Journal of Mathematical Chemistry 5(1990)99-120

ENUMERATIONS OF CHEMICAL STRUCTURES BY SUBDUCTION OF COSET REPRESENTATIONS. CORRELATION OF UNIT SUBDUCED CYCLE INDICES TO PÓLYA'S CYCLE INDICES

Shinsaku FUJITA
Research Laboratories, Ashigara, Fuji Photo Film Co., Ltd., Minami-Ashigara, Kanagawa, 250-01 Japan

Received 18 May 1989

Abstract

Subduction of the coset representations and the related concepts such as unit subduced cycle indices and subduced cycle indices yields the foundation for a new type of generating function for enumerating chemical structures. This method is related to Pólya's theorem.

1. Introduction

Pólya's theorem [1,2] has had a profound influence on the progress of solving enumeration problems. There has thus emerged a vast number of papers which are devoted to its extension [3-5] and various applications, in particular to isomer enumerations [6]. Ruch et al. [7] have reported enumerations based on double cosets. Recently, Hässelbarth [8] has presented an excellent method using tables of marks. Brocas [9] has mentioned another method that is based on double cosets and the framework group. Mead [10] has compared these methods by using common problems.

A typical question in enumeration has been how to obtain the number of isomers with ligands (or atoms) selected from a given set on the basis of a parent skeleton. This question, however, overlooks the fact that each position (vertex) of the skeleton cannot always take all ligands from the set. Especially in the case of chemical applications, this type of restriction is an important consideration, since each position has an obligatory minimum valency (OMV) [11-13].

In previous papers [13], we have reported subduction of coset representations and its application to such enumeration problems. In particular, we have proposed unit subduced cycle indices (USCIs), which are foundations for qualitative discussions on molecular symmetry as well as for introducing a new type of generating functions. In a continuation of that work, the present paper deals with discussions on the relationship between USCIs and Pólya's cycle indices.

2. Subduction of coset representations and unit subduced cycle indices

Let $\boldsymbol{G}$ be a finite group that keeps a given skeleton invariant. The group $\boldsymbol{G}$ thus acts on the set (Δ) of positions of the skeleton to give a permutation representation $\boldsymbol{P}_G$

on Δ. If P_G is intransitive, the domain Δ is divided into orbits. This division is accomplished by theorem 1, which derives from Burnside [14].

THEOREM 1

Any permutation representation P_G is reduced to a set of (transitive) coset representations (CRs) in the form of

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

in which the symbol $(G(/G_i))$ denotes a coset representation (CR) of G by the subgroup G_i. The multiplicities α_i are determined by solving the following equations:

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

where μ_j is the mark of G_j in P_G.

The multiplicities α_i are obtained by solving the s equations expressed by eq. (2). When the symbol $(\bar{m}_{ji})$ denotes the inverse of a mark table (m_{ij}), eq. (2) is transformed into

$$\alpha_i = \sum_{k=1}^{s} \mu_j \overline{m}_{ji}, \quad j = 1, 2, \ldots, s. \tag{3}$$

Table 1 lists coset representations for the C_{2v} group. Table 2 shows the table of marks for the C_{2v} group, which can be easily constructed from the concrete forms of the coset representations of C_{2v}.

Equation (1) corresponds to the division of the domain Δ into orbits, i.e.

$$\Delta_{i\alpha} \quad \text{for } i = 1, 2, \ldots, s \quad \text{and} \quad \alpha = 1, 2, \ldots, \alpha_i, \tag{4}$$

on which $G(/G_i)$ acts (fig. 1). The number of orbits is

$$\sum_{i=1}^{s} \alpha_i . \tag{5}$$

The length of $\Delta_{i\alpha}$ is equal to the degree of the corresponding $G(/G_i)$, i.e.

$$|\Delta_{i\alpha}| = |G|/|G_i|. \tag{6}$$

Each of the CRs represented by eq. (1) is transitive. However, if it is subduced to a subgroup, the resulting subduced representation (SR) for the subgroup is generally intransitive. Let $G(/G_i)\downarrow G_j$ denote the subduced representation of $G(/G_i)$ by the subgroup G_j. The SR is reduced to a set of CRs in terms of:

Table 1

Coset representations of $\boldsymbol{C}_{2v}$ and $\boldsymbol{D}_2$ by the subgroups

D_2	C_{2v}	$D_2(/C_1)$ $C_{2v}(/C_1)$	$D_2(/C_2)$ $C_{2v}(/C_2)$	$D_2(/C_{2'})$ $C_{2v}(/C_s)$	$D_2(/C_{2''})$ $C_{2v}(/C_{s'})$	$D_2(/D_2)$ $C_{2v}(/C_{2v})$
I	I	(1) (2) (3) (4)	(1) (2)	(1) (2)	(1) (2)	(1)
$C_{2(3)}$	C_2	(1 2) (3 4)	(1) (2)	(1 2)	(1 2)	(1)
$C_{2(1)}$	$\sigma_{v(1)}$	(1 3) (2 4)	(1 2)	(1) (2)	(1 2)	(1)
$C_{2(2)}$	$\sigma_{v(2)}$	(1 4) (2 3)	(1 2)	(1 2)	(1) (2)	(1)

Table 2

Mark table for $\boldsymbol{C}_{2v}$ and $\boldsymbol{D}_2$

i \ j		C_1 C_1	C_2 C_2	$C_{2'}$ C_s	$C_{2''}$ $C_{s'}$	D_2 C_{2v}
$D_2(/C_1)$	$C_{2v}(/C_1)$	4	0	0	0	0
$D_2(/C_2)$	$C_{2v}(/C_2)$	2	2	0	0	0
$D_2(/C_{2'})$	$C_{2v}(/C_s)$	2	0	2	0	0
$D_2(/C_{2''})$	$C_{2v}(/C_{s'})$	2	0	0	2	0
$D_2(/D_2)$	$C_{2v}(/C_{2v})$	1	1	1	1	1

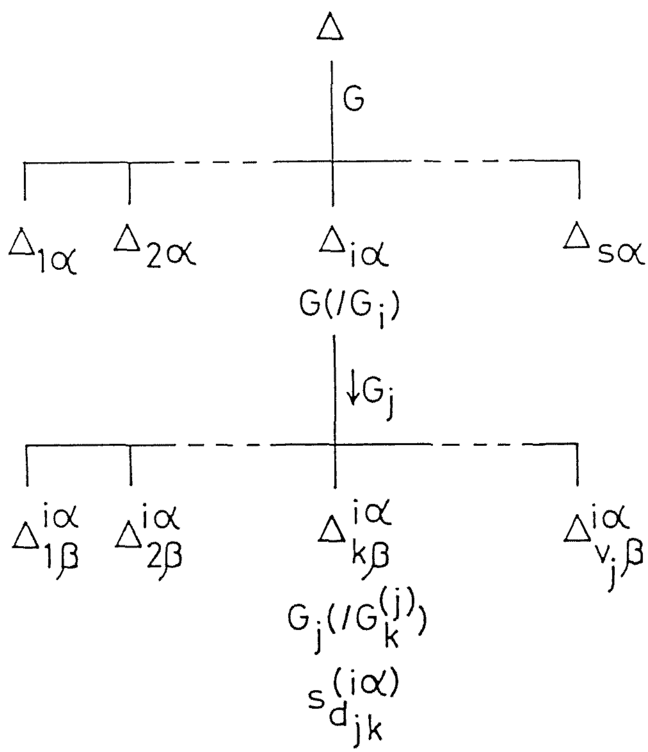


Fig. 1. Subdivision of the orbit $\Delta_{i\alpha}$ into $\Delta^{i\alpha}_{k\beta}$ by the subduction of $G(/G_i)$ by G_j.

COROLLARY 1-1

$$G(/G_i) \downarrow G_j = \sum_{k=1}^{\upsilon_j} \beta_k^{(ij)} G_j(/G_k^{(j)}), \quad i = 1,2,\ldots,s \text{ and } j = 1,2,\ldots,s, \tag{7}$$

in which $G_k^{(j)}$ is a set of υ_j subgroups of G_j in a similar way as in theorem 1, $G_1^{(j)}$ is an identity representation, and $G_{\upsilon_j}^{(j)} = G_j$. The multiplicities $\beta_k^{(ij)}$ are calculated in the light of

$$\nu_l = \sum_{k=1}^{\upsilon_j} \beta_k^{(ij)} m_{kl}^{(j)}, \quad i = 1,2,\ldots,s, \; j = 1,2,\ldots,s \text{ and } l = 1,2,\ldots,\upsilon_j, \tag{8}$$

in which $(m_{kl}^{(j)})$ is a table of marks for G_j and ν_l are the marks of $G_l^{(j)}$ in $G(/G_i)\downarrow G_j$.

The subduction of $G(/G_i)$ by G_j yields a subdivision of the orbit $\Delta_{i\alpha}$ into $\Delta_{k\beta}^{i\alpha}$ ($\beta = 1, 2, \ldots, \beta_k^{(ij)}$) by means of corollary 1-1 (fig. 1). The length of the sub-orbit ($\Delta_{k\beta}^{i\alpha}$) is equal to the degree of $G_j(/G_k^{(j)})$, i.e.

$$d_{jk} = |G_j| / |G_k^{(j)}|, \tag{9}$$

since the sub-orbit is subject to $G_j(/G_k^{(j)})$.

We next assign a variable $s_{d_{jk}}^{(i\alpha)}$ to each orbit $\Delta_{k\beta}^{i\alpha}$ and define a unit subduced cycle index (USCI). Note that $G_j(/G_k^{(j)})$ is a CR on the orbit $\Delta_{k\beta}^{i\alpha}$. Thereby, we arrive at:

DEFINITION 1

The unit subduced cycle index (USCI) for $G(/G_i)\downarrow G_j$ is represented by

$$Z\left(G(/G_i) \downarrow G_j \,;\, s_{d_{jk}}^{(i\alpha)}\right) = \prod_{k=1}^{\upsilon_j} \left(s_{d_{jk}}^{(i\alpha)}\right)^{\beta_k^{(ij)}}, \quad \text{for } i = 1,2,\ldots,s, \; j = 1,2,\ldots,s, \tag{10}$$

in which the superscript $(i\alpha)$ is concerned with the sub-orbit ($\Delta_{k\beta}^{i\alpha}$). Since USCIs can be pre-estimated by eq. (8), a table of USCIs that collects them over all i and j (table 3) is convenient for further applications. Table 4 is an example for the C_{2v} group.

Table 3

Unit subduced cycle indices for $G(/G_i)\downarrow G_j$

i \ j	$\downarrow G_1$	. . .	$\downarrow G_j$	. . .	$\downarrow G_s$
$G(/G_1)$			. . .		
. . .					
$G(/G_i)$	. . .		$\prod_{k=1}^{\upsilon_j} (s_{d_{jk}})^{\beta_k^{(ij)}}$		. . .
. . .					
$G(/G_s)$			. . .		

Table 4

Unit subduced cycle indices of C_{2v} and D_2

i \ j		$\downarrow C_1$ $\downarrow C_1$	$\downarrow C_2$ $\downarrow C_2$	$\downarrow C_{2'}$ $\downarrow C_s$	$\downarrow C_{2''}$ $\downarrow C_{s'}$	$\downarrow D_2$ $\downarrow C_{2v}$
$D_2(/C_1)$	$C_{2v}(/C_1)$	s_1^4	s_2^2	s_2^2	s_2^2	s_4
$D_2(/C_2)$	$C_{2v}(/C_2)$	s_1^2	s_1^2	s_2	s_2	s_2
$D_2(/C_{2'})$	$C_{2v}(/C_s)$	s_1^2	s_2	s_1^2	s_2	s_2
$D_2(/C_{2''})$	$C_{2v}(/C_{s'})$	s_1^2	s_2	s_2	s_1^2	s_2
$D_2(/D_2)$	$C_{2v}(/C_{2v})$	s_1	s_1	s_1	s_1	s_1
$\Sigma_i \bar{m}_{ji}$		1/4	1/4	1/4	1/4	0

3. Enumeration by using USCIs

We explicitly consider a partition of positions of a given skeleton. We then provide different sets of weights to different orbits of the skeleton. Suppose that $\Delta = \{\delta_1, \delta_2, \ldots, \delta_{|\Delta|}\}$ is a domain which contains vertices of the skeleton and $\boldsymbol{X} = \{X_1, X_2, \ldots, X_{|\boldsymbol{X}|}\}$ is a co-domain which contains atoms or ligands. Let a finite group $\boldsymbol{G}$ act on Δ in the form of the permutation representation $\boldsymbol{P}_G$ on Δ. The action of $\boldsymbol{G}$ on Δ yields a partition illustrated by fig. 1. Suppose that a weight $w_{i\alpha}(X_r)$ (for $i = 1, 2, \ldots, s$, $\alpha = 1, 2, \ldots, \alpha_i$ and $r = 1, 2, \ldots, |\boldsymbol{X}|$) is assigned to each orbit $\Delta_{i\alpha}$. We then define the weight of a function (configuration) as follows.

DEFINITION 2 (weight of function)

$$W(f) = \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \prod_{\delta \in \Delta_{i\alpha}} w_{i\alpha}(f(\delta)), \tag{11}$$

for a function $f: \Delta \to \boldsymbol{X}$, where $w_{i0}(X_r) = 1$. Then the following lemma can be proved (appendix B).

LEMMA 1

If two functions f_γ and f_ε: $\Delta \to \boldsymbol{X}$ are equivalent to each other, then

$$W(f_\gamma) = W(f_\varepsilon), \tag{12}$$

where the weights are given by eq. (8).

Let $\boldsymbol{F}^{(\theta)}$ be a set of configurations with a given weight W_θ, i.e.

$$\boldsymbol{F}^{(\theta)} = \{f_1^{(\theta)}, \ldots, f_\gamma^{(\theta)}, \ldots, f_\varepsilon^{(\theta)}, \ldots, f_{|\boldsymbol{F}|}^{(\theta)}\}. \tag{13}$$

Lemma 1 indicates that $\boldsymbol{F}^{(\theta)}$ contains one or more equivalence classes. Since eq. (8) is considered to be a mapping of $f_\gamma^{(\theta)}$ to $f_\varepsilon^{(\theta)}$ in $\boldsymbol{F}^{(\theta)}$, we can define a permutation,

$$\pi_g^{(\theta)} = \begin{pmatrix} f_1^{(\theta)} P_g^{-1} & , \ldots , & f_F^{(\theta)} P_g^{-1} \\ f_1^{(\theta)} & , \ldots , & f_F^{(\theta)} \end{pmatrix}, \tag{14}$$

which corresponds to $g \in \boldsymbol{G}$. The permutation group,

$$\Pi_{\boldsymbol{G}}^{(\theta)} = \{ \pi_g^{(\theta)} \mid \forall g \in \boldsymbol{G} \},$$

is homomorphic to $\boldsymbol{G}$ (or, equivalently, to $\boldsymbol{P}_{\boldsymbol{G}}$), since $\pi_{g'}^{(\theta)} \pi_g^{(\theta)} = \pi_{g'g}^{(\theta)}$ can be proved for $\forall g, g' \in \boldsymbol{G}$ [15].

Since $\Pi_{\boldsymbol{G}}^{(\theta)}$ is a permutation representation of $\boldsymbol{G}$, we can apply theorem 1 to this case. We thus obtain:

THEOREM 2

$$\Pi_{\boldsymbol{G}}^{(\theta)} = \sum_{i=1}^{s} A_{\theta i} \boldsymbol{G}(/\boldsymbol{G}_i), \tag{15}$$

where the multiplicities $A_{\theta i}$ are the solution of the following equation:

$$\rho_{\theta j} = \sum_{i=1}^{s} A_{\theta i} m_{ij}, \quad j = 1, 2, \ldots, s. \tag{16}$$

The values ($A_{\theta i}$) can be proved to be the numbers of configurations of $\boldsymbol{G}_i$-subsymmetry and with a weight W_θ. They are obtained by solving the set of equations (eq. (16)), once the $\rho_{\theta j}$'s are evaluated. The latter task can be accomplished by using USCIs (eq. (10)). The multiplication of USCIs over α and i yields the definition of a subduced cycle index.

DEFINITION 3

The subduced cycle index (SCI) for $\boldsymbol{G}_j$ is represented by

$$\begin{aligned} Z_G\left(\boldsymbol{G}_j ; s_{d_{jk}}^{(i\alpha)}\right) &= \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} Z\left(\boldsymbol{G}(/\boldsymbol{G}_i) \downarrow \boldsymbol{G}_j ; s_{d_{jk}}^{(i\alpha)}\right) \\ &= \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \prod_{k=1}^{v_j} \left(s_{d_{jk}}^{(i\alpha)}\right)^{\beta_k^{(ij)}}, \quad j = 1, 2, \ldots, s. \end{aligned} \tag{17}$$

In terms of definition 3, we have obtained the generating function of $\rho_{\theta j}$ in the form of:

THEOREM 3

A generating function for calculating the mark $\rho_{\theta j}$ is expressed by

$$\sum_{\theta} \rho_{\theta j} W_\theta = Z_G\left(G_j \,; s_{d_{jk}}^{(i\alpha)}\right), \tag{18}$$

wherein the right-hand side is substituted by

$$s_{d_{jk}}^{(i\alpha)} = \sum_{r=1}^{|X|} w_{i\alpha}(X_r)^{d_{jk}}. \tag{19}$$

Our target is a derivation of a novel generating function for the number (A_θ) of configurations (isomers). Equation (16) can be converted into

$$A_{\theta i} = \sum_{j=1}^{s} \rho_{\theta j} \overline{m}_{ji} , \tag{20}$$

in terms of the inverse of a mark table. Equation (20) yields an equation to give the total number of orbits of $\boldsymbol{F}^{(\theta)}$, i.e.

$$A_\theta = \sum_{i=1}^{s} A_{\theta i} = \sum_{i=1}^{s} \sum_{j=1}^{s} \rho_{\theta j} \overline{m}_{ji} . \tag{21}$$

Equation (21) leads to a generating function for A_θ as follows:

$$\begin{aligned} \sum_{\theta} A_\theta W_\theta &= \sum_{\theta}\left(\sum_{i=1}^{s} \sum_{j=1}^{s} \rho_{\theta j} \overline{m}_{ji}^{(j)}\right) W_\theta \\ &= \sum_{j=1}^{s}\left(\left(\sum_{i=1}^{s} \overline{m}_{ji}^{(j)}\right) \sum_{\theta} \rho_{\theta j} W_\theta\right). \end{aligned} \tag{22}$$

Obviously, the last term of eq. (22),

$$\sum_{\theta} \rho_{\theta j} W_\theta ,$$

is a generating function for $\rho_{\theta j}$'s, which are the marks of the subgroup $\boldsymbol{G}$ in $\Pi_G^{(\theta)}$. These have already been evaluated in theorem 3 (eq. (18)). By introducing eq. (18) into eq. (22), we find the definition of a cycle index for $\boldsymbol{G}$.

DEFINITION 4

The cycle index (CI) for $\boldsymbol{G}$ is represented by

$$Z\left(G; s_{d_{jk}}^{(i\alpha)}\right) = \sum_{j=1}^{s}\left(\left(\sum_{i=1}^{s} \overline{m}_{ji}^{(j)}\right) Z\left(G_j; s_{d_{jk}}^{(i\alpha)}\right)\right). \tag{23}$$

This CI will be proved to be equivalent to Pólya's original CI. It should be emphasized that the present definition (eq. (23)) involves variables ($s_{d_{jk}}^{(i\alpha)}$) which are pre-estimated by the subduction of CRs. We now arrive at:

THEOREM 4

A generating function for the total number of orbits of $\boldsymbol{F}^{(\theta)}$ (i.e. the number of isomers with W_θ) is represented by

$$\sum_{\theta} A_\theta W_\theta = Z\left(G; s_{d_{jk}}^{(i\alpha)}\right), \tag{24}$$

where

$$s_{d_{jk}}^{(i\alpha)} = \sum_{r=1}^{|X|} w_{i\alpha}(X_r)^{d_{jk}}. \tag{25}$$

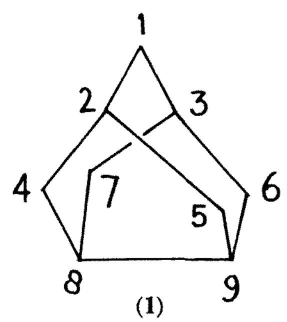
The right-hand side of eq. (24) is a novel generating function that is based on the concept of USCI and SCI.

A procedure for the enumeration discussed in this section contains the following steps:

(1) determination of the symmetry G of a parent skeleton;
(2) counting of fixed points (marks) in the G-set of the skeleton on each operation of symmetry G;
(3) determination of coset representations (CRs) by means of eqs. (1) and (2);
(4) use of USCIs corresponding to the CRs (definition 1 and table 2) and construction of an SCI in terms of definition 3 (eq. (17));
(5) calculation of the factor of each of the subduced cycle indices by summing up the elements of each row contained in the inverse of the mark table;
(6) construction of a generating function by definition 4 (eq. (23)); and
(7) introduction of figure inventories into eq. (24) (theorem 4).

The following example illustrates the procedure.

Example 1: A noradamantane skeleton (**1**) of C_{2v} symmetry.



(**1**)

We use the name *noradamantane* for octahydro-2,5-methanopentalene (**1**). The skeleton has nine positions, which are subject to $P_{C_{2v}}$ of degree 9. Its marks are obtained by counting fixed points on the action of each subgroup. Hence,

$$\mu_{C_1} = 9, \ \mu_{C_2} = 1, \ \mu_{C_s} = 3, \ \mu_{C_{s'}} = 3, \text{ and } \mu_{C_{2v}} = 1.$$

These values are introduced into eq. (2) to yield

$$(\alpha_{C_1} \ \alpha_{C_2} \ \alpha_{C_s} \ \alpha_{C_{s'}} \ \alpha_{C_{2v}})$$

$$= (9 \ 1 \ 3 \ 3 \ 1)\begin{pmatrix} 1/4 & 0 & 0 & 0 & 0 \\ -1/4 & 1/2 & 0 & 0 & 0 \\ -1/4 & 0 & 1/2 & 0 & 0 \\ -1/4 & 0 & 0 & 1/2 & 0 \\ 1/2 & -1/2 & -1/2 & -1/2 & 1 \end{pmatrix} = (1 \ 0 \ 1 \ 1 \ 1).$$

This result indicates the reduction of P_G into four coset representations, i.e.

$$P_{G_{2v}} = C_{2v}(/C_1) + C_{2v}(/C_s) + C_{2v}(/C_{s'}) + C_{2v}(/C_{2v}).$$

These CRs are permutation groups on orbits $\Delta_1 = \{4, 5, 6, 7\}$, $\Delta_2 = \{2, 3\}$, $\Delta_3 = \{8, 9\}$, and $\Delta_4 = \{1\}$, respectively. The orbits can be easily understood if we directly examine the skeleton and classify its nine positions into equivalence classes. It should be noted that the above treatment reveals the action of the CRs on the orbits.

The inverse of the mark table of C_{2v} has been found and is shown in table 5. By summing up each row of the inverse, we obtain the corresponding factors, as shown in

Table 5
The inverse of a mark table for C_{2v} and D_2

D_2	C_{2v}	$D_2(/C_1)$ $C_{2v}(/C_1)$	$D_2(/C_2)$ $C_{2v}(/C_2)$	$D_2(C_{2'})$ $C_{2v}(/C_s)$	$D_2(C_{2''})$ $C_{2v}(/C_{s'})$	$D_2(/D_2)$ $C_{2v}(/C_{2v})$	$\sum_{i=1}^{s} \bar{m}_{ji}$
C_1	C_1	1/4	0	0	0	0	1/4
C_2	C_2	−1/4	1/2	0	0	0	1/4
$C_{2'}$	C_s	−1/4	0	1/2	0	0	1/4
$C_{2''}$	$C_{s'}$	−1/4	0	0	1/2	0	1/4
D_2	C_{2v}	1/2	−1/2	−1/2	−1/2	1	0

the rightmost column of table 5. Since the above reduction indicates the use of the rows ($C_{2v}(/C_1)$, $C_{2v}(/C_s)$, $C_{2v}(/C_{s'})$ and $C_{2v}(/C_{2v})$) of table 4, definition 4 yields

$$\begin{aligned}Z(\boldsymbol{P}_{G_{2v}}) = (1/4)\{&(s_1^2)^{(1)}(s_1^2)^{(2)}(s_1^2)^{(3)}(s_1)^{(4)}\\ &+ (s_2^2)^{(1)}(s_2)^{(2)}(s_2)^{(3)}(s_1)^{(4)}\\ &+ (s_2^2)^{(1)}(s_1^2)^{(2)}(s_2)^{(2)}(s_1)^{(4)}\\ &+ (s_2^2)^{(1)}(s_2)^{(2)}(s_1^2)^{(3)}(s_1)^{(4)}\}.\end{aligned}$$

The superscripts (1) to (4) correspond to the orbits Δ_1 to Δ_4, respectively.

The OMVs of the skeleton (**1**) are 2 for Δ_1 and Δ_4, and 3 for Δ_2 and Δ_3. If we select a co-domain $\boldsymbol{X} = \{\mathrm{C, N, O}\}$, the orbits Δ_1 and Δ_4 can take C, N, and O, but the orbits Δ_2 and Δ_3 take only C and N. Hence, we determine the following weights:

$$\begin{array}{llll} w_1(\mathrm{C}) = x, & w_1(\mathrm{N}) = y, & w_1(\mathrm{O}) = z, & \text{for } \Delta_1,\\ w_2(\mathrm{C}) = x, & w_2(\mathrm{N}) = y, & w_2(\mathrm{O}) = 0, & \text{for } \Delta_2,\\ w_3(\mathrm{C}) = x, & w_3(\mathrm{N}) = y, & w_3(\mathrm{O}) = 0, & \text{for } \Delta_3,\\ w_4(\mathrm{C}) = x, & w_4(\mathrm{N}) = y, & w_4(\mathrm{O}) = z, & \text{for } \Delta_4.\end{array}$$

Hence, we obtain the following figure inventories:

$$\begin{array}{ll} s_\tau^{(1)} = x^\tau + y^\tau + y^\tau + z^\tau, & \text{for } \Delta_1,\\ s_\tau^{(2)} = x^\tau + y^\tau, & \text{for } \Delta_2,\\ s_\tau^{(3)} = x^\tau + y^\tau, & \text{for } \Delta_3,\\ s_\tau^{(4)} = x^\tau + y^\tau + z^\tau, & \text{for } \Delta_4.\end{array}$$

These equations are introduced into eq. (24) to give a generating function:

$$\begin{aligned}\sum_\theta A_\theta W_\theta = (1/4)\{&(x+y+z)^5(x+y)^4\\ &+(x^2+y^2+z^2)^2(x+y+z)(x^2+y^2)^2\\ &+(x^2+y^2+z^2)^2(x+y+z)(x+y)^2(x^2+y^2)\\ &+(x^2+y^2+z^2)^2(x+y+z)(x^2+y^2(x+y)^2\}\\ = x^9 &+ 4x^8y + 2x^8z + 13x^7y^2 + 11x^7yz + 4x^7z^2 + 27x^6y^3\\ &+38x^6y^2z + 21x^6yz^2 + 4x^6z^3 + 39x^5y^4 + 73x^5y^3z\\ &+59x^5y^2z^2 + 17x^5yz^3 + 2x^5z^4 + 39x^4y^5 + 92x^4y^4z\\ &+96x^4y^3z^2 + 42x^4y^2z^3 + 8x^4yz^4 + x^4z^5 + 27x^3y^6\end{aligned}$$

$$
\begin{aligned}
&+73x^3y^5z+96x^3y^4z^2+54x^3y^3z^3+15x^3y^2z^4+2x^3yz^5\\
&+13x^2y^7+38x^2y^6z + 59x^2y^5z^2+42x^2y^4z^3+15x^2y^3z^4\\
&+3x^2y^2z^5+4xy^8+11xy^7z+21xy^6z^2+17xy^5z^3\\
&+8xy^4z^4+2xy^3z^5+y^9+2y^8z+4y^7z^2+4y^6z^3\\
&+2y^5z^4+y^4z^5.
\end{aligned}
$$

The coefficient of the term $x^ly^mz^n$ indicates the number of isomers with $C_lN_mO_n$. Figure 2 collects C_7N_2 and C_7O_2 isomers based on the skeleton (**1**), in which unmarked vertices denote carbon atoms. The number (13) of C_7N_2 isomers appears as the coefficient of x^7y^2. The coefficient of x^7z^2 indicates that there are 4 isomers corresponding to C_7O_2. The difference between the numbers comes from the OMV restriction.

Some simplification is available so as to derive equations for special cases that do not take OMVs into account (appendix C).

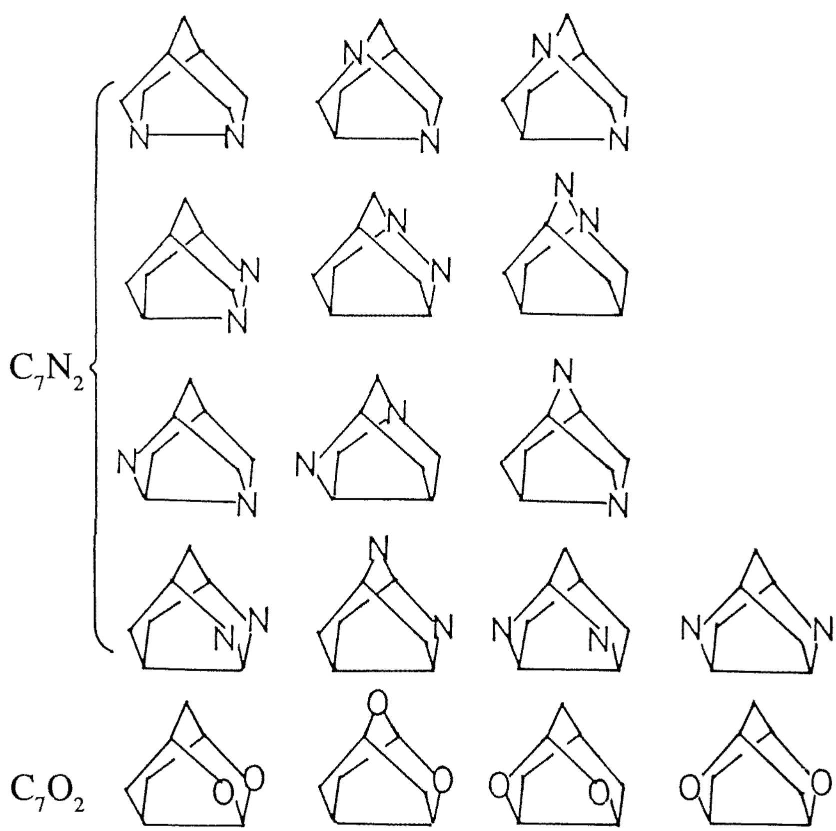


Fig. 2. Collection of C_7N_2 and C_7O_2 isomers based on the skeleton (**1**).

4. Correlation of the present method to Pólya's theorem

Equation (1) yields a partition of Δ into $\Delta_{i\alpha}$. Each coset representation $\boldsymbol{G}(/\boldsymbol{G}_i)$ is a permutation representation on $\Delta_{i\alpha}$. Suppose that $G(/G_i)_g \in \boldsymbol{G}(/\boldsymbol{G}_i)$ has a cycle structure,

$$(i_1, i_2, \ldots, i_m),$$

where

$$\sum_{\tau=1}^{m} \tau i_\tau = m \tag{26}$$

and

$$m = |\boldsymbol{G}|/|\boldsymbol{G}_i| = |\Delta_{i\alpha}|. \tag{27}$$

Note that m is dependent upon i. We then assign a variable s_τ to a cycle of length τ. Thereby, we define a unit cycle index as

$$z_g^{(i\alpha)} = \left(\prod_{\tau=1}^{m} s_\tau^{i_\tau}\right)_{(g)}^{(i\alpha)}, \tag{28}$$

for $G(/G_i)_g$. The superscript $(i\alpha)$ is concerned with the orbit $\Delta_{i\alpha}$ on which $\boldsymbol{G}(/\boldsymbol{G}_i)$ acts. By using $z_g^{(i\alpha)}$, we obtain the definition of the cycle index.

DEFINITION 5

$$\begin{aligned} Z\left(\boldsymbol{P}_G; s_\tau^{(i\alpha)}\right) &= (1/|\boldsymbol{G}|) \sum_{g\in G} \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} z_g^{(i\alpha)} \\ &= (1/|\boldsymbol{G}|) \sum_{g\in G} \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \left(\prod_{\tau=1}^{m} s_\tau^{i_\tau}\right)_{(g)}^{(i\alpha)}, \end{aligned} \tag{29}$$

where $z_g^{(i0)} = 1$. Appendix D proves the following theorem, in which Pólya's theorem is generalized to meet our requirements.

THEOREM 5

The number (A_θ) of configurations with weight W_θ is obtained in terms of a generating function:

$$\sum_{\theta} A_\theta W_\theta = Z\left(\boldsymbol{P}_G; s_\tau^{(i\alpha)}\right), \tag{30}$$

where the corresponding figure inventories are represented by

$$s_{\tau}^{(i\alpha)} = \sum_{r=1}^{|X|} w_{i\alpha}(X_r)^{\tau}. \tag{31}$$

The above two methods have yielded eq. (24) (theorem 4) and eq. (30) (theorem 5), respectively, as generating functions. These equations are different in their explicit forms. However, since both equations are generating functions for the same A_{θ}, their right-hand sides should be equal to each other. Thus, we find

$$(1/|G|) \sum_{g \in G} \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \left(\prod_{\tau=1}^{m} s_{\tau}^{i_\tau} \right)_{(g)}^{(i\alpha)}$$

$$= \sum_{j=1}^{s} \left(\left(\sum_{i=1}^{s} \overline{m}_{ji} \right) \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \prod_{k=1}^{v_j} \left(s_{d_{jk}}^{(i\alpha)} \right)^{\beta_k^{(ij)}} \right). \tag{32}$$

In order to characterize eq. (32), we should clarify the correspondence between g of the left-hand side and the subgroup G_j that is implied by the right-hand side. The following lemma (appendix D) is important in clarifying this correspondence.

LEMMA 2

(1) Suppose that $G(/G_i)$ is a coset representation on Δ. Let $h = G(/G_i)_g$ for $g \in G$ have a cycle structure:

$$(i_1, i_2, \ldots, i_m),$$

where

$$\sum_{\tau=1}^{m} \tau i_\tau = m. \tag{33}$$

Suppose that h is represented by a product of cycles,

$$h = \prod_{\tau=1}^{m} \prod_{a=1}^{i_\tau} (a_1 a_2, \ldots, a_\tau). \tag{34}$$

Let n be the least common multiple of τ (for $i_\tau \neq 0$; $\tau = 1, 2, \ldots, m$). The subgroup generated from the element h:

$$\boldsymbol{H} = \{\mathrm{I}, h, h^2, \ldots, h^{n-1}\}$$

is a cyclic group. The cyclic group ($\boldsymbol{H}$) provides a partition of $\Delta_{i\alpha}$ into i_τ orbits: $(a_1, a_2, \ldots, a_\tau)$, the length of which is τ.

(2) If q $(1 \leq q \leq n)$ is any divisor of n, an element (h^q) of $\boldsymbol{H}$ generates a cyclic subgroup,

$$\boldsymbol{H}' = \{h^q, h^{2q}, \ldots, h^{wq}(=\mathrm{I})\},$$

where $w = n/q$. This provides a further partition of $\Delta_{i\alpha}$ in which the orbit $(a_1, a_2, \ldots, a_\tau)$ is subdivided if $1 \leq q \leq \tau$ and q is a multiple of a divisor of τ.

(3) Consider the case where q' $(1 \leq q' < n)$ is no divisor of n and where q' and n have at least one common divisor. Suppose that q is the greatest common divisor of n and q'. The element $h^{q'}$ generates a cyclic subgroup which is equal to $\boldsymbol{H}'$.

(4) If q and n are co-prime, the element (h^q) has the same cycle structure as h and generates a cyclic group $\boldsymbol{H}$ that is equal to that generated by h. Note that $h^q \notin \boldsymbol{H}'$.

The above process is identical to the operation that selects the element of $\boldsymbol{H}$ from $\boldsymbol{G}(/\boldsymbol{G}_i)$. This means a consideration of $\boldsymbol{G}(/\boldsymbol{G}_i)\downarrow\boldsymbol{H}$. As a result, lemma 2 can be considered to show the reduction of $\boldsymbol{G}(/\boldsymbol{G}_i)\downarrow\boldsymbol{H}$. Hence, $\boldsymbol{G}(/\boldsymbol{G}_i)\downarrow\boldsymbol{H}$ provides i_τ orbits of length τ. If we consider that $\boldsymbol{G}_j = \boldsymbol{H}$, eq. (7) holds for this case. This fact combined with lemma 2 permits us to recognize that $\boldsymbol{G}_j(/\boldsymbol{G}_k^{(j)})$ denotes a coset representation on the orbit $(a_1, a_2, \ldots, a_\tau)$. The number of such orbits is i_τ. It follows that

$$|\boldsymbol{G}_j|/|\boldsymbol{G}_k^{(j)}| = \tau \tag{35}$$

and

$$\beta_k^{(ij)} = i_\tau, \tag{36}$$

since the degree of $\boldsymbol{G}_j(/\boldsymbol{G}_k^{(j)})$ is $|\boldsymbol{G}_j|/|\boldsymbol{G}_k^{(j)}|$, which is equal to the length of the orbit. Equation (35) combined with eq. (9) gives

$$d_{jk} = \tau. \tag{37}$$

The USCI (eq. (10)) is converted as follows in the light of eqs. (36) and (37):

$$Z\left(\boldsymbol{G}(/\boldsymbol{G}_i) \downarrow \boldsymbol{G}_j; s_{d_{jk}}\right) = \prod_{k=1}^{v_j} \left(s_{d_{jk}}^{(i\alpha)}\right)^{\beta_k^{(ij)}}$$

$$= \left(\prod_{\tau=1}^{m} s_\tau^{i_\tau}\right)_{(g)}^{(i\alpha)} = z_g^{(i\alpha)}, \tag{38}$$

where the product over k can be converted into that over τ. The superscript $i\alpha$ concerns the orbit $\Delta_{i\alpha}$. The subscript g represents the term related to $G(/G_i)_g$ $(=h)$. The subgroup $\boldsymbol{G}_j$ corresponds to g through $\boldsymbol{G}_j = \boldsymbol{H} = \{\mathrm{I}, h, h^2, \ldots, h^{n-1}\}$. Note that eq. (38) is true only if $\boldsymbol{G}_j = \boldsymbol{H}$, i.e. if $\boldsymbol{G}_j$ is a cyclic group.

If $g' \in \boldsymbol{G}$ is conjugate to $g \in \boldsymbol{G}$ or, equivalently, if the corresponding $G(/G_i)_{g'}$ $(=h')$ is conjugate to $G(/G_i)_g$ $(=h)$, the cycle structure of h is equal to that of h'. Hence,

$$z_g^{(i\alpha)} = z_{g'}^{(i\alpha)}. \tag{39}$$

The conjugate elements h and h' generate cyclic groups $\boldsymbol{H}$ and $\boldsymbol{H}'$ that are conjugate to each other.

If $g^{\tau} = g'$ ($\tau = 1, 2, \ldots,$ or m) for g and $g' \in \boldsymbol{G}$ and $G(/G_i)_g$ (=h) and $G(/G_i)_{g'}$ (=h') have the same cycle structures, the cyclic group $\boldsymbol{H}$ generated from h is obviously equal to that generated from h'.

Suppose that a cyclic group $\boldsymbol{G}_j$ has cyclic subgroups $\boldsymbol{G}_k^{(j)}$ ($k = 1, 2, \ldots, \upsilon_j - 1$). Since $|\boldsymbol{G}_k^{(j)}|$ is a divisor of $|\boldsymbol{G}_j|$, lemma 2(4) indicates that (a) if $g \in \boldsymbol{G}_j$ corresponds to the generator $h = G(/G_i)_g$ which generates $\boldsymbol{G}_j$ (=$\boldsymbol{H}$), it is not an element of any $\boldsymbol{G}_k^{(j)}$. Hence,

$$g \in \boldsymbol{G}_j - \bigcup_{k=1}^{\upsilon-1} \boldsymbol{G}_k^{(j)},$$

and (b) if $h' = G(/G_i)_{g'}$ has the same cycle structure as h,

$$g' \in \boldsymbol{G}_j - \bigcup_{k=1}^{\upsilon-1} \boldsymbol{G}_k^{(j)} \quad \text{or} \quad g' \in \boldsymbol{G}_{j'} - \bigcup_{k=1}^{\upsilon-1} \boldsymbol{G}_k^{(j')},$$

where $\boldsymbol{G}_{j'}$ is a conjugate group of $\boldsymbol{G}_j$. Hence, if σ denotes the number of groups conjugate to $\boldsymbol{G}_j$ in $\boldsymbol{G}$, the number of elements that have the same cycle structure as h is represented by

$$\sigma \left| \boldsymbol{G}_j - \bigcup_{k=1}^{\upsilon-1} \boldsymbol{G}_k^{(j)} \right| = |\boldsymbol{G}|\, \varphi(|\boldsymbol{G}_j|)/|N_G(\boldsymbol{G}_j)|,$$

where $\varphi(n)$ is the Euler function and $N_G(\boldsymbol{G}_j)$ denotes a normalizer of $\boldsymbol{G}_j$. Note that

$$\left| \boldsymbol{G}_j - \bigcup_{k=1}^{\upsilon-1} \boldsymbol{G}_k^{(j)} \right| = \varphi(|\boldsymbol{G}_j|),$$

where lemma 2(4) shows this term to be equal to the number of integers from 1 to n which are co-prime to n. The term σ has proven to be $\sigma = |\boldsymbol{G}: N_G(\boldsymbol{G}_j)| = |\boldsymbol{G}|/|N_G(\boldsymbol{G}_j)|$ [16].

If cyclic groups are generated from all $g \in \boldsymbol{G}$, they can be easily proved to construct a complete set of cyclic subgroups of $\boldsymbol{G}$. This means that the summation over $g \in \boldsymbol{G}$ on the left-hand side of eq. (32) corresponds to that over all cyclic subgroups of $\boldsymbol{G}$. Hence, on the right-hand side of eq. (32), the summation over j (or $\boldsymbol{G}_j$) is effective if and only if $\boldsymbol{G}_j$ is a cyclic group. These results can be summarized as:

THEOREM 6

$$\sum_{i=1}^{s} \overline{m}_{ji} = \frac{\varphi(|G_j|)}{|N_G(G_j)|} \quad \text{for any cyclic } G_j,$$

$$\sum_{i=1}^{s} \overline{m}_{ji} = 0 \qquad \text{for others.} \tag{40}$$

This equation is equivalent to that derived independently by Kerber [17]. The following equations are easily proved.

$$\sum_{j=1}^{s} \overline{m}_{ji} = 0, \quad i \neq s,$$
$$= 1, \quad i = s. \tag{41}$$

5. Conclusions

A novel enumeration that explicitly considers the transitivity of a given group acting on a domain is accomplished by subduction of coset representations. This method is based on novel concepts such as unit subduced cycle indices and subduced cycle indices, all of which also stem from the coset representations. The relationship between the present method and that of Pólya is discussed.

Appendix A

Coset representations and tables of marks. Let G_i be a subgroup of a finite group G. The subgroup G_i provides a coset decomposition of G, i.e.

$$G = G_i g_1 + G_i g_2 + \ldots + G_i g_m,$$

where $g_1 = \mathrm{I}$ (identity) and $g_j \in G$ (for $j = 1, 2, \ldots, m$). The set of permutations of degree m:

$$G(/G_i)_g = \begin{pmatrix} G_i g_1, & G_i g_2 & , \ldots, & G_i g_m \\ G_i g_1 g, & G_i g_2 g & , \ldots, & G_i g_m g \end{pmatrix} \quad \text{for } \forall g \in G$$

constructs a permutation representation of G. This is called a coset representation (CR) of G by G_i, which is denoted as $G(/G_i)$ in the present paper. The CR is transitive and its degree is $|G|/|G_i|$. It should be noted that two conjugate subgroups provide equivalent coset representations.

Suppose that a series of subgroups G_i ($i = 1, 2, \ldots, s$) of G are selected in such a way that conjugate subgroups are counted once. They are arranged in ascending order of their orders, where G_1 is an identity group and $G_s = G$. The corresponding CRs, i.e.

$G(/G_i)$'s, construct a complete set of transitive representations of G. The group $G(/G_1)$ is a regular representation of degree $|G|$. Obviously, $G(/G_s)$ is an identity group.

The mark of a subgroup H in G is the number of fixed points of a G set on the action of H. The symbol m_{ij} indicates the mark of subgroup G_j in $G(/G_i)$, which is the number of fixed points in the domain of $G(/G_i)$ by the action of G_j. Each element m_{ij} is constant, since G_j and $G(/G_i)$ are given. A list of m_{ij} for $\forall j$ and $\forall i$ is called a table of marks [14].

Appendix B

Proof of lemma 1. Since f_γ and f_ε are equivalent, there is a $P_g \in P_G$ that satisfies

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

Hence,

$$W(f_\gamma) = \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \prod_{\delta \in \Delta_{i\alpha}} w_{i\alpha}(f_\gamma(\delta)) = \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \prod_{\delta \in \Delta_{i\alpha}} w_{i\alpha}[f_\varepsilon(P_g(\delta))].$$

On the other hand,

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

Since the right-hand sides of these equations are equal except for the sequences of $f_\varepsilon(P_g(\delta))$ and $f_\varepsilon(\delta)$,

$$W(f_\gamma) = W(f_\varepsilon).$$

Appendix C

Special cases. If we do not consider the OMVs, we can obtain a simpler generating function. In this case, we can abbreviate the superscript $(i\alpha)$ that denotes the correspondence to each orbit. Thereby, definition 3 is converted as follows:

$$Z_G\left(G_j; s_{d_{jk}}^{(i\alpha)}\right) = \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \prod_{k=1}^{v_j} \left(s_{d_{jk}}^{(i\alpha)}\right)^{\beta_k^{(ij)}} = \prod_{k=1}^{v_j} \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \left(s_{d_{jk}}^{(i\alpha)}\right)^{\beta_k^{(ij)}}$$

$$= \prod_{k=1}^{v_j} \prod_{i=1}^{s} (s_{d_{jk}})^{\alpha_i \beta_k^{(ij)}} = \prod_{k=1}^{v_j} (s_{d_{jk}})^{\sum_{i=1}^{s} \alpha_i \beta_k^{(ij)}}.$$

Hence, we arrive at:

DEFINITION 6

(1) The SCI for this case is defined as

$$Z'_G(G_j; s_{d_{jk}}) = \prod_{k=1}^{v_j} (s_{d_{jk}})^{\sum_{i=1}^{s} \alpha_i \beta_k^{(ij)}}. \tag{C.1}$$

(2) By using the SCI (eq. (C.1)), the CI for this case is defined as

$$Z'(G; s_{d_{jk}}) = \sum_{j=1}^{s} \left(\left(\sum_{i=1}^{s} \overline{m}_{ji} \right) Z'_G(G_j; s_{d_{jk}}) \right). \tag{C.2}$$

Thereby, theorem 4 is transformed into corollary 4-1 in order to treat the present special case.

COROLLARY 4-1

A generating function without considering the OMV restriction is represented by

$$\sum_{\theta} A_\theta W_\theta = Z'(G; s_{d_{jk}}), \tag{C.3}$$

where

$$s_{d_{jk}} = \sum_{r=1}^{|X|} X_r^{d_{jk}}. \tag{C.4}$$

Note that the power:

$$\sum_{i=1}^{s} \alpha_i \beta_k^{(ij)} \tag{C.5}$$

appearing in eq. (C.1) is available from a summation of the powers contained in the unit subduced cycle indices under multiplication by α_i.

Suppose that $X_r = 1$ for all r in eq. (C.4). Then, we obtain $s_{d_{jk}} = |X|$. As a result, eq. (C.4) can be converted into corollary 4-2. which gives the total number of configurations.

COROLLARY 4-2

$$\begin{aligned} \sum_{\theta} A_\theta &= \sum_{j=1}^{s} \left(\sum_{i=1}^{s} \overline{m}_{ji} \right) \prod_{k=1}^{v_j} |X|^{\sum_{i=1}^{s} \alpha_i \beta_k^{(ij)}} \\ &= \sum_{j=1}^{s} \left(\sum_{i=1}^{s} \overline{m}_{ji} \right) |X|^{\sum_{i=1}^{s} \alpha_i \beta_{ij}}, \end{aligned} \tag{C.6}$$

where

$$\beta_{ij} = \sum_{k=1}^{s} \beta_k^{(ij)}. \tag{C.7}$$

The left-hand side of eq. (C.6), i.e. $\Sigma_\theta A_\theta$, is the total number of configurations. The term β_{ij} in eq. (C.7) is the number of sub-orbits that are derived by eq. (8).

Appendix D

Proof of theorem 5. Let $\psi(\pi_g^{(\theta)})$ be the total number of configurations with weight W_θ that are invariant under a permutation $\pi_g^{(\theta)}$ ($\in \Pi_G^{(\theta)}$). For a configuration to be invariant, the positions corresponding to each cycle of length τ have to take the same ligands, i.e. τX_1 or $\tau X_2, \ldots,$ or τX_r. Hence, the generating function for this part is obtained as follows:

$$s_\tau^{(i\alpha)} = \sum_{r=1}^{|X|} w_{i\alpha}(X_r)^\tau. \tag{D.1}$$

Since this is true for all cycles, we find the generating function for $\Delta_{i\alpha}$ on which $G(/G_i)_g$ operates, i.e.

$$\left(\prod_{\tau=1}^{m} s_\tau^{i_\tau}\right)_{(g)}^{(i\alpha)}. \tag{D.2}$$

Multiplication of this term over α and i provides a generating function:

$$\sum_\theta \psi(\pi_g^{(\theta)}) W_\theta = \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \left(\prod_{\tau=1}^{m} s_\tau^{i_\tau}\right)_{(g)}^{(i\alpha)}. \tag{D.3}$$

Note that the term s_τ of eqs. (D.2) and (D.3) is concretely expressed by eq. (D.1).

The number of fixed points $\psi(\pi_g^{(\theta)})$ of $\boldsymbol{F}^{(\theta)}$ on the action of $\pi_g^{(\theta)}$ provides the number of orbits of $\boldsymbol{F}^{(\theta)}$ through the *Cauchy–Frobenius* (so-called *Burnside*) *Lemma*:

$$A_\theta = (1/|\boldsymbol{G}|) \sum_{g \in \boldsymbol{G}} \psi(\pi_g^{(\theta)}), \tag{D.4}$$

where A_θ is the number of orbits of $\boldsymbol{F}^{(\theta)}$. The Cauchy–Frobenius Lemma (eq. (D.4)) gives the generating function for A_θ:

$$\begin{aligned}\sum_\theta A_\theta W_\theta &= \sum_\theta \left((1/|\boldsymbol{G}|) \sum_{g \in \boldsymbol{G}} \psi(\pi_g^{(\theta)}) \right) W_\theta \\ &= (1/|\boldsymbol{G}|) \sum_{g \in \boldsymbol{G}} \left(\sum_\theta \psi(\pi_g^{(\theta)}) W_\theta \right).\end{aligned} \tag{D.5}$$

The introduction of eq. (D.2) into eq. (D.3) yields

$$\sum_{\theta} A_{\theta} W_{\theta} = (1/|\boldsymbol{G}|) \sum_{g \in \boldsymbol{G}} \prod_{i=1}^{s} \prod_{\alpha=0}^{\alpha_i} \left(\prod_{\tau=1}^{m} s_{\tau}^{i_{\tau}} \right)_{(g)}^{(i\alpha)} . \tag{D.6}$$

A comparison between eqs. (29) and (D.6) yields theorem 5, which is a generalization of Pólya's theorem.

Appendix E

Proof of lemma 2. Consider $h = \boldsymbol{G}(/\boldsymbol{G}_i)_g \in \boldsymbol{G}(/\boldsymbol{G}_i)$ for a given $g \in \boldsymbol{G}$. We then construct a series of elements:

$$\boldsymbol{H} = \{h, h^2, \ldots, h^{n-1}, h^n(=\mathrm{I})\}.$$

Obviously, $\boldsymbol{H}$ is a cyclic group that is a subgroup of $\boldsymbol{G}(/\boldsymbol{G}_i)$ generated from the generator h. Let us first consider the case where h consists of a single cycle, i.e.

$$h = (a_1\ a_2, \ldots, a_n) = \begin{pmatrix} a_1, a_2 & , \ldots, & a_{n-1}, a_n \\ a_2, a_3 & , \ldots, & a_n, \ \ a_1 \end{pmatrix}.$$

As a result,

$$h^2 = \begin{pmatrix} a_1, & a_2 & , \ldots, & a_{n-2}, & a_{n-1}, & a_n \\ a_3, & a_4 & , \ldots, & a_n, & a_1, & a_2 \end{pmatrix},$$

$$h^3 = \begin{pmatrix} a_1, & a_2 & , \ldots, & a_{n-2}, & a_{n-1}, & a_n \\ a_4, & a_5 & , \ldots, & a_1, & a_2, & a_3 \end{pmatrix},$$

...

$$h^n = \begin{pmatrix} a_1, & a_2 & , \ldots, & a_{n-2}, & a_{n-1}, & a_n \\ a_1, & a_2 & , \ldots, & a_{n-2}, & a_{n-1}, & a_n \end{pmatrix} = \mathrm{I}.$$

This process implies that each of these permutations can be represented by a product of several cycles, all of which have length n or less. Therefore, the cyclic group $\boldsymbol{H} = \{\mathrm{I}, h, \ldots, h^{n-1}\}$ on $\Delta = \{1, 2, \ldots, n\}$ provides a single orbit of Δ, which has a length n.

A cyclic group of finite order generally has only one subgroup of which the order is equal to any divisor of the order of the cyclic group. The set of such subgroups is the complete set of the subgroup of the cyclic group. Now, we consider h^q $(1 \leq q < n)$ to be a generator of such a cyclic group. As a result, when q $(1 \leq q < n)$ is a divisor of n, the generator h^q yields

$$H' = \{h^q, h^{2q}, \ldots, h^{wq}(=\mathrm{I})\},$$

which is a subgroup of $\boldsymbol{H}$, where $w = n/q$. Note that $|\boldsymbol{H}'| = w$. In this case, if we divide the permutation h^q into w parts of equal length q, we obtain the following relation:

$$h^q = \begin{pmatrix} a_1 & ,\ldots, & a_{q+1} & ,\ldots, & a_{2q+1} & ,\ldots, & \ldots, & a_{(w-1)q+1}, & \ldots \\ a_{q+1} & ,\ldots, & a_{2q+1} & ,\ldots, & a_{3q+1} & ,\ldots, & \ldots, & a_1, & \ldots \end{pmatrix}$$
$$= (a_1\, a_{q+1} \ldots a_{n-q+1})(a_2 \ldots a_{n-q+2}) \ldots (a_q \ldots a_n).$$

This indicates that h^q is the product of q cycles of length w. Hence, $\boldsymbol{H}'$ on $\Delta_{i\alpha}$ provides q orbits, each of which has a length w.

Let us next consider the case in which q' $(1 \le q' < n)$ is no divisor of n but that we can suppose that n and q' have common divisors. Let q be the greatest common divisor of n and q', where $q' = aq$. Since q is a divisor of n, we can assume that $h^{wq} = \mathrm{I}$. Hence, we can obtain $(h^{q'})^w = (h^{aq})^w = \mathrm{I}$ and $(h^{q'})^{w+b} = (h^{q'})^w (h^{q'})^b = (h^{q'})^b$, where a and b are integers. These equations indicate that $h^{q'}$ generates $\boldsymbol{H}'$, which is equal to the cyclic group generated by h^q.

The third case is that q' $(1 \le q' < n)$ is not a multiple of any q (i.e. q' and n are co-prime). The permutation $h^{q'}$ has the same cycle structure as h, since such a division as above is impossible. Therefore, $h^{q'}$ generates H, which is the same as the cyclic group generated by h. In terms of the definition, $h^{q'} \notin \boldsymbol{H}'$. Obviously, the generator h is not an element of any $\boldsymbol{H}'$.

Let us next extend these results to a more general case. Suppose that h has a cycle structure $(i_1, i_2, \ldots, i_m)$. This cycle structure means that h contains i_τ cycles of length τ, i.e.

$$h = \prod_{\tau=1}^{m} \prod_{a=1}^{i_\tau} (a_1\, a_2, \ldots, a_\tau).$$

Let n be the least common multiple of τ's in which the τ's are selected from $1, 2, \ldots, m$ if $i_\tau \ne 0$. If we consider $h^2, h^3, \ldots, h^n(=\mathrm{I})$, the above discussion on a single cycle applies to each of the cycles of the present case. Therefore, the cyclic group $\boldsymbol{H} = \{\mathrm{I}, h, h^2, \ldots, h^{n-1}\}$ on Δ provides a partitioning of Δ into orbits, the lengths of which are τ $(\tau = 1, 2, \ldots, m)$ if $i_\tau \ne 0$. The above discussions have proved lemma 2.

References

[1] G. Pólya, Acta Math. 68(1937)145.

[2] (a) G. Pólya and R.C. Read, *Combinatorial Enumeration of Groups, Graphs and Chemical Compounds* (Springer, New York–Berlin–Heidelberg, 1987);
(b) C.L. Liu, *Introduction to Combinatorial Mathematics* (McGraw–Hill, New York, 1969) Ch. 5.

[3] N.G. De Bruijn, Indag. Math. 21(1959)59.

[4] F. Harary and E. Palmer, J. Comb. Theory 1(1966)157.
[5] W. Hässelbarth, Theor. Chim. Acta 66(1984)91.
[6] (a) A.T. Balaban (ed.), *Chemical Application of Graph Theory* (Academic Press, London, 1976);
(b) D.H. Rouvray, Chem. Soc. Rev. 3(1974)355;
(c) S. Fujita, J. Chem. Inf. Comput. Sci. 26(1986)212, 224; 27(1987)99, 104.
[7] E. Ruch, W. Hässelbarth and B. Richter, Theor. Chim. Acta 19(1970)288.
[8] W. Hässelbarth, Theor. Chim. Acta 67(1985)339.
[9] J. Brocas, J. Amer. Chem. Soc. 108(1986)1135.
[10] C.A. Mead, J. Amer. Chem. Soc. 109(1987)2130.
[11] J.B. Hendrickson, Angew. Chem., Int. Ed. 13(1974)47.
[12] D.H. McDaniel, Inorg. Chem. 11(1972)2678.
[13] (a) S. Fujita, Bull. Chem. Soc. Japan 61(1988)4189;
(b) S. Fujita, Theor. Chim. Acta 76(1989)247;
(c) S. Fujita, Bull. Chem. Soc. Japan 62(1989)3771;
(d) S. Fujita, Tetrahedron 46(1990)365;
(e) S. Fujita, Bull. Chem. Soc. Japan 63(1990)203.
[14] W. Burnside, *Theory of Groups of Finite Order*, 2nd Ed. (Cambridge University Press, Cambridge, 1911).
[15] For the proof, see ref. [13(a)].
[16] T. Oyama, *Yugen Chikan-Gun (Theory of Permutation Groups of Finite Order)* (Shokabo, Tokyo, 1981).
[17] A. Kerber and K.-J, Thürlings, in: *Lecture Notes in Mathematics*, Vol. 969 (Springer, New York, 1982), p. 191.