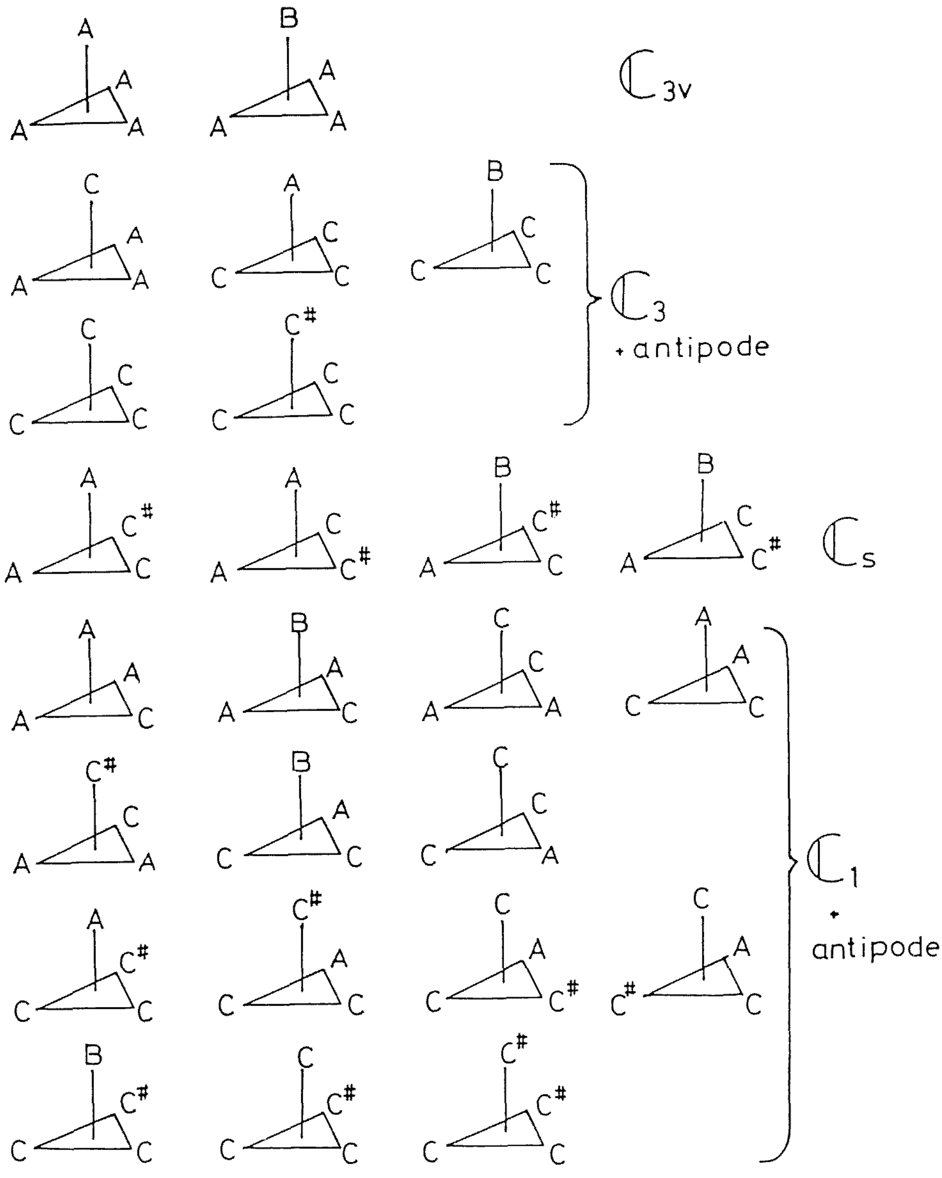

Fig. 4. Isomers based on a trigonal pyramid.

This provides

$$B_{C_1} = 14,\ B_{C_s} = 4,\ B_{C_3} = 5,\ \text{and}\ B_{C_{3v}} = 2.$$

Figure 4 lists the isomers derived by the enumeration of example 1.

6. Enumeration of configurations with a given symmetry as well as a given weight. The most general case which takes the OMV into consideration

In this section, we enumerate the number of configurations with a given symmetry as well as a given weight on the basis of a given skeleton. We start from:

LEMMA 1

Let $f_\gamma: \Delta \rightarrow \boldsymbol{X}$ and $f_\varepsilon: \Delta \rightarrow \boldsymbol{X}$ be equivalent. Then

$$W(f_\gamma) = W(f_\varepsilon), \tag{24}$$

where the weights are given by eq. (14) (appendix H).

Let $\boldsymbol{F}^{(\theta)}$ be a set of functions ($f: \Delta \rightarrow \boldsymbol{X}$), all of which have the same weight $W_\theta(f)$:

$$\boldsymbol{F}^{(\theta)} = \{f_1^{(\theta)}, f_2^{(\theta)}, \ldots, f_\gamma^{(\theta)}, \ldots, f_\varepsilon^{(\theta)}, \ldots, f_\psi^{(\theta)}\}, \tag{25}$$

where $\psi = |\boldsymbol{F}^{(\theta)}|$. Then, we can obtain a permutation:

$$\lambda_g^{(\theta)} = \begin{pmatrix} Q_g f_1^{(\theta)} P_g^{-1}, & \ldots, & Q_g f_\gamma^{(\theta)} P_g^{-1}, & \ldots, & Q_g f_\psi^{(\theta)} P_g^{-1} \\ f_1^{(\theta)} & , \ldots, & f_\gamma^{(\theta)} & , \ldots, & f_\psi^{(\theta)} \end{pmatrix}. \tag{26}$$

Let the symbol $\Lambda_{\boldsymbol{G}}^{(\theta)}$ denote the set of $\lambda_g^{(\theta)}$ for $g \in \boldsymbol{G}$. It can be proven that $\Lambda_{\boldsymbol{G}}^{(\theta)}$ is a permutation representation of $\boldsymbol{G}$ (appendix I) This result allows us to apply theorem 1 to $\Lambda_{\boldsymbol{G}}^{(\theta)}$. Thereby, we end up with:

THEOREM 4

$$\Lambda_{\boldsymbol{G}}^{(\theta)} = \sum_{i=1}^{s} B_{\theta i}\, \boldsymbol{G}\,(/\boldsymbol{G}_i), \tag{27}$$

and

$$\rho_{\theta j} = \sum_{i=1}^{s} B_{\theta i}\, m_{ij}, \quad j = 1, 2, \ldots, s. \tag{28}$$

The symbol $(B_{\theta i})$, which originally denotes the multiplicity of a transitive coset representation $(\boldsymbol{G}(/\boldsymbol{G}_i))$, also indicates the number of isomeric configurations with $\boldsymbol{G}_i$ symmetry as well as a weight W_θ. The values of the $B_{\theta i}$ can be calculated with eq. (28), if the marks $\rho_{\theta j}$ are estimated.

By using a fixed-point (FP) matrix $(\rho_{\theta j})$, an isomer-counting matrix $(B_{\theta i})$, and a mark table (m_{ij}), eq. (28) can be alternatively expressed as follows:

$$\underset{(\rho_{\theta j})}{\begin{pmatrix} \rho_{11} & \cdots & \rho_{1j} & \cdots & \rho_{1s} \\ \rho_{21} & \cdots & \rho_{2j} & \cdots & \rho_{2s} \\ & & \cdots & & \\ \rho_{\theta 1} & \cdots & \rho_{\theta j} & \cdots & \rho_{\theta s} \\ & & \cdots & & \\ \rho_{|\theta|1} & \cdots & \rho_{|\theta|j} & \cdots & \rho_{|\theta|s} \end{pmatrix}} = \underset{(B_{\theta i})}{\begin{pmatrix} B_{11} & \cdots & B_{1s} \\ B_{21} & \cdots & B_{2s} \\ & \cdots & \\ & \cdots & \\ & \cdots & \\ B_{|\theta|1} & \cdots & B_{|\theta|s} \end{pmatrix}} \underset{(m_{ij})}{\begin{pmatrix} m_{11} & \cdots & m_{1s} \\ m_{22} & \cdots & m_{2s} \\ & \cdots & \\ m_{s1} & \cdots & m_{ss} \end{pmatrix}}. \tag{29}$$

The next task is the evaluation of $\rho_{\theta j}$. Let us now define a subduced cycle index with chirality fittingness using eq. (9).

DEFINITION 3

A subduced cycle index with chirality fittingness (SCI-CF) is defined as

$$\begin{aligned} Z(\mathbf{G}_j\,;\, a, b, c) &= \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} Z(\mathbf{G}\,(/\mathbf{G}_i) \downarrow \mathbf{G}_j\,;\, a, b, c) \\ &= \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \prod_{k=1}^{v_j} \left[\left(a_{d_{jk}}^{(\alpha)}\right)^{\chi_{ak}^{(j)} \beta_k^{(ij)}} \left(b_{d_{jk}}^{(\alpha)}\right)^{\chi_{bk}^{(j)} \beta_k^{(ij)}} \left(c_{d_{jk}}^{(\alpha)}\right)^{\chi_{ck}^{(j)} \beta_k^{(ij)}} \right], \end{aligned} \tag{30}$$

for $j = 1, 2, \ldots, s$.

The SCI-CF is the product of USCI-CFs (definition 1) over all i and α. Now we arrive at lemma 2 (appendix J).

LEMMA 2

The generating function for marks $\rho_{\theta j}$ with a weight W_θ is given by the following figure inventories:

$$\sum_{\theta} \rho_{\theta j} W_\theta = Z(\mathbf{G}_j\,;\, a, b, c), \tag{31}$$

wherein the right-hand side is substituted by

$$a_{d_{jk}}^{(\alpha)} = \sum_{r=1}^{|X|} w_{i\alpha} \left(X_r^{(\mathrm{a})}\right)^{d_{jk}}, \tag{32}$$

$$b_{d_{jk}}^{(\alpha)} = \sum_{r=1}^{|X|} w_{i\alpha} (X_r)^{d_{jk}}, \tag{33}$$

and

$$c_{d_{jk}}^{(\alpha)} = \sum_{r=1}^{|X|} w_{i\alpha}\left(X_r^{(a)}\right)^{d_{jk}} + 2\sum_{r=1}^{|X|}\left[w_{i\alpha}\left(X_r^{(c)}\right)w_{i\alpha}\left(X_r^{(c\#)}\right)\right]^{d_{jk}/2}. \tag{34}$$

Lemma 2 gives a generating function for calculating marks $\rho_{\theta j}$, which are in turn introduced into eq. (28) or (29) to yield the number ($B_{\theta i}$) of configurations of symmetry G_i. It should be noted that an SCI of definition 2 can be practically obtained by an appropriate multiplication of such USCIs as collected in table 6. The following example illustrates these procedures.

Example 2. The enumeration of isomers based on a trigonal bipyramid (example 1) is re-examined by the method of this section. We pick up the rows of $\boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v})$ and $\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)$ from table 4. Generating functions are obtained in terms of lemma 2, i.e.

$$(b_1)^{(1)}(b_1^3)^{(2)} = (A + B + C + C^\#)(A + C + C^\#)^3, \qquad \text{for } \boldsymbol{C}_1,$$

$$(a_1)^{(1)}(a_1c_2)^{(2)} = (A + B)A(A + 2CC^\#), \qquad \text{for } \boldsymbol{C}_s,$$

$$(b_1)^{(1)}(b_3)^{(2)} = (A + B + C + C^\#)(A^3 + C^3 + C^{\#3}), \qquad \text{for } \boldsymbol{C}_3, \text{ and}$$

$$(b_1)^{(1)}(a_3)^{(2)} = (A + B)A^3, \qquad \text{for } \boldsymbol{C}_{3v}.$$

The terms with superscript (1) are concerned with the row of $\boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v})$. The other terms, with superscript (2), stem from the row of $\boldsymbol{C}_3(/\boldsymbol{C}_s)$. These generating functions are expanded and the coefficients of two terms for each pair of mirror images are collected to give a matrix ($\rho_{\theta j}$). The number of isomers are obtained by multiplication of the matrix ($\rho_{\theta j}$) with the inverse of the table of marks derived from table 1 (fig. 5). Obviously, the sum of the values for each subgroup (with respect to each column) is equal to that obtained in example 1. We have already illustrated the isomers in fig. 4.

A slight modification of lemma 2 gives a method for counting isomers in the case that forbids chiral ligands (appendix K). This is illustrated by the following example.

Example 3. The adamantane skeleton (**2**) of $\boldsymbol{T}_d$ symmetry has ten positions, which are divided into two orbits (six methylene and four methine positions) in accord with

$$\boldsymbol{P}_{T_d} = \boldsymbol{T}_d(/\boldsymbol{C}_{2v}) + \boldsymbol{T}_d(/\boldsymbol{C}_{3v}).$$

This reduction allows us to use $\boldsymbol{T}_d(/\boldsymbol{C}_{2v})$ and $\boldsymbol{T}_d(/\boldsymbol{C}_{3v})$ rows of a table of USCIs (table 6). We select $\boldsymbol{X} = \{C, N, O\}$ as a co-domain and determine weights:

$$w_1(C) = x,\ w_1(N) = y,\ w_1(O) = z, \quad \text{for } \Delta_1, \text{ and}$$

$$w_2(C) = x,\ w_2(N) = y,\ w_2(O) = 0, \quad \text{for } \Delta_2,$$

	C_1	C_s	C_3	C_{3v}
A^4	1	1	1	1
A^3B	1	1	1	1
$A^3C + A^3C^\#$	8	0	2	0
$A^2BC + A^2BC^\#$	6	0	0	0
$A^2C^2 + A^2C^{\#2}$	12	0	0	0
$A^2CC^\#$	12	2	0	0
$ABC^2 + ABC^{\#2}$	6	0	0	0
$ABCC^\#$	6	2	0	0
$AC^3 + AC^{\#3}$	8	0	2	0
$AC^2C^\# + ACC^{\#2}$	24	0	0	0
$BC^3 + BC^{\#3}$	2	0	2	0
$BC^2C^\# + BCC^{\#2}$	6	0	0	0
$C^4 + C^{\#4}$	2	0	2	0
$C^3C^\# + CC^{\#3}$	8	0	2	0
$C^2C^{\#2}$	6	0	0	0

$(\rho_{\theta j})$

$$\times \begin{pmatrix} 1/6 & 0 & 0 & 0 \\ -1/2 & 1 & 0 & 0 \\ -1/6 & 0 & 1/2 & 0 \\ 1/2 & -1 & -1/2 & 1 \end{pmatrix} =$$

the inverse of the table of marks

C_1	C_s	C_3	C_{3v}
0	0	0	1
0	0	0	1
1	0	1	0
1	0	0	0
2	0	0	0
1	2	0	0
1	0	0	0
0	2	0	0
1	0	1	0
4	0	0	0
0	0	1	0
1	0	0	0
0	0	1	0
1	0	1	0
1	0	0	0

numbers of isomers

Fig. 5. Isomer counting based on a trigonal pyramid under the OMV restriction.

in accordance with the OMV restriction of the skeleton. We then find figure inventories,

$$s_\tau^{(1)} = x^\tau + y^\tau + z^\tau, \quad \text{for } \Delta_1 \text{ and}$$
$$s_\tau^{(2)} = x^\tau + y^\tau, \quad \text{for } \Delta_2.$$

Lemma 4 (appendix K) gives the following generating functions for the $\rho_{\theta j}$'s:

$$(s_1^6)^{(1)}(s_1^4)^{(2)} = (x + y + z)^6(x + y)^4, \quad \text{for } \boldsymbol{C}_1,$$
$$(s_1^2 s_2^2)^{(1)}(s_2^2)^{(2)} = (x + y + z)^2(x^2 + y^2 + z^2)^2(x^2 + y^2)^2, \quad \text{for } \boldsymbol{C}_2,$$
$$(s_1^2 s_2^2)^{(1)}(s_1^2 s_2)^{(2)} = (x + y + z)^2(x^2 + y^2 + z^2)^2(x + y)^2(x^2 + y^2), \quad \text{for } \boldsymbol{C}_s,$$
$$(s_3^2)^{(1)}(s_1 s_3)^{(2)} = (x^3 + y^3 + z^3)^2(x + y)(x^3 + y^3), \quad \text{for } \boldsymbol{C}_3,$$
$$(s_2 s_4)^{(1)}(s_4)^{(2)} = (x^2 + y^2 + z^2)(x^4 + y^4 + z^4)(x^4 + y^4), \quad \text{for } \boldsymbol{S}_4,$$

$$(s_2^3)^{(1)}(s_4)^{(2)} = (x^2 + y^2 + z^2)^3(x^4 + y^4), \qquad \text{for } \boldsymbol{D}_2,$$

$$(s_1^2 s_4)^{(1)}(s_2^2)^{(2)} = (x + y + z)^2(x^4 + y^4 + z^4)(x^2 + y^2)^2, \qquad \text{for } \boldsymbol{C}_{2\mathrm{v}},$$

$$(s_3^2)^{(1)}(s_1 s_3)^{(2)} = (x^3 + y^3 + z^3)^2(x + y)(x^3 + y^3), \qquad \text{for } \boldsymbol{C}_{3\mathrm{v}},$$

$$(s_2 s_4)^{(1)}(s_4)^{(2)} = (x^2 + y^2 + z^2)(x^4 + y^4 + z^4)(x^4 + y^4), \qquad \text{for } \boldsymbol{D}_{2\mathrm{d}},$$

$$(s_6)^{(1)}(s_4)^{(2)} = (x^6 + y^6 + z^6)(x^4 + y^4), \qquad \text{for } \boldsymbol{T},$$

$$(s_6)^{(1)}(s_4)^{(2)} = (x^6 + y^6 + z^6)(x^4 + y^4), \qquad \text{for } \boldsymbol{T}_{\mathrm{d}},$$

in which the superscripts (1) and (2) correspond to the $\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{C}_{2\mathrm{v}})$ and $\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{C}_{3\mathrm{v}})$ rows of table 6.

Table 6
Unit subduced cycle indices for $\boldsymbol{T}_{\mathrm{d}}$

i \ j	$\boldsymbol{C}_1$	$\boldsymbol{C}_2$	$\boldsymbol{C}_s$	$\boldsymbol{C}_3$	$\boldsymbol{S}_4$	$\boldsymbol{D}_2$	$\boldsymbol{C}_{2\mathrm{v}}$	$\boldsymbol{C}_{3\mathrm{v}}$	$\boldsymbol{D}_{2\mathrm{d}}$	$\boldsymbol{T}$	$\boldsymbol{T}_{\mathrm{d}}$
$\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{C}_1)$	s_1^{24}	s_2^{12}	s_2^{12}	s_3^{8}	s_4^{6}	s_4^{6}	s_4^{6}	s_6^{4}	s_8^{3}	s_{12}^{2}	s_{24}
$\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{C}_2)$	s_1^{12}	$s_1^{4}s_2^{4}$	s_2^{6}	s_3^{4}	$s_2^{2}s_4^{2}$	s_2^{6}	$s_2^{2}s_4^{2}$	s_6^{2}	s_4^{3}	s_6^{2}	s_{12}
$\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{C}_s)$	s_1^{12}	s_2^{6}	$s_1^{2}s_2^{5}$	s_3^{4}	s_4^{3}	s_4^{3}	$s_2^{2}s_4^{2}$	$s_3^{2}s_6$	$s_4 s_8$	s_{12}	s_{12}
$\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{C}_3)$	s_1^{8}	s_2^{4}	s_2^{4}	$s_1^{2}s_3^{2}$	s_4^{2}	s_4^{2}	s_4^{2}	$s_2 s_6$	s_8	s_4^{2}	s_8
$\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{S}_4)$	s_1^{6}	$s_1^{2}s_2^{2}$	s_2^{3}	s_2^{3}	$s_1^{2}s_4$	s_2^{3}	$s_2 s_4$	s_6	$s_2 s_4$	s_6	s_6
$\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{D}_2)$	s_1^{6}	s_1^{6}	s_2^{3}	s_3^{2}	s_2^{3}	s_1^{6}	s_2^{3}	s_6	s_2^{3}	s_3^{2}	s_6
$\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{C}_{2\mathrm{v}})$	s_1^{6}	$s_1^{2}s_2^{2}$	$s_1^{2}s_2^{2}$	s_3^{2}	$s_2 s_4$	s_2^{3}	$s_1^{2}s_4$	s_3^{2}	$s_2 s_4$	s_6	s_6
$\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{C}_{3\mathrm{v}})$	s_1^{4}	s_2^{2}	$s_1^{2}s_2$	$s_1 s_3$	s_4	s_4	s_2^{2}	$s_1 s_3$	s_4	s_4	s_4
$\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{D}_{2\mathrm{d}})$	s_1^{3}	s_1^{3}	$s_1 s_2$	s_3	$s_1 s_2$	s_1^{3}	$s_1 s_2$	s_3	$s_1 s_2$	s_3	s_3
$\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{T})$	s_1^{2}	s_1^{2}	s_2	s_1^{2}	s_2	s_1^{2}	s_2	s_2	s_2	s_1^{2}	s_2
$\boldsymbol{T}_{\mathrm{d}}(/\boldsymbol{T}_{\mathrm{d}})$	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1

The expansion of these generating functions gives the values of $\rho_{\theta j}$, which construct an FP matrix. The FP matrix is multiplied by the inverse of the mark table for $\boldsymbol{T}_{\mathrm{d}}$ (table 7) to yield $A_{\theta i}$. The values thus obtained are found in table 8, which shows the number of isomers with $W_\theta = x^{p_1}y^{p_2}z^{p_3}$ (the row) and $\boldsymbol{G}_j$ (the column).

As an illustration of the result, fig. 6 collects C_8N_2 as well as C_8O_2 isomers based on the adamantane skeleton. The coefficient of x^8y^2 reveals that there are five isomers with C_8N_2. That of x^8z^2 is the number of C_8O_2 isomers. This difference comes from the OMV restriction, by which an oxygen is forbidden to occupy the bridgehead positions

Table 7
The inverse ($\bar{M}$) of the mark table of $\boldsymbol{T}_d$

j \ i	$T_d(/C_1)$	$T_d(/C_2)$	$T_d(/C_s)$	$T_d(/C_3)$	$T_d(/S_4)$	$T_d(/D_2)$	$T_d(/C_{2v})$	$T_d(/C_{3v})$	$T_d(/D_{2d})$	$T_d(/T)$	$T_d(/T_d)$
C_1	1/24	0	0	0	0	0	0	0	0	0	0
C_2	−1/8	1/4	0	0	0	0	0	0	0	0	0
C_s	−1/4	0	1/2	0	0	0	0	0	0	0	0
C_3	−1/6	0	0	1/2	0	0	0	0	0	0	0
S_4	0	−1/4	0	0	1/2	0	0	0	0	0	0
D_2	1/12	−1/4	0	0	0	1/6	0	0	0	0	0
C_{2v}	1/4	−1/4	−1/2	0	0	0	1/2	0	0	0	0
C_{3v}	1/2	0	−1	−1/2	0	0	0	1	0	0	0
D_{2d}	0	1/2	0	0	−1/2	−1/2	−1/2	0	1	0	0
T	1/6	0	0	−1/2	0	−1/6	0	0	0	1/2	0
T_d	−1/2	0	1	1/2	0	1/2	0	−1	−1	−1/2	1

Table 8

Enumeration of isomers based on an adamantane skeleton (2)

p_1 (C)	p_2 (N)	p_3 (O)	C_1	C_2	C_s	C_3	S_4	D_2	C_{2v}	C_{3v}	D_{2d}	T	T_d
10	0	0	0	0	0	0	0	0	0	0	0	0	0
9	1	0	0	0	0	0	0	0	1	1	0	0	0
9	0	1	0	0	0	0	0	0	1	0	0	0	0
8	2	0	0	0	3	0	0	0	1	0	1	0	0
8	1	1	1	0	2	0	0	0	1	0	0	0	0
8	0	2	0	0	1	0	0	0	0	0	1	0	0
7	3	0	2	1	3	0	0	0	2	3	0	0	0
7	2	1	6	1	4	0	0	0	2	0	0	0	0
7	1	2	2	1	5	0	0	0	0	0	0	0	0
7	0	3	0	1	0	0	0	0	0	2	0	0	0
6	4	0	4	1	7	0	0	0	1	2	1	0	1
6	3	1	16	1	8	0	0	0	2	0	0	0	0
6	2	2	12	1	9	0	0	1	1	0	0	0	0
6	1	3	3	1	4	0	0	0	0	2	0	0	0
6	0	4	0	0	1	0	0	0	0	0	1	0	0
5	5	0	4	2	10	0	0	0	2	0	0	0	0
5	4	1	25	2	10	0	0	0	2	0	0	0	0
5	3	2	26	3	15	0	0	0	0	0	0	0	0
5	2	3	11	3	10	0	0	0	0	0	0	0	0
5	1	4	2	3	10	0	0	0	1	0	0	0	0
5	0	5	0	0	0	0	0	0	1	0	0	0	0
4	6	0	4	1	7	0	0	0	1	2	1	0	1
4	5	1	25	2	10	0	0	0	2	0	0	0	0
4	4	2	34	3	16	0	0	0	0	0	2	0	0
4	3	3	22	3	10	0	0	0	0	4	0	0	0
4	2	4	6	1	5	0	0	0	1	0	1	0	0
4	1	5	0	0	2	0	0	0	1	0	0	0	0
4	0	6	0	0	0	0	0	0	0	0	0	0	1
3	7	0	2	1	3	0	0	0	2	3	0	0	0
3	6	1	16	1	8	0	0	0	2	0	0	0	0
3	5	2	26	3	15	0	0	0	0	0	0	0	0
3	4	3	22	3	10	0	0	0	0	4	0	0	0
3	3	4	9	0	6	0	0	0	2	0	0	0	0
3	2	5	1	0	2	0	0	0	2	0	0	0	0
3	1	6	0	0	0	0	0	0	0	1	0	0	0
2	8	0	0	0	3	0	0	0	1	0	1	0	0
2	7	1	6	1	4	0	0	0	2	0	0	0	0
2	6	2	12	1	9	0	0	1	1	0	0	0	0
2	5	3	11	3	10	0	0	0	0	0	0	0	0
2	4	4	6	1	5	0	0	0	1	0	1	0	0
2	3	5	1	0	2	0	0	0	2	0	0	0	0
2	2	6	0	0	0	0	0	0	1	0	0	0	0

Table 8 (continued)

Enumeration of isomers based on an adamantane skeleton (**2**)

p_1 (C)	p_2 (N)	p_3 (O)	$\boldsymbol{C}_1$	$\boldsymbol{C}_2$	$\boldsymbol{C}_s$	$\boldsymbol{C}_3$	$\boldsymbol{S}_4$	$\boldsymbol{D}_2$	$\boldsymbol{C}_{2v}$	$\boldsymbol{C}_{3v}$	$\boldsymbol{D}_{2d}$	$\boldsymbol{T}$	$\boldsymbol{T}_d$
1	9	0	0	0	0	0	0	0	1	1	0	0	0
1	8	1	1	0	2	0	0	0	1	0	0	0	0
1	7	2	2	1	5	0	0	0	0	0	0	0	0
1	6	3	3	1	4	0	0	0	0	2	0	0	0
1	5	4	2	0	3	0	0	0	1	0	0	0	0
1	4	5	0	0	2	0	0	0	1	0	0	0	0
1	3	6	0	0	0	0	0	0	0	1	0	0	0
0	10	0	0	0	0	0	0	0	0	0	0	0	1
0	9	1	0	0	0	0	0	0	1	0	0	0	0
0	8	2	0	0	1	0	0	0	0	0	1	0	0
0	7	3	0	1	0	0	0	0	0	2	0	0	0
0	6	4	0	0	1	0	0	0	0	0	1	0	0
0	5	5	0	0	0	0	0	0	1	0	0	0	0
0	4	6	0	0	0	0	0	0	0	0	0	0	1

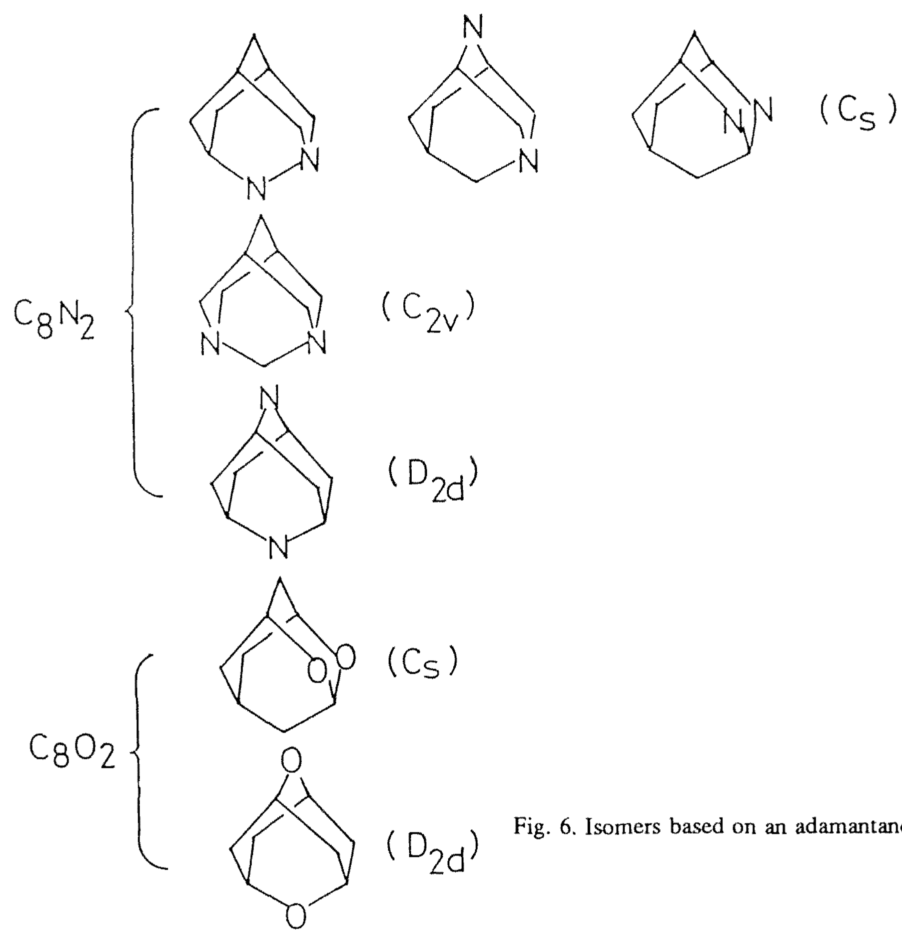

Fig. 6. Isomers based on an adamantane skeleton.

of the skeleton. Figure 6 also shows that the five C_8N_2 isomers are classified into three $\boldsymbol{C}_s$ isomers, one $\boldsymbol{C}_{2v}$ isomer and one $\boldsymbol{D}_{2d}$ isomer. The two C_8O_2 isomers are divided into one $\boldsymbol{C}_s$ and one $\boldsymbol{D}_{2d}$ isomer. These numbers appear as the values collected in table 8.

7. Special cases

This section deals with the derivation of a special case in which the OMV is not considered. For this purpose, all weights given by eq. (13) are redefined as follows:

$$w_{i\alpha}(X_r) = X_r, \tag{35}$$

for $i = 1, 2, \ldots, s$; $\alpha = 1, 2, \ldots, \alpha_i$; and $r = 1, 2, \ldots, |X|$. Thereby, the weight of a function (configuration) is found to be

$$W(f) = \prod_{\delta \in \Delta} w_{i\alpha}(f(\delta)). \tag{36}$$

Suppose that $|\boldsymbol{X}_{i\alpha}^{(a)}| = |\boldsymbol{X}^{(a)}|$ and $|\boldsymbol{X}_{i\alpha}^{(b)}| = |\boldsymbol{X}_{i\alpha}^{(c)}| = |\boldsymbol{X}|$. Then, we can apply corollary 3-1 to the special case. Hence, we end up with:

COROLLARY 3-2

$$\left[|\boldsymbol{X}^{(a)}|^{\sum_{i=1}^{s} \alpha_i \beta_{ij}^{(a)}}\right]\left[|\boldsymbol{X}|^{\sum_{i=1}^{s} \alpha_i (\beta_{ij}^{(b)} + \beta_{ij}^{(c)})}\right] = \sum_{i=1}^{s} B_i m_{ij}, \quad j = 1, 2, \ldots, s. \tag{37}$$

This corollary is more informative than Hässelbarth's counterpart [3], since the present result contains the number of orbits in the explicit powers that are derived from a novel treatment of subduced representations.

The definitions of this section indicate that the variables

$$a_{d_{jk}}^{(\alpha)}, \ b_{d_{jk}}^{(\alpha)}, \ \text{and} \ c_{d_{jk}}^{(\alpha)}$$

are independent of their orbits. Thus, we can omit the superscript (α), i.e.

$$a_{d_{jk}}^{(\alpha)} = a_{d_{jk}}, \ b_{d_{jk}}^{(\alpha)} = b_{d_{jk}}, \ \text{and} \ c_{d_{jk}}^{(\alpha)} = c_{d_{jk}}. \tag{38}$$

By using these variables, we transform the right-hand side of definition 3 into a simpler form that is suitable for the special case. Hence, we find a new definition for a subduced cycle index:

DEFINITION 4

A subduced cycle index (SCI) without consideration of OMVs is defined as

$$Z'(G_j\,;\, a, b, c) = \prod_{k=1}^{v_j} \left[(a_{d_{jk}})^{q_{ak}^{(j)}} (b_{d_{jk}})^{q_{bk}^{(j)}} (c_{d_{jk}})^{q_{ck}^{(j)}} \right], \tag{39}$$

where the powers of the respective terms are represented by

$$q_{ak}^{(j)} = \sum_{i=1}^{s} \alpha_i \chi_{ak}^{(j)} \beta_k^{(ij)}, \tag{40}$$

$$q_{bk}^{(j)} = \sum_{i=1}^{s} \alpha_i \chi_{bk}^{(j)} \beta_k^{(ij)}, \tag{41}$$

and

$$q_{ck}^{(j)} = \sum_{i=1}^{s} \alpha_i \chi_{ck}^{(j)} \beta_k^{(ij)}. \tag{42}$$

Using the subduced cycle index, we transform lemma 2 into lemma 3 that is suitable for the special case of this section (see appendix J).

LEMMA 3

If $G_j \leq G$ acts on Δ and no OMVs are considered, a generating function for marks $\rho_{\theta j}$ with a weight W_θ is as follows:

$$\sum_{\theta} \rho_{\theta j} W_\theta = Z'(G_j\,; a, b, c), \tag{43}$$

where

$$a_{d_{jk}} = \sum_{r=1}^{|X|} (X_r^{(\mathrm{a})})^{d_{jk}}, \tag{44}$$

$$b_{d_{jk}} = \sum_{r=1}^{|X|} (X_r)^{d_{jk}} = \sum_{r=1}^{|X|} (X_r^{(\mathrm{a})})^{d_{jk}} + \sum_{r=1}^{|X|} (X_r^{(\mathrm{c})})^{d_{jk}} + \sum_{r=1}^{|X|} (X_r^{(\mathrm{c\#})})^{d_{jk}}, \tag{45}$$

and

$$c_{d_{jk}} = \sum_{r=1}^{|X|} (X_r^{(\mathrm{a})})^{d_{jk}} + 2 \sum_{r=1}^{|X|} (X_r^{(\mathrm{c})} X_r^{(\mathrm{c\#})})^{d_{jk}/2}. \tag{46}$$

Lemma 3 yields a set of marks $\rho_{\theta j}$ that is necessary to enumerate isomers with a subsymmetry $G_j \leq G$ and a weight θ based on a parent skeleton of symmetry G. The values of $\rho_{\theta j}$ are introduced into theorem 4 (eq. (27) or (28)) in order to obtain the number ($B_{\theta i}$) of isomers of symmetry G_i. A more special case that enumerates isomers only with achiral ligands and without consideration of OMVs is similarly manipulated (appendix L). This case will be reported elsewhere, in particular for the purpose of clarifying the relationship between the present result and Pólya's theorem.

8. Conclusions

Enumerations with and without the effect of obligatory minimum valency (OMV) have been discussed. Each position of a given skeleton has the OMV that determines the mode of substitution at its position. The OMV can be treated with the idea that different weights are assigned to different orbits of positions. This yields several new concepts such as chirality fittingness and a subduced cycle index with three parts.

Appendix A

Coset representations as transitive ones. Coset representations (CRs) are a kind of permutation representations that play an important role in the present enumeration. Let $\boldsymbol{G}$ be a finite group. Let $\boldsymbol{H}$ be a subgroup of $\boldsymbol{G}$. The set of (left) cosets of $\boldsymbol{H}$ in $\boldsymbol{G}$ provide a partition of $\boldsymbol{G}$. If we adopt a set of $\{g_1, g_2, \ldots, g_m\}$ as a transversal (i.e. a system of representatives), we obtain the partition:

$$\boldsymbol{G} = \boldsymbol{H}g_1 + \boldsymbol{H}g_2 + \ldots + \boldsymbol{H}g_m, \tag{A.1}$$

where $g_1 = I$ (identity) and $g_i \in \boldsymbol{G}$. Let us next consider the set of the cosets:

$$\{\boldsymbol{H}g_1, \boldsymbol{H}g_2, \ldots, \boldsymbol{H}g_m\}. \tag{A.2}$$

The coset representation (CR) of $\boldsymbol{G}$ by $\boldsymbol{H}$ that is denoted as $\boldsymbol{G}(/\boldsymbol{H})$ is a set of permutations of degree m:

$$\boldsymbol{G}(/\boldsymbol{H})_g = \begin{pmatrix} \boldsymbol{H}g_1, & \boldsymbol{H}g_2 & ,\ldots, & \boldsymbol{H}g_m \\ \boldsymbol{H}g_1 g, & \boldsymbol{H}g_2 g & ,\ldots, & \boldsymbol{H}g_m g \end{pmatrix}, \tag{A.3}$$

for any $g \in \boldsymbol{G}$. The degree of $\boldsymbol{G}/(/\boldsymbol{H})$ is $m = |\boldsymbol{G}|/|\boldsymbol{H}|$. Obviously, the coset representation $\boldsymbol{G}(/\boldsymbol{H})$ is transitive and, in other words, has one orbit. When $\boldsymbol{H}$ and $\boldsymbol{H}'$ are conjugate subgroups of $\boldsymbol{G}$, the corresponding coset representations $\boldsymbol{G}(/\boldsymbol{H})$ and $\boldsymbol{G}(/\boldsymbol{H}')$ are equivalent to each other.

Representatives of conjugate groups. Suppose that the number of representatives of conjugate subgroups in a finite group $\boldsymbol{G}$ is s, where an appropriate representative is selected from a set of conjugate subgroups. We select a system of representatives,

$$\mathrm{SSG} = \{\boldsymbol{G}_1, \boldsymbol{G}_2, \ldots, \boldsymbol{G}_s\}, \tag{A.4}$$

in an ascending order of their orders, i.e.

$$|G_1| \leq |G_2| \leq \ldots \leq |G_s|,$$

where $G_1 = I$ (identity) and $G_s = G$. We call this sytem a system of subgroups (SSG). The set of corresponding CRs, $G(/G_i)$ ($i = 1, 2, \ldots, s$), is the complete set of different transitive representations of G. Obviously, $G(/G_1)$ is a regular representation and $G(/G_s)$ is an identity group.

A table of marks. A mark of H ($\leq G$) in a permutation representation of G is defined as the number of fixed points of a G-set on the action of the subgroup H. Suppose that G_i ($i = 1, 2, \ldots, s$) is an SSG of a finite group G, as defined above. Let $G(/G_i)$ be a coset representation. The mark of G_j in $G(/G_i)$ is a constant for each i and j and is denoted as m_{ij}. The table of marks m_{ij} for all i and j will be used in theorem 1.

An orbit subject to a coset representation. The feature of $G(/G_i)$ can be understood by the following explanation. The coset partition of G by G_i yields the corresponding transversal $\{g_1, g_2, \ldots, g_\tau, \ldots, g_m\}$, where $m = |G|/|G_i|$. Let G_i be a stabilizer of $\exists \delta_1^{(i)}$ of Δ. This means that G_i holds $\delta_1^{(i)}$ to be constant. We can consider that g_τ ($\in G$) converts $\delta_1^{(i)}$ into $\delta_\tau^{(i)}$. Hence, $G_i g_\tau$ corresponds to $\delta_\tau^{(i)}$ in a one-to-one fashion. As a result, $G(/G_i)$ that originally acts on $\{G_i g_\tau | \tau = 1, 2, \ldots, m\}$ can be considered to act also on $\Delta_{i\alpha} = \{\delta_\tau^{(i)} | \tau = 1, 2, \ldots, m\}$, where α denotes one of such equivalent orbits.

Appendix B

Orbits in a trigonal pyramid (C_{3v}). Let us consider the set of vertices of a trigonal pyramid to be $\Delta = \{1, 2, 3, 4\}$, whose apex is vertex 4. The C_{3v} group contains six elements, i.e.

$$G = C_{3v} = \{\mathrm{I}, C_3, C_3^2, \sigma_{v(1)}, \sigma_{v(2)}, \sigma_{v(3)}\}.$$

By counting fixed points for the respective subgroups, we can obtain marks as follows:

$$\mu_{C_1} = 4, \ \mu_{C_s} = 2, \ \mu_{C_3} = 1, \ \text{and} \ \mu_{C_{3v}} = 1.$$

If we introduce these marks into eq. (2), we find

$$(4\ 2\ 1\ 1) = (\alpha_{C_1}\ \alpha_{C_s}\ \alpha_{C_3}\ \alpha_{C_{3v}}) \begin{bmatrix} 6 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 \\ 2 & 0 & 2 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix},$$

which in turn yields

$$\alpha_{C_1} = 0, \ \alpha_{C_s} = 1, \ \alpha_{C_3} = 0, \ \text{and} \ \alpha_{C_{3v}} = 1.$$

Hence, the permutation representation has been reduced to the form of

$$P_{C_{3v}} = C_{3v}(/C_s) + C_{3v}(/C_{3v}).$$

The result is in agreement with two orbits, $\Delta_1 = \{4\}$ and $\Delta_2 = \{1, 2, 3\}$, in which Δ_1 is acted on by $C_{3v}(/C_{3v})$ and Δ_2 by $C_{3v}(/C_s)$, as shown in fig. 3. The concrete forms of the CRs have been collected in table 2.

Appendix C

Proof of eq. (3). Since the subduced representation $G(/G_1)\downarrow G_j$ is a permutation representation, eqs. (1) and (2) hold for this case. Hence,

$$G(/G_1)\downarrow G_j = \sum_{k=1}^{\upsilon_j} \beta_k^{(1j)} G_j(/H_k^{(j)}), \tag{C.1}$$

where $H_k^{(j)}$ denote a subgroup of a conjugacy class of G_j; $G_j(/H_k^{(j)})$ is the CR of G_j by $H_k^{(j)}$; $\beta_k^{(1j)}$ are non-negative integers; and υ_j is the number of conjugacy classes of subgroups. The multiplicities $\beta_k^{(1j)}$ are obtained by

$$\nu_l = \sum_{k=1}^{\upsilon_j} \beta_k^{(1j)} m_{kl}^{(j)}, \quad l = 1, 2, \ldots, \upsilon_j, \tag{C.2}$$

where ν_l is the mark of $H_l^{(j)}$ in $G(/G_l)\downarrow G_j$. In the case of $G(/G_1)\downarrow G_j$, the mark of $H_k^{(j)}$ in $G(/G_1)\downarrow G_j$ is obtained as follows:

$$\nu_1 = |G|/|G_j| \quad \text{and} \quad \nu_2 = \nu_3 = \ldots = \nu_j = 0.$$

These values, as well as $m_{kl}^{(j)} = 0$ $(l > k)$, provide

$$\beta_1^{(1j)} = |G|/|G_j| \quad \text{and} \quad \beta_2^{(1j)} = \beta_3^{(1j)} = \ldots = \beta_{\upsilon_j}^{(ij)} = 0.$$

Hence, eq. (C.1) is converted into

$$G(/G_1)\downarrow G_j = (|G|/|G_j|)G_j(/H_1^{(j)}), \tag{C.3}$$

where $H_1^{(j)}$ is an identity group.

Appendix D

A system of imprimitive blocks. Let P_G be a transitive permutation representation on Δ by the action of a finite group G on Δ. If a subset Ω ($\neq\varnothing$) of Δ satisfies the condition of $P_g\Omega = \Omega$ or $P_g\Omega \cap \Omega = \varnothing$ for $\forall P_g \in \boldsymbol{P}_G$, the subset Ω is defined as an imprimitive block of the group $\boldsymbol{P}_G$ (or of the group $\boldsymbol{G}$) [11]. Suppose that the group $\boldsymbol{P}_G$ on Δ is transitive, that the subset Ω of Δ is an imprimitive block, and that the group $\boldsymbol{G}_{\langle\Omega\rangle}$ is a stabilizer for the subset Ω. Let $\boldsymbol{H}$ denote the permutation representation corresponding to $\boldsymbol{G}_{\langle\Omega\rangle}$, i.e.

$$\boldsymbol{P}_{\boldsymbol{G}_{\langle\Omega\rangle}} = \boldsymbol{H}.$$

The set of (left) cosets of $\boldsymbol{H}$ in $\boldsymbol{P}_G$ provide a partition of $\boldsymbol{P}_G$. That is

$$\boldsymbol{P}_G = \boldsymbol{H}t_1 + \boldsymbol{H}t_2 + \ldots + \boldsymbol{H}t_r, \tag{D.1}$$

where $t_1 = I$ (identity) and $t_k \in \boldsymbol{P}_G$ for $k = 1, 2, \ldots, r$. This equation gives a system of primitive blocks $\Gamma = \{\Omega_1, \Omega_2, \ldots, \Omega_r\}$, where $\Omega_1 = \Omega$ and $t_k\Omega = \Omega_k$.

LEMMA D.1

Let $\Gamma = \{\Omega_1, \Omega_2, \ldots, \Omega_r\}$ be a system of imprimitive blocks of a transitive representation $\boldsymbol{P}_G$ by the action of $\boldsymbol{G}$ on Δ. Since $P_g\Omega_\tau \in \Gamma$ $(\tau = 1, 2, \ldots r)$ for $P_g \in \boldsymbol{P}_G$ $(\forall g \in \boldsymbol{G})$, a permutation represented by

$$G_g^{\#} = \begin{pmatrix} \Omega_1, & \Omega_2, & \ldots, & \Omega_r \\ P_g\,\Omega_1, & P_g\,\Omega_2, & \ldots, & P_g\,\Omega_r \end{pmatrix} \tag{D.2}$$

can be defined. The $\boldsymbol{G}^{\#} = \{G_g^{\#} \mid \forall g \in \boldsymbol{G}\}$ is a permutation representation which is equivalent to the coset representation of $\boldsymbol{G}$ by the stabilizer $\boldsymbol{G}_{\langle\Omega\rangle}$, i.e.

$$\boldsymbol{G}^{\#} = \boldsymbol{G}(/\boldsymbol{G}_{\langle\Omega\rangle}).$$

Appendix E

A system of imprimitive blocks with respect to a regular representation. A stabilizer of each sub-orbit $(\omega_1, \omega_2, \ldots, \omega_r)$ is $\boldsymbol{G}(/\boldsymbol{G}_1)\downarrow\boldsymbol{G}_j$, since this is faithful to $\boldsymbol{G}_j$. The sub-orbit ω_1 $(=\Omega_1)$ thereby is an imprimitive block in Δ. Equation (D.1) holds for this case, if we take $\boldsymbol{P}_G = \boldsymbol{G}(/\boldsymbol{G}_1)$ and $\boldsymbol{H} = \boldsymbol{G}(/\boldsymbol{G}_1)\downarrow\boldsymbol{G}_j$. Hence, this fact gives a system of imprimitive blocks $\Gamma = \{\Omega_1, \Omega_2, \ldots, \Omega_r\}$, where each representative t_τ is selected from $\boldsymbol{P}_G$ to yield $t_\tau\Omega_1 = \Omega_\tau$ $(\tau = 1, 2, \ldots, r)$ as shown in appendix D. It should be noted that the set of orbits ω_k are not always identical to Γ except Ω_1. In terms of lemma D.1, let $\boldsymbol{G}^{\#}$ be a permutation group on the system Γ. Lemma D.1 indicates $\boldsymbol{G}^{\#} = \boldsymbol{G}(/\boldsymbol{H})$. On the other hand, $\boldsymbol{P}_G(/\boldsymbol{H}) = \boldsymbol{G}(/\boldsymbol{G}_j)$, because $\boldsymbol{P}_G$ and $\boldsymbol{H}$ are isomorphic to $\boldsymbol{G}$ and $\boldsymbol{G}_j$, respectively. Hence, $\boldsymbol{G}^{\#} = \boldsymbol{G}(/\boldsymbol{G}_j)$. As a result, the coset representation $\boldsymbol{G}(/\boldsymbol{G}_j)$, which originally acts on the corresponding set of cosets (appendix A), can be considered to act on $\Gamma = \{\Omega_1, \Omega_2, \ldots, \Omega_r\}$.

Appendix F

Proof of theorem 2. The object of this appendix is to examine the mode of action of $\boldsymbol{G}(/\boldsymbol{G}_j)$ on $\Gamma = \{\Omega_1, \Omega_2, \ldots, \Omega_r\}$ from a chemical point of view. We discuss this in the following three cases:

(a) $\boldsymbol{G}$ is a group having improper rotations and $\boldsymbol{G}_j$ is a subgroup also having improper rotations.

(b) Both $\boldsymbol{G}$ and $\boldsymbol{G}_j \leq \boldsymbol{G}$ are groups of proper rotations.

(c) $\boldsymbol{G}$ is a group having improper rotations and $\boldsymbol{G}_j$ is a subgroup of proper rotations.

The subgroup $\boldsymbol{G}_j$ is a stabilizer of the block $\Omega_1 = \omega_1$, as shown in the above discussions. Hence, the homomorphic $\boldsymbol{G}(/\boldsymbol{G}_j)\downarrow\boldsymbol{G}_j$ is a subgroup that stabilizes Ω_1. In other words, the subgroup $\boldsymbol{G}_j$, or equivalently $\boldsymbol{G}(/\boldsymbol{G}_j)\ \downarrow\boldsymbol{G}_j$, keeps Ω_1 constant.

Case (a). If we assign a chiral ligand C to Ω_1, the subgroup $\boldsymbol{G}_j$ converts this into the antipode $C^{\#}$, since $\boldsymbol{G}_j$ contains improper rotations in case (a). In order for Ω_1 to be a constant, we obtain the relationship $C = C^{\#}$, which indicates that C (and $C^{\#}$) should be achiral. In case (a), therefore, $\boldsymbol{G}(/\boldsymbol{G}_j)$ acts on the domain that takes only achiral ligands.

Case (b). This is more straightforward. Since the group $\boldsymbol{G}(/\boldsymbol{G}_j)$ is not concerned with improper rotations, any ligands can be available.

Case (c). Let $\boldsymbol{P}_G$ be $\boldsymbol{G}$ and let $\boldsymbol{H}$ be $\boldsymbol{G}_j$ in eq. (D.1). Since $\boldsymbol{H}$ contains only proper rotations, eq. (D.1) indicates that the transversal $\{t_1, t_2, \ldots, t_r\}$ consists of $r/2$ improper rotations and $r/2$ proper ones. Note that $t_\tau\Omega_1 = \Omega_\tau$. Hence, if we assign a chiral ligand (C) to Ω_1, the $r/2$ blocks of Γ can be assigned to C and the remaining $r/2$ ones to the antipode ($C^{\#}$). On the other hand, if we assign an achiral ligand to Ω_1, all of the r blocks in Γ can be assigned to achiral ligands. Therefore, $\boldsymbol{G}(/\boldsymbol{G}_j)$ acts on the domain that takes achiral ligands as well as chiral ones. The mode of substitution with chiral ligands is illustrated in the text.

Appendix G

Proof of Λ_G being homomorphic to $\boldsymbol{G}$. Let us consider a mapping $\lambda_g : f_\varepsilon \to f_\gamma$, i.e. $\lambda_g : Q_g f_\gamma P_g^{-1} \to f_\gamma$ or $f_\gamma \to Q_g^{-1} f_\gamma P_g$. Suppose that both f_γ and f_ε ($f_\gamma \neq f_\varepsilon$) are mapped by λ_g to the same function, i.e.

$$Q_g^{-1} f_\gamma(P_g(\delta)) = Q_g^{-1} f_\varepsilon(P_g(\delta)) \quad \text{for} \quad \forall\, \delta \in \Delta.$$

This indicates that $f_\gamma(P_g(\delta)) = f_\varepsilon(P_g(\delta))$. In other words, $f_\gamma = f_\varepsilon$, which is contrary to the presumption. Hence, this mapping λ_g is a permutation on $\boldsymbol{F}$:

$$\lambda_g = \begin{pmatrix} Q_g f_1 P_g^{-1} & ,\ldots, & Q_g f_{|F|} P_g^{-1} \\ f_1 & ,\ldots, & f_{|F|} \end{pmatrix}$$

$$= \begin{pmatrix} f_1 & ,\ldots, & f_{|F|} \\ Q_g^{-1} f_1 P_g & ,\ldots, & Q_g^{-1} f_{|F|} P_g \end{pmatrix}. \qquad \text{(G.1)}$$

Equation (G.1) indicates that $g \in G$ corresponds to the permutation λ_g. Let Λ_G be the set that contains λ_g for $\forall g \in G$. For any $g' \in G$,

$$\lambda_{g'} \lambda_g = \begin{pmatrix} \cdots & f_\gamma & \cdots \\ \cdots & Q_{g'}^{-1} f_\gamma P_{g'} & \cdots \end{pmatrix} \begin{pmatrix} \cdots & Q_g f_\gamma P_g^{-1} & \cdots \\ \cdots & f_\gamma & \cdots \end{pmatrix}$$

$$= \begin{pmatrix} \cdots & Q_g f_\gamma P_g^{-1} & \cdots \\ \cdots & Q_{g'} f_\gamma P_{g'} & \cdots \end{pmatrix}$$

$$= \begin{pmatrix} \cdots & (Q_{g'} Q_g) f_\gamma (P_{g'} P_g)^{-1} & \cdots \\ \cdots & f_\gamma & \cdots \end{pmatrix} = \lambda_{g'g}.$$

This indicates that the group Λ_G is homomorphic to G. In other words, Λ_G is a permutation representation of G.

Appendix H

Proof of lemma 1. Since $f_\gamma \sim f_\varepsilon$, the definition (eq. (15)) shows that there is an appropriate g ($\in G$) which satisfies

$$Q_g f_\gamma(\delta) = f_\varepsilon(P_g(\delta)) \qquad \text{for } \forall \delta \in \Delta.$$

Hence, we find

$$W(Q_g f_\gamma)$$

$$= \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \left[\prod_{\delta \in \Delta_{k\beta a}^{i\alpha}} w_{i\alpha}(f_\varepsilon P_g(\delta)) \prod_{\delta \in \Delta_{k\beta b}^{i\beta}} w_{i\alpha}(f_\varepsilon P_g(\delta)) \prod_{\delta \in \Delta_{k\beta c}^{i\alpha}} w_{i\alpha}(f_\varepsilon P_g(\delta)) \right]. \qquad \text{(H.1)}$$

On the other hand,

$$W(Q_g f_\varepsilon)$$

$$= \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \left[\prod_{\delta \in \Delta_{k\beta a}^{i\alpha}} w_{i\alpha}(Q_g f_\varepsilon(\delta)) \prod_{\delta \in \Delta_{k\beta b}^{i\alpha}} w_{i\alpha}(Q_g f_\varepsilon(\delta)) \prod_{\delta \in \Delta_{k\beta c}^{i\alpha}} w_{i\alpha}(Q_g f_\varepsilon(\delta)) \right]$$

$$= \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \left[\prod_{\delta \in \Delta_{k\beta a}^{i\alpha}} w_{i\alpha}(f_\varepsilon(\delta)) \prod_{\delta \in \Delta_{k\beta b}^{i\alpha}} w_{i\alpha}(f_\varepsilon(\delta)) \prod_{\delta \in \Delta_{k\beta c}^{i\alpha}} w_{i\alpha}(f_\varepsilon(\delta)) \right], \qquad \text{(H.2)}$$

since a set of $Q_g f_\varepsilon(\delta)$'s is the same as that of $f_\varepsilon(\delta)$'s except for the sequence. A comparison between the right-hand sides of eqs. (H.1) and (H.2) reveals that $W(Q_g f_\gamma) = W(Q_g f_\varepsilon)$, since a set of $P_g(\delta)$'s and one of δ's are the same except for their sequences. This equation indicates that $W(Q_g f_\varepsilon) = W(f_\varepsilon)$. Similarly, $W(Q_g f_\gamma)$. Therefore, $W(f_\gamma) = W(f_\varepsilon)$.

Appendix I

Proof of $\Lambda_G^{(\theta)}$ being homomorphic to G. Let $F^{(\theta)}$ be a set of functions ($f : \Delta \to X$), all of which have the same weight $W_\theta(f)$:

$$F^{(\theta)} = \{f_1^{(\theta)}, f_2^{(\theta)}, \ldots, f_\gamma^{(\theta)}, \ldots, f_\varepsilon^{(\theta)}, \ldots, f_\psi^{(\theta)}\}, \qquad \text{(I.1)}$$

where $\psi = |F^{(\theta)}|$. We can obtain a permutation,

$$\lambda_g^{(\theta)} = \begin{pmatrix} Q_g f_1^{(\theta)} P_g^{-1} & ,\ldots, & Q_g f_\gamma^{(\theta)} P_g^{-1} & ,\ldots, & Q_g f_\psi^{(\theta)} P_g^{-1} \\ f_1^{(\theta)} & ,\ldots, & f_\gamma^{(\theta)} & ,\ldots, & f_\psi^{(\theta)} \end{pmatrix}$$

$$= \begin{pmatrix} f_1^{(\theta)} & ,\ldots, & f_\gamma^{(\theta)} & ,\ldots, & f_\psi^{(\theta)} \\ Q_g^{-1} f_1^{(\theta)} P_g & ,\ldots, & Q_g^{-1} f_\gamma^{(\theta)} P_g & ,\ldots, & Q_g^{-1} f_\psi^{(\theta)} P_g \end{pmatrix}. \qquad \text{(I.2)}$$

Let the symbol $\Lambda_G^{(\theta)}$ denote the set of $\lambda_g^{(\theta)}$ for $\forall g \in G$. The next issue is to prove that $\lambda_G^{(\theta)}$ is a permutation representation of G.

$$\lambda_g^{(\theta)} = \begin{pmatrix} \ldots, & f_\gamma^{(\theta)}(\delta) & ,\ldots \\ \ldots, & Q_g^{-1} f_\gamma^{(\theta)}(P_g(\delta)) & ,\ldots \end{pmatrix}$$

$$\lambda_{g'}^{(\theta)} = \begin{pmatrix} \ldots, & f_\gamma^{(\theta)}(\delta) & ,\ldots \\ \ldots, & Q_{g'}^{-1} f_\gamma^{(\theta)}(P_{g'}(\delta)) & ,\ldots \end{pmatrix} = \begin{pmatrix} \ldots, & f_\gamma^{(\theta)}(P_g(\delta)) & ,\ldots \\ \ldots, & Q_{g'}^{-1} f_\gamma^{(\theta)}(P_{g'} P_g(\delta)) & ,\ldots \end{pmatrix}$$

$$= \begin{pmatrix} \ldots, & Q_g^{-1} f_\gamma^{(\theta)}(P_g(\delta)) & ,\ldots \\ \ldots, & Q_g^{-1} Q_{g'}^{-1} f_\gamma^{(\theta)}(P_{g'} P_g(\delta)) & ,\ldots \end{pmatrix}$$

$$= \begin{pmatrix} \ldots, & Q_g^{-1} f_\gamma^{(\theta)}(P_g(\delta)) & ,\ldots \\ \ldots, & Q_{g'g}^{-1} f_\gamma^{(\theta)}(P_{g'g}(\delta)) & ,\ldots \end{pmatrix},$$

since $P_{g'} P_g = P_{g'g}$ and $Q_{g'} Q_g = Q_{g'g}$. Hence,

$$\lambda_{g'}^{(\theta)} \lambda_g^{(\theta)} = \begin{pmatrix} \ldots, & f_\gamma^{(\theta)}(\delta) & ,\ldots \\ \ldots, & Q_{g'g}^{-1} f_\gamma^{(\theta)}(P_{g'g}(\delta)) & ,\ldots \end{pmatrix} = \lambda_{g'g}\,. \tag{I.3}$$

This equation indicates that the mapping of $\boldsymbol{G}$ (or $\boldsymbol{P}_G$) onto $\Lambda_G^{(\theta)}$ is homomorphic. In other words, the group $\Lambda_G^{(\theta)}$ is a permutation representation of $\boldsymbol{G}$.

Appendix J

Proof of lemma 2. In order to find marks $\rho_{\theta j}$, we consider a series of $\rho_{\theta j}$'s in column j of $(\rho_{\theta j})$ of eq. (29). These elements are the numbers of fixed configurations of symmetry $\boldsymbol{G}_j$. Figure 2 holds for this case. Hence, the above discussion on eq. (7) indicates that $\chi_{ak}^{(j)} \beta_k^{(ij)}$ or $\chi_{bk}^{(j)} \beta_k^{(ij)}$ or $\chi_{ck}^{(j)} \beta_k^{(ij)}$ orbits of length d_{jk} emerge during this operation. For the purpose of constructing a fixed configuration, each of the $\boldsymbol{G}_j$-achiral orbits of length d_{jk} has the same achiral ligands. Hence, the corresponding generating function is found as follows:

$$a_{d_{jk}}^{(\alpha)} = \sum_{r=1}^{|X|} w_{i\alpha} (X_r^{(\mathrm{a})})^{d_{jk}}, \tag{J.1}$$

where $X_r^{(\mathrm{a})}$ denotes an achiral ligand. For each of the $\boldsymbol{G}_j$-neutral sub-orbits, all types of ligands are available. Hence,

$$b_{d_{jk}}^{(\alpha)} = \sum_{r=1}^{|X|} w_{i\alpha} (X_r)^{d_{jk}} = \sum_{r=1}^{|X|} w_{i\alpha} (X_r^{(\mathrm{a})})^{d_{jk}} + \sum_{r=1}^{|X|} w_{i\alpha} (X_r^{(\mathrm{c})})^{d_{jk}} + \sum_{r=1}^{|X|} w_{i\alpha} / X_r^{(\mathrm{c\#})})^{d_{jk}}, \tag{J.2}$$

where X_r denotes any type of ligands.

Each of the G_j-chiral orbits finds the same situation as eq. (21) and hence yields the following generating function:

$$c_{d_{jk}}^{(\alpha)} = \sum_{r=1}^{|X|} w_{i\alpha}(X_r^{(\mathrm{a})})^{d_{jk}} + 2\sum_{r=1}^{|X|} [w_{i\alpha}(X_r^{(\mathrm{c})} w_{i\alpha}(X_r^{(\mathrm{c}\#)})]^{d_{jk}/2}, \tag{J.3}$$

where $X_r^{(\mathrm{c})}$ and $X_r^{(\mathrm{c}\#)}$ denote a pair of chiral ligands. Since these equations are true for all orbits of $\Delta_{i\alpha}$, the product over all sub-orbits of $\Delta_{i\alpha}$ (i.e. over all subgroups $\boldsymbol{H}_k^{(j)}$) yields a generating function:

$$\prod_{k=1}^{v_j}\left[\sum_{r=1}^{|X|} w_{i\alpha}(X_r^{(\mathrm{a})})^{d_{jk}}\right]^{\chi_{ak}^{(j)}\beta_k^{(ij)}}\left[\sum_{r=1}^{|X|} w_{i\alpha}(X_r)^{d_{jk}}\right]^{\chi_{bk}^{(j)}\beta_k^{(ij)}}$$
$$\times\left[\sum_{r=1}^{|X|} w_{i\alpha}(X_r^{(\mathrm{a})})^{d_{jk}} + 2\sum_{r=1}^{|X|}\left[w_{i\alpha}(X_r^{(\mathrm{c})})w_{i\alpha}(X_r^{(\mathrm{c}\#)})\right]^{d_{jk}/2}\right]^{\chi_{ck}^{(j)}\beta_k^{(ij)}}. \tag{J.4}$$

Equation (J.4) is alternatively obtained by the introduction of eqs. (J.1) to (J.3) into eq. (9). Since eq. (J.4) is true for all orbits of Δ, the product over all α and i provides a generating function that contains monomials of total powers of $d_{jk}\beta_{ij}^{(\mathrm{a})}$, $d_{jk}\beta_{ij}^{(\mathrm{b})}$ and $d_{jk}\beta_{ik}^{(\mathrm{c})}$. Thus, these monomials are in accord with the definition of weights (eq. (14)); therefore, the resulting polynomial is a generating function for enumeration of the marks $\rho_{\theta j}$. Examination of the concrete form of the generating function shows that it is equal to the equation which is derived by the introduction of eqs. (J.1) to (J.3) into eq. (30).

Appendix K

A special case with achiral ligands only and with consideration of OMVs [12]. Suppose that β_{ij} is the number of sub-orbits concerned with $\boldsymbol{G}(/\boldsymbol{G}_i)\downarrow\boldsymbol{G}_j$. Then, eqs. (10), (11), and (12) yield the following result:

$$\begin{aligned}\beta_{ij} &= \beta_{ij}^{(\mathrm{a})} + \beta_{ij}^{(\mathrm{b})} + \beta_{ij}^{(\mathrm{c})} \\ &= \sum_{k=1}^{v_j}(\chi_{ak}^{(j)} + \chi_{bk}^{(j)} + \chi_{ck}^{(j)})\beta_k^{(ij)} = \sum_{k=1}^{v_j}\beta_k^{(ij)}.\end{aligned} \tag{K.1}$$

If we assume $|\boldsymbol{X}_{i\alpha}^{(\mathrm{a})}| = |\boldsymbol{X}_{i\alpha}^{(\mathrm{b})}| = |\boldsymbol{X}_{i\alpha}^{(\mathrm{c})}| = |\boldsymbol{X}_{i\alpha}|$ in corollary 3-1 (eq. (22) or (23)), we can obtain an equation for the special case.

COROLLARY 3-3

$$\prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} |X_{i\alpha}|^{\beta_{ij}} = \sum B_i m_{ij} . \tag{K.2}$$

Under the conditions of this section, we can suppose that

$$a_{d_{jk}} = b_{d_{jk}} = c_{d_{jk}} = s_{d_{jk}} .$$

Hence, eq. (30) converts definition 3 into:

DEFINITION 5

A subduced cycle index (SCI) with permission for only achiral ligands under consideration of OMVs is defined as

$$Z''(G_j ; s_{d_{jk}}^{(\alpha)}) = \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \prod_{k=1}^{v_j} (s_{d_{jk}}^{(\alpha)})^{\beta_k^{(ij)}}, \qquad j = 1, 2, \ldots, s. \tag{K.3}$$

Note that eq. (K.3) contains the following unit subduced cycle index (USCI):

$$Z''(G(/G_i) \downarrow G_j ; s_{d_{jk}}^{(\alpha)}) = \prod_{k=1}^{v_j} (s_{d_{jk}}^{(\alpha)})^{\beta_k^{(ij)}}, \quad j = 1, 2, \ldots, s, \tag{K.4}$$

which corresponds to eq. (9) (definition 1).

Since we permit achiral ligands only, lemma 2 can be converted into lemma 4 by using the SCI of definition 5.

LEMMA 4

$$\sum_{\theta} \rho_{\theta j} W_\theta = Z''(G_j ; s_{d_{jk}}^{(\alpha)}), \tag{K.5}$$

where

$$s_{d_{jk}}^{(\alpha)} = \sum_{r=1}^{|X|} w_{i\alpha}(X_r)^{d_{jk}}. \tag{K.6}$$

This lemma gives a set of $\rho_{\theta j}$, which in turn yields $B_{\theta i}$ in terms of theorem 4.

Appendix L

A special case with achiral ligands only and without consideration of OMVs [12]. In this case, the term β_{ij} is also given by eq. (K.1). If we assume $|X^{(a)}| = |X|$, we can convert corollary 3-2 into corollary 3-5 for this case.

COROLLARY 3-5

$$|X|^{\sum_{i=1}^{s} \alpha_i \beta_{ij}} = \sum_{i=1}^{s} B_i m_{ij}, \quad j = 1, 2, \ldots, s. \tag{L.1}$$

Suppose that $q_k^{(j)}$ is the number of sub-orbits concerned in $G_j(/H_k^{(j)})$. This term is represented by eqs. (40), (41), and (42) to be

$$q_k^{(j)} = q_{ak}^{(j)} + q_{bk}^{(j)} + q_{ck}^{(j)} = \sum_{i=1}^{s} \alpha_i (\chi_{ak}^{(j)} + \chi_{bk}^{(j)} + \chi_{ck}^{(j)}) \beta_k^{(ij)} = \sum_{i=1} \alpha_i \beta_k^{(ij)}. \tag{L.2}$$

Under the conditions of this section, we can suppose that

$$s_{d_{jk}} = a_{d_{jk}} = b_{d_{jk}} = c_{d_{jk}}. \tag{L.3}$$

Equations (L.2) and (L.3) convert definition 4 into:

$$Z'''(G_j; s_{d_{jk}}) = \prod_{k=1}^{v_j} (s_{d_{jk}})^{q_k^{(j)}}, \quad \text{for } j = 1, 2, \ldots, s, \tag{L.4}$$

where $q_k^{(j)}$ is given by eq. (L.3).

Since we permit achiral ligands only, we can obtain the following lemma by using the SCI defined in definition 6.

LEMMA 5

When only achiral ligands are permitted and no OMVs are considered, a generating function for marks ($\rho_{\theta j}$) is represented by

$$\sum_{\theta} \rho_{\theta j} W_\theta = Z'''(G_j; s_{d_{jk}}), \quad \text{for } j = 1, 2, \ldots, s, \tag{L.5}$$

where

$$s_{d_{jk}} = \sum_{r=1}^{|X|} X_r^{d_{jk}}. \tag{L.6}$$

A matrix of $\rho_{\theta i}$ obtained by lemma 5 was introduced into theorem 4 (eq. (28) or (29)). Then the number ($B_{\theta i}$) of isomers of symmetry G_i can be obtained.

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