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Direct subduction of Q-conjugacy representations to give characteristic monomials for combinatorial enumeration

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Abstract. Characteristic monomials for a finite group are obtained by direct subductions of **Q**-conjugate representations. They are shown to give a generating function that is capable of solving enumeration problems.

Key words: Characteristic monomial table – Direct subduction – Isomer enumeration – **Q**-conjugacy character table – Markaracter table

1 Introduction

Major problems of chemical group theory are concerned with electronic and vibrational spectra, symmetry properties of molecular orbitals, stereochemical properties of molecules, etc. They have been treated mainly by means of approaches based on linear representations and irreducible representations [1]. Such types of approach have been the central topics of most textbooks on chemical group theory [2–10].

On the other hand, an alternative type of approach based on permutation representations and coset representations [11–14] has been applied to such problems as combinatorial enumeration of isomers [15–23].

Throughout a series of papers [24–28], we have been aiming at integrating both types of approach so as to obtain a broader prospect of chemical symmetry. As a result, the first type of approach has been extended to be capable of being applied to enumeration problems of no original territory. Thus, we have reported a method of combinatorial enumeration based on characteristic monomial tables, where the subduction of **Q**-conjugacy representations has been a key concept for deriving such characteristic monomial tables from **Q**-conjugacy character tables [26–28]. Although the subduction process reported gives a full set of mathematical derivations [28], it is so indirect that (1) each **Q**-conjugacy character of **G** is converted into a linear combination of dominant markaracters $[\mathbf{G}(/\mathbf{G}_i)]$ and (2) each dominant markaracter is in turn subducted into respective cyclic subgroups $\mathbf{G}_j$ to give a linear combination of the markaracters of $\mathbf{G}_j$. In particular, it is a disadvantage for the indirect subduction to involve rather tedious calculations, because the coefficients in the linear combination of step (1) are rational numbers.

The subduction of **Q**-conjugacy representations can be performed directly if each **Q**-conjugacy character of **G** is subducted into a cyclic subgroup $\mathbf{G}_j$ to give a linear combination of the markaracters of $\mathbf{G}_j$. The present paper deals with direct subductions, which are as useful as, but simpler than indirect subductions for deriving characteristic monomials.

2 Direct subductions versus indirect subductions

2.1 Indirect subductions

As shown in the next subsection, direct subductions are derived by omitting intermediate steps of the indirect subductions reported in a previous paper [28]. In order to show the intermediate steps omitted, the indirect subductions are formulated with matrix expressions in place of the previous expressions by linear equations [28]. Suppose a finite group **G** has a **Q**-conjugacy representation $\widehat{\Theta}_\ell$ with a **Q**-conjugacy character $\widehat{\theta}_\ell$, which appears as a row vector in a **Q**-conjugacy character table of **G**:

$$D_{\mathbf{G}} = \begin{pmatrix} \widehat{\theta}_1 \\ \widehat{\theta}_2 \\ \vdots \\ \widehat{\theta}_\ell \\ \vdots \\ \widehat{\theta}_s \end{pmatrix} = \begin{array}{c} \\ \widehat{\Theta}_1 \\ \widehat{\Theta}_2 \\ \vdots \\ \widehat{\Theta}_\ell \\ \vdots \\ \widehat{\Theta}_s \end{array} \begin{array}{c} \begin{array}{ccccccc} \downarrow \mathbf{G}_1 & \downarrow \mathbf{G}_2 & & \downarrow \mathbf{G}_j & & \downarrow \mathbf{G}_s \end{array} \\ \begin{pmatrix} \widehat{\theta}_{11} & \widehat{\theta}_{12} & \cdots & \widehat{\theta}_{1j} & \cdots & \widehat{\theta}_{1s} \\ \widehat{\theta}_{21} & \widehat{\theta}_{22} & \cdots & \widehat{\theta}_{2j} & \cdots & \widehat{\theta}_{2s} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ \widehat{\theta}_{\ell 1} & \widehat{\theta}_{\ell 2} & \cdots & \widehat{\theta}_{\ell j} & \cdots & \widehat{\theta}_{\ell s} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ \widehat{\theta}_{s1} & \widehat{\theta}_{s2} & \cdots & \widehat{\theta}_{sj} & \cdots & \widehat{\theta}_{ss} \end{pmatrix} \end{array} \tag{1}$$

Since such a **Q**-conjugacy representation $\widehat{\Theta}_\ell$ is a matured representation, its character $\widehat{\theta}_\ell$ is expressed by a linear combination of dominant markaracters:

$$\widehat{\theta}_\ell = \sum_{i=1}^{\mathrm{s}} \alpha_{\ell i} \mathbf{G}(/\mathbf{G}_i) \tag{2}$$

for $\ell = 1, 2, \ldots, \mathrm{s}$, where each coefficient $\alpha_{\ell i}$ is a rational number. For simplicity, the symbol $\mathbf{G}(/\mathbf{G}_i)$ is used for denoting dominant representations as well as the corresponding dominant markaracters. When the coefficients are collected to give a row vector called a mutliplicity vector,

$$\alpha_\ell = (\alpha_{\ell 1}, \alpha_{\ell 2}, \ldots, \alpha_{\ell \mathrm{s}}) \tag{3}$$

for $\ell = 1, 2, \ldots, \mathrm{s}$, the coefficients are obtained by solving linear equations or equivalently by calculating a matrix equation,

$$\widehat{\theta}_\ell \widetilde{M}^{-1}{}_{\mathbf{G}} = \alpha_\ell \tag{4}$$

for $\ell = 1, 2, \ldots, \mathrm{s}$, where the matrix $\widetilde{M}_{\mathbf{G}}^{-1}$ appearing in the left-hand side is the inverse of a markaracter table of $\mathbf{G}$, i.e.,

$$\widetilde{M}_{\mathbf{G}} = \begin{array}{c} \\ \mathbf{G}(/\mathbf{G}_1) \\ \mathbf{G}(/\mathbf{G}_2) \\ \vdots \\ \mathbf{G}(/\mathbf{G}_i) \\ \vdots \\ \mathbf{G}(/\mathbf{G}_\mathrm{s}) \end{array} \begin{array}{c} \begin{array}{cccccc} \downarrow \mathbf{G}_1 & \downarrow \mathbf{G}_2 & & \downarrow \mathbf{G}_i & & \downarrow \mathbf{G}_\mathrm{s} \end{array} \\ \begin{pmatrix} m_{11} & & & & & \\ m_{21} & m_{22} & & & & \\ \vdots & \vdots & \ddots & & & \\ m_{i1} & m_{i2} & \cdots & m_{ii} & & \\ \vdots & \vdots & & \vdots & \ddots & \\ m_{\mathrm{s}1} & m_{\mathrm{s}2} & \cdots & m_{\mathrm{s}i} & \cdots & m_{\mathrm{ss}} \end{pmatrix} \end{array} \tag{5}$$

Equation 4 is transformed into

$$\widehat{\theta}_\ell = \alpha_\ell \widetilde{M}_{\mathbf{G}} \tag{6}$$

for $\ell = 1, 2, \ldots, \mathrm{s}$, which is formally related to Eq. (2) by regarding each row of $\widetilde{M}_{\mathbf{G}}$ as a row vector denoted by the symbol $\mathbf{G}(/\mathbf{G}_i)$. The method reported in the previous paper [28] is based on Eq. (4) or Eq. (6), in which such coefficients of rational numbers are calculated.

By collecting the multiplicity vectors (Eq. 3), we construct an $\mathrm{s} \times \mathrm{s}$ multiplicity matrix A as follows:

$$A = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \\ \vdots \\ \alpha_\mathrm{s} \end{pmatrix} = \begin{array}{c} \begin{array}{cccccc} \mathbf{G}(/\mathbf{G}_1) & \mathbf{G}(/\mathbf{G}_2) & & \mathbf{G}(/\mathbf{G}_i) & & \mathbf{G}(/\mathbf{G}_\mathrm{s}) \end{array} \\ \begin{pmatrix} \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1i} & \cdots & \alpha_{1\mathrm{s}} \\ \alpha_{21} & \alpha_{22} & \cdots & \alpha_{2i} & \cdots & \alpha_{2\mathrm{s}} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ \alpha_{\ell 1} & \alpha_{\ell 2} & \cdots & \alpha_{\ell i} & \cdots & \alpha_{\ell \mathrm{s}} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ \alpha_{\mathrm{s}1} & \alpha_{\mathrm{s}2} & \cdots & \alpha_{\mathrm{s}i} & \cdots & \alpha_{\mathrm{ss}} \end{pmatrix} \end{array} \tag{7}$$

Thereby, Eq. (6) is transformed into a matrix expression,

$$D_{\mathbf{G}} = A\widetilde{M}_{\mathbf{G}} \ . \tag{8}$$

The subduction of each dominant representation $\mathbf{G}(/\mathbf{G}_\ell) \downarrow \mathbf{G}_j$ gives a linear combination of the dominant representations of $\mathbf{G}_j$.

$$\mathbf{G}(/\mathbf{G}_\ell) \downarrow \mathbf{G}_j = \sum_{k=1}^{r} \beta_{\ell k}^{(j)} \mathbf{G}_j(/\mathbf{G}_k^{(j)}) \tag{9}$$

The coefficients $\beta_{\ell k}(j)$ $(k = 1, 2, \ldots, r)$ of the linear combination are calculated by

$$\widetilde{M}_{\mathbf{G}\downarrow\mathbf{G}_j} \widetilde{M}^{-1}{}_{\mathbf{G}_j} = B_{\mathbf{G}_j} \tag{10}$$

The symbol $\widetilde{M}_{\mathbf{G}\downarrow\mathbf{G}_j}$ in the left-hand side of Eq. (10) represents an $\mathrm{s} \times r$ subducted matrix, in which the columns corresponding to the subgroups of $\mathbf{G}_j$ are collected from $\widetilde{M}_{\mathbf{G}}$, i.e.,

$$\widetilde{M}_{\mathbf{G}\downarrow\mathbf{G}_j} = \begin{array}{c} \\ \mathbf{G}(/\mathbf{G}_1) \downarrow \mathbf{G}_j \\ \mathbf{G}(/\mathbf{G}_2) \downarrow \mathbf{G}_j \\ \vdots \\ \mathbf{G}(/\mathbf{G}_k) \downarrow \mathbf{G}_j \\ \vdots \\ \mathbf{G}(/\mathbf{G}_r) \downarrow \mathbf{G}_j \\ \vdots \\ \mathbf{G}(/\mathbf{G}_\mathrm{s}) \downarrow \mathbf{G}_j \end{array} \begin{array}{c} \begin{array}{cccccc} \downarrow \mathbf{G}_1^{(j)} & \downarrow \mathbf{G}_2^{(j)} & & \downarrow \mathbf{G}_k^{(j)} & & \downarrow \mathbf{G}_r^{(j)} \end{array} \\ \begin{pmatrix} m_{11}^{(j)} & & & & & \\ m_{21}^{(j)} & m_{22}^{(j)} & & & & \\ \vdots & \vdots & \ddots & & & \\ m_{k1}^{(j)} & m_{k2} & \cdots & m_{kk}^{(j)} & & \\ \vdots & \vdots & & \vdots & \ddots & \\ m_{r1}^{(j)} & m_{r2}^{(j)} & \cdots & m_{rk}^{(j)} & \cdots & m_{rr}^{(j)} \\ \vdots & \vdots & & \vdots & & \vdots \\ m_{\mathrm{s}1}^{(j)} & m_{\mathrm{s}2}^{(j)} & \cdots & m_{\mathrm{s}k}^{(j)} & \cdots & m_{\mathrm{s}r}^{(j)} \end{pmatrix} \end{array}, \tag{11}$$

and the symbol $\widetilde{M}_{\mathbf{G}_j}^{-1}$ represents the inverse matrix of the dominant markaracter table of the subgroup $\mathbf{G}_j$. The symbol $B_{\mathbf{G}_j}$ in the right-hand side of Eq. (10) represents an $\mathrm{s} \times r$ multiplicity matrix,

$$B_{\mathbf{G}_j} = \begin{array}{c} \begin{array}{cccccc} \mathbf{G}_j(/\mathbf{G}_1^{(j)}) & \mathbf{G}_j(/\mathbf{G}_2^{(j)}) & & \mathbf{G}_j(/\mathbf{G}_k^{(j)}) & & \mathbf{G}_j(/\mathbf{G}_r^{(j)}) \end{array} \\ \begin{pmatrix} \beta_{11}^{(j)} & \beta_{12}^{(j)} & \cdots & \beta_{1k}^{(j)} & \cdots & \beta_{1r}^{(j)} \\ \beta_{21}^{(j)} & \beta_{22}^{(j)} & \cdots & \beta_{2k}^{(j)} & \cdots & \beta_{2r}^{(j)} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ \beta_{\ell 1}^{(j)} & \beta_{\ell 2}^{(j)} & \cdots & \beta_{\ell k}^{(j)} & \cdots & \beta_{\ell r}^{(j)} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ \beta_{\mathrm{s}1}^{(j)} & \beta_{\mathrm{s}2}^{(j)} & \cdots & \beta_{\mathrm{s}k}^{(j)} & \cdots & \beta_{\mathrm{s}r}^{(j)} \end{pmatrix} \end{array} \tag{12}$$

For convenience, we use a row vector $\beta_\ell^{(j)}$ selected from the matrix $B_{\mathbf{G}_j}$, i.e.,

$$\beta_\ell^{(j)} = (\beta_{\ell 1}^{(j)}, \beta_{\ell 2}^{(j)}, \ldots, \beta_{\ell r}^{(j)}) \tag{13}$$

for $\ell = 1, 2, \ldots, \mathrm{s}$. Both sides of Eq. (10) are multiplied by the multiplicity matrix A to give

$$A\widetilde{M}_{\mathbf{G}\downarrow\mathbf{G}_j} \widetilde{\mathrm{M}}_{\mathbf{G}_j}^{-1} = AB_{\mathbf{G}_j} = X_{\mathbf{G}_j}, \tag{14}$$

where the symbol $X_{\mathbf{G}_j}$ represents an $\mathrm{s} \times r$ multiplicity matrix,

$$X_{\mathbf{G}_j} = \begin{array}{c} \begin{array}{cccccc} \mathbf{G}_j(/\mathbf{G}_1^{(j)}) & \mathbf{G}_j(/\mathbf{G}_2^{(j)}) & & \mathbf{G}_j(/\mathbf{G}_k^{(j)}) & & \mathbf{G}_j(/\mathbf{G}_r^{(j)}) \end{array} \\ \begin{pmatrix} \chi_{11}^{(j)} & \chi_{12}^{(j)} & \cdots & \chi_{1k}^{(j)} & \cdots & \chi_{1r}^{(j)} \\ \chi_{21}^{(j)} & \chi_{22}^{(j)} & \cdots & \chi_{2k}^{(j)} & \cdots & \chi_{2r}^{(j)} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ \chi_{\ell 1}^{(j)} & \chi_{\ell 2}^{(j)} & \cdots & \chi_{\ell k}^{(j)} & \cdots & \chi_{\ell r}^{(j)} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ \chi_{\mathrm{s}1}^{(j)} & \chi_{\mathrm{s}2}^{(j)} & \cdots & \chi_{\mathrm{s}k}^{(j)} & \cdots & \chi_{\mathrm{s}r}^{(j)} \end{pmatrix} \end{array} \tag{15}$$

2.2 Direct subductions

In Sect 2.1 we calculated the multiplicity matrix A, which we introduced into Eq. (14) to obtain $X_{\mathbf{G}_j}$. However, the following discussion will show that calculation of A is unnecessary for obtaining $X_{\mathbf{G}_j}$.

Compare $A\widetilde{M}_{\mathbf{G}\downarrow\mathbf{G}_j}$ in the left-hand side of Eq. (14) with $A\widetilde{M}_{\mathbf{G}}$ in the right-hand side of Eq. (8). Since the former can be derived from the latter by subduction, Eq. (8) gives

$$D_{\mathbf{G}\downarrow\mathbf{G}_j} = A\widetilde{M}_{\mathbf{G}\downarrow\mathbf{G}_j} \quad , \tag{16}$$

where $D_{\mathbf{G}\downarrow\mathbf{G}_j}$ in the left-hand side is generated from $D_{\mathbf{G}}$ (Eq. 1) by collecting the columns related to the subgroups of $\mathbf{G}_j$, i.e.,

$$D_{\mathbf{G}\downarrow\mathbf{G}_j} = \begin{array}{c} \\ \widehat{\Theta}_1 \downarrow \mathbf{G}_j \\ \widehat{\Theta}_2 \downarrow \mathbf{G}_j \\ \vdots \\ \widehat{\Theta}_\ell \downarrow \mathbf{G}_j \\ \vdots \\ \widehat{\Theta}_s \downarrow \mathbf{G}_j \end{array} \begin{array}{c} \begin{array}{ccccccc} \downarrow \mathbf{G}_1^{(j)} & \downarrow \mathbf{G}_2^{(j)} & & \downarrow \mathbf{G}_k^{(j)} & & \downarrow \mathbf{G}_r^{(j)} \end{array} \\ \left(\begin{array}{ccccccc} \widehat{\theta}_{11}^{(j)} & \widehat{\theta}_{12}^{(j)} & \cdots & \widehat{\theta}_{1k}^{(j)} & \cdots & \widehat{\theta}_{1r}^{(j)} \\ \widehat{\theta}_{21}^{(j)} & \widehat{\theta}_{22}^{(j)} & \cdots & \widehat{\theta}_{2k}^{(j)} & \cdots & \widehat{\theta}_{2r}^{(j)} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ \widehat{\theta}_{\ell 1}^{(j)} & \widehat{\theta}_{\ell 2}^{(j)} & \cdots & \widehat{\theta}_{\ell k}^{(j)} & \cdots & \widehat{\theta}_{\ell r}^{(j)} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ \widehat{\theta}_{s1}^{(j)} & \widehat{\theta}_{s2}^{(j)} & \cdots & \widehat{\theta}_{sk}^{(j)} & \cdots & \widehat{\theta}_{sr}^{(j)} \end{array} \right) \end{array} . \tag{17}$$

By introducing Eq. (16) into Eq. (14), we obtain

$$D_{\mathbf{G}\downarrow\mathbf{G}_j}\widetilde{M}^{-1}{}_{\mathbf{G}_j} = X_{\mathbf{G}_j} \quad . \tag{18}$$

The matrix expression (Eq. 18) does not contain the intermediate matrix A [eq. (7)]. This fact is the basis of naming the method "direct subduction". The disscussion is summarized into a theorem, in which the matrix expression is transformed into another formulation using row vectors.

Theorem 1: *The multiplicity vectors represented by*

$$\chi_\ell^{(j)} = (\chi_{\ell 1}^{(j)}, \chi_{\ell 2}^{(j)}, \ldots, \chi_{\ell k}^{(j)}, \ldots, \chi_{\ell r}^{(j)}) \tag{19}$$

are obtained by

$$[\widehat{\theta}_\ell \downarrow \mathbf{G}_j]\widetilde{M}^{-1}{}_{\mathbf{G}_j} = \chi_\ell^{(j)} \tag{20}$$

for $\ell = 1, 2, \ldots, s$. *The symbol* $[\widehat{\theta}_\ell \downarrow \mathbf{G}_j]$ *represents the row vector obtained by the subduction* ($D_{\mathbf{G}\downarrow\mathbf{G}_j}$).

This theorem gives a direct method of subduction of **Q**-conjugacy representations with characters $\widehat{\theta}_\ell$ into a cyclic subgroup $\mathbf{G}_j$.

Each element of the multiplicity vector [$\chi_{\ell k}^{(j)}$ in Eq. (19)] represents the multiplicity of the coset representation $\mathbf{G}_j(/\mathbf{G}_k^{(j)})$, the degree of which is equal to $d_{jk} = |\mathbf{G}_j|/|\mathbf{G}_k^{(j)}|$. This value represents the size of the corresponding orbit, to which a dummy variable $s_{d_{jk}}$ is assigned. Thereby, we define a characteristic monomial as follows by using the multiplicity vector (Eq. 19).

$$Z(\widehat{\theta}_\ell \downarrow \mathbf{G}_j; s_{d_{jk}}) = \prod_{k=1}^{r} s_{d_{jk}}^{\chi_{\ell k}^{(j)}} \tag{21}$$

Example 1: Let us examine the point group **T**, which has a **Q**-conjugacy character table:

$$D_{\mathbf{T}} = \begin{array}{c} \\ A \\ E \\ T \end{array} \begin{array}{c} \begin{array}{ccc} \downarrow \mathbf{C}_1 & \downarrow \mathbf{C}_2 & \downarrow \mathbf{C}_3 \end{array} \\ \left(\begin{array}{ccc} 1 & 1 & 1 \\ 2 & 2 & -1 \\ 3 & -1 & 0 \end{array} \right) \end{array} \tag{22}$$

The monomials for the column $\downarrow \mathbf{C}_2$ are obtained by direct subduction. We select the $\downarrow \mathbf{C}_1$ and $\downarrow \mathbf{C}_2$ columns from the **Q**-conjugacy character table of **T** to form a 3×2 matrix. This matrix is multiplied by the inverse ($\widetilde{M}^{-1}{}_{\mathbf{C}_2}$) of the markaracter table of $\mathbf{C}_2$.

$$\begin{aligned} & \begin{pmatrix} 1 & 1 \\ 2 & 2 \\ 3 & -1 \end{pmatrix} \begin{array}{c} \widetilde{M}^{-1}{}_{\mathbf{C}_2} \\ \begin{pmatrix} \frac{1}{2} & 0 \\ -\frac{1}{2} & 1 \end{pmatrix} \end{array} \\ & = \begin{array}{c} \\ A \\ E \\ T \end{array} \begin{array}{c} \begin{array}{cc} \mathbf{C}_2(/\mathbf{C}_1) & \mathbf{C}_2(/\mathbf{C}_2) \end{array} \\ \left(\begin{array}{cc} 0 & 1 \\ 0 & 2 \\ 2 & -1 \end{array} \right) \end{array} \begin{array}{c} \\ \cdots \\ \cdots \\ \cdots \end{array} \begin{array}{c} \underline{\downarrow \mathbf{C}_2} \\ s_1 \\ s_1^2 \\ s_1^{-1}s_2^2 \end{array} \end{aligned} \tag{23}$$

The resulting 3×2 matrix contains the multiplicities of dominant markaracters of $\mathbf{C}_2$:

$$A \downarrow \mathbf{C}_2 = \mathbf{C}_2(/\mathbf{C}_2)$$
$$E \downarrow \mathbf{C}_2 = 2\mathbf{C}_2(/\mathbf{C}_2)$$
$$T \downarrow \mathbf{C}_2 = 2\mathbf{C}_2(/\mathbf{C}_1) + \mathbf{C}_2(/\mathbf{C}_2)$$

Since the sizes of orbits are calculated to be $|\mathbf{C}_2|/|\mathbf{C}_1| = 2$ and $|\mathbf{C}_2|/|\mathbf{C}_2| = 1$, we obtain characteristic monomials, as shown after dotted lines in Eq. (23).

The monomials for the column $\downarrow \mathbf{C}_3$ are also obtained by direct subduction. We use the inverse ($\widetilde{M}^{-1}{}_{\mathbf{C}_3}$) of the markaracter table of $\mathbf{C}_3$.

$$\begin{aligned} & \begin{pmatrix} 1 & 1 \\ 2 & -1 \\ 3 & 0 \end{pmatrix} \begin{array}{c} \widetilde{M}^{-1}{}_{\mathbf{C}_3} \\ \begin{pmatrix} \frac{1}{3} & 0 \\ -\frac{1}{3} & 1 \end{pmatrix} \end{array} \\ & = \begin{array}{c} \\ A \\ E \\ T \end{array} \begin{array}{c} \begin{array}{cc} \mathbf{C}_3(/\mathbf{C}_1) & \mathbf{C}_3(/\mathbf{C}_3) \end{array} \\ \left(\begin{array}{cc} 0 & 1 \\ 1 & -1 \\ 1 & 0 \end{array} \right) \end{array} \begin{array}{c} \\ \cdots \\ \cdots \\ \cdots \end{array} \begin{array}{c} \underline{\downarrow \mathbf{C}_3} \\ s_1 \\ s_1^{-1}s_3 \\ s_3 \end{array} \end{aligned} \tag{24}$$

The monomials for $\downarrow \mathbf{C}_1$ are obtained directly from the first column of $D_{\mathbf{T}}$ (Eq. 22) to be s_1, s_1^2, and s_1^3, the powers of which appear in the first column. All the monomials obtained above are collected to give a characteristic nomomial table for **T** (Table 1). □

Example 2: Let us examine the point group $\mathbf{D}_{2d}$, which has a **Q**-conjugacy character table:

$$D_{\mathbf{D}_{2d}} = \begin{array}{c} \\ A_1 \\ A_2 \\ B_1 \\ B_2 \\ E \end{array} \begin{array}{c} \begin{array}{ccccc} \downarrow \mathbf{C}_1 & \downarrow \mathbf{C}_2 & \downarrow \mathbf{C}_2' & \downarrow \mathbf{C}_s & \downarrow \mathbf{S}_4 \end{array} \\ \left(\begin{array}{ccccc} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 & -1 \\ 2 & -2 & 0 & 0 & 0 \end{array} \right) \end{array} \tag{25}$$

Table 1. Characteristic monomials for **T**

T	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_2$	$\downarrow \mathbf{C}_3$
A	s_1	s_1	s_1
E	s_1^2	s_1^2	$s_1^{-1}s_3$
T	s_1^3	$s_1^{-1}s_2^2$	s_3

The monomials for the column $\downarrow \mathbf{S}_4$ are obtained by direct subduction. We select $\downarrow \mathbf{C}_1$, $\downarrow \mathbf{C}_2$ and $\downarrow \mathbf{S}_4$ and columns from the **Q**-conjugacy character table of $\mathbf{D}_{2d}$ to form a 5×3 matrix. This matrix is multiplied by the inverse ($\widetilde{M}^{-1}{}_{\mathbf{S}_4}$) of the markaracter table of $\mathbf{S}_4$.

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & -1 \\ 2 & -2 & 0 \end{pmatrix} \times \begin{array}{c} \widetilde{M}^{-1}{}_{\mathbf{S}_4} \\ \begin{pmatrix} \frac{1}{4} & 0 & 0 \\ -\frac{1}{4} & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 1 \end{pmatrix} \end{array}$$

$$= \begin{array}{c} \\ A_1 \\ A_2 \\ B_1 \\ B_2 \\ E \end{array} \begin{array}{c} \begin{array}{ccc} \mathbf{S}_4(/\mathbf{C}_1) & \mathbf{S}_4(/\mathbf{C}_2) & \mathbf{S}_4(/\mathbf{S}_4) \end{array} \\ \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 1 & -1 \\ 0 & 1 & -1 \\ 1 & -1 & 0 \end{pmatrix} \end{array} \begin{array}{c} \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \cdots \end{array} \begin{array}{c} \underline{\downarrow \mathbf{S}_4} \\ s_1 \\ s_1 \\ s_1^{-1}s_2 \\ s_1^{-1}s_2 \\ s_2^{-1}s_4 \end{array}. \tag{26}$$

We obtain characteristic monomials, as shown after dotted lines in Eq. (26).

The monomials for cyclic subgroups are directly obtained in a similar way. All the monomials are collected to give a characteristic monomial table for $\mathbf{D}_{2d}$ (Table 2).

3 Combinatorial enumeration with obligatory minimum valency

We proposed the combinatorial enumeration of isomers under the influence of obligatory minimum valency (OMV) [29, 30]. This enumeration is formulated to assign a distinct ligand inventory to each orbit governed by a coset representation. This formulation is able to be combined with the characteristic monomials defined in the present paper.

Suppose that a skeleton has a set of positions placed under the action of the group **G**, which gives a permutation representation **P**. The permutation representation is subdivied into a set of coset representations:

Table 2. Characteristic monomials for $\mathbf{D}_{2d}$

$\mathbf{D}_{2d}$	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_2$	$\downarrow \mathbf{C}_2'$	$\downarrow \mathbf{C}_s$	$\downarrow \mathbf{S}_4$
A_1	s_1	s_1	s_1	s_1	s_1
A_2	s_1	s_1	$s_1^{-1}s_2$	$s_1^{-1}s_2$	s_1
B_1	s_1	s_1	s_1	$s_1^{-1}s_2$	$s_1^{-1}s_2$
B_2	s_1	s_1	$s_1^{-1}s_2$	s_1	$s_1^{-1}s_2$
E	s_1^2	$s_1^{-2}s_2^2$	s_2	s_2	$s_2^{-1}s_4$
N_j	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$

$$\mathbf{P} = \sum_{i=1}^{t} \alpha_i \mathbf{G}(/\mathbf{G}_i) \tag{27}$$

Each coset representation $\mathbf{G}(/\mathbf{G}_i)$ corresponds to an orbit $\Delta_{i\alpha}$ with $|\mathbf{G}|/|\mathbf{G}_i|$ positions, where $\alpha = 1, 2, \ldots, \alpha_i$ and $i = 1, 2, \ldots, t$. Note that t represents the number of a nonredundant set of subgroups. This value is in general unequal to the value (s) concerning cyclic subgroups only. The multiplicities α_i can be calculated in the light of Theorem 1 or Ref. [30]. Each coset representation (as a matrix form) appearing in Eq. (27) is reduced into a set of **Q**-conjugacy representations as follows:

$$\mathbf{G}(/\mathbf{G}_i) = \sum_{\ell=1}^{s} a_\ell^{(i)} \widehat{\Theta}_\ell \tag{28}$$

To treat OMVs, we assign a distinct ligand inventory to each orbit $\Delta_{i\alpha}$, where we give a dummy variable $s_{d_{jk}}^{(i\alpha)}$ to the orbit $\Delta_{i\alpha}$ governed by $\mathbf{G}(/\mathbf{G}_i)$. Thereby, Eq. (21) is transformed into

$$Z(\widehat{\theta}_\ell \downarrow \mathbf{G}_j; s_{d_{jk}}^{(i\alpha)}) = \prod_{k=1}^{r} (s_{d_{jk}}^{(i\alpha)})^{\chi_{\ell k}^{(j)}} \tag{29}$$

The collection of characteristic monomials labeled with $(i\alpha)$ (Eq. 29) in accord with Eq. (28) generates the following monomial

$$\begin{aligned} Z(\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j; s_{d_{jk}}^{(i\alpha)}) &= \prod_{\ell=1}^{s} \left(Z(\widehat{\theta}_\ell \downarrow \mathbf{G}_j; s_{d_{jk}}^{(i\alpha)}) \right)^{a_\ell^{(i)}} \\ &= \prod_{\ell=1}^{s} \left(\prod_{k=1}^{r} (s_{d_{jk}}^{(i\alpha)})^{\chi_{\ell k}^{(j)}} \right)^{a_\ell^{(i)}} \\ &= \prod_{k=1}^{r} (s_{d_{jk}}^{(i\alpha)})^{\chi_k^{(ij)}} \end{aligned} \tag{30}$$

where we place

$$\chi_k^{(ij)} = \sum_{\ell=1}^{s} a_\ell^{(i)} \chi_{\ell k}^{(j)}. \tag{31}$$

The monomial (Eq. 30) is concerned with the orbit $\Delta_{i\alpha}$ governed by $\mathbf{G}(/\mathbf{G}_i)$. Since the orbit takes the same inventory, the two products appearing in Eq. (30) are allowed to be exchanged. As a result, the product concerning (s) is converted into the sum in the power of the dummy variable, as shown in Eq. (31). When i runs from 1 to t, the product of the monomials (Eq. 30) gives the definition of a subducted cycle index (SCI) concerning the subduction into $\mathbf{G}_j$:

$$\begin{aligned} SCI(\mathbf{G} \downarrow \mathbf{G}_j; s_{d_{jk}}^{(i\alpha)}) &= \prod_{i=1}^{t} \prod_{\alpha=0}^{\alpha_i} Z(\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j; s_{d_{jk}}^{(i\alpha)}) \\ &= \prod_{i=1}^{t} \prod_{\alpha=0}^{\alpha_i} \prod_{\ell=1}^{s} \left(Z(\widehat{\theta}_\ell \downarrow \mathbf{G}_j; s_{d_{jk}}^{(i\alpha)}) \right)^{a_\ell^{(i)}} \\ &= \prod_{i=1}^{t} \prod_{\alpha=0}^{\alpha_i} \prod_{k=1}^{r} (s_{d_{jk}}^{(i\alpha)})^{\chi_k^{(ij)}} \quad , \end{aligned} \tag{32}$$

where we place $s_{d_{jk}}^{(i0)} = 1$ for $\alpha = 0$ for remedying the case of $\alpha_i = 0$. In a similar way to Def. 4 of Ref. [30], we have the definition of a cycle index (CI) by starting from Eq. (32)

$$CI(\mathbf{G}; s_{d_{jk}}^{(i\alpha)}) = \sum_{j=1}^{s} N_j \left(\prod_{i=1}^{t} \prod_{\alpha=0}^{\alpha_i} Z(\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j; s_{d_{jk}}^{(i\alpha)}) \right)$$
$$= \sum_{j=1}^{s} N_j \left(\prod_{i=1}^{t} \prod_{\alpha=0}^{\alpha_i} \prod_{k=1}^{r} (s_{d_{jk}}^{(i\alpha)})^{\chi_k^{(ij)}} \right) , \tag{33}$$

where we place

$$N_j = \sum_{i=1}^{s} \overline{m}_{ji} = \frac{\varphi(|\mathbf{G}_j|)}{|\mathbf{N_G}(\mathbf{G}_j)|} \tag{34}$$

in the light of Eq. (54) of Ref. [24]. The cycle index (Eq. 33) based on characteristic monomials is easily shown to be equal to the counterpart based on unit subduced cycle indices (USCIs) [30]. Hence, Theorem 4 of Ref. [30] is restated in terms of the present formulation.

Theorem 2: *Suppose η_γ of ligands X_γ ($\gamma = 1, 2, \ldots, v$) are selected from a set of ligands*:

$$\mathbf{X} = \{X_1, X_2, \ldots, X_v\} \ , \tag{35}$$

where we have a partition:

$$[\eta] = \eta_1 + \eta_2 + \cdots + \eta_v = n \ . \tag{36}$$

They are placed on n of the positions in a skeleton to give isomers with the weight

$$W_\eta = \prod_{i=1}^{t} \prod_{\alpha=0}^{\alpha_i} \prod_{v} w_{i\alpha}(X_\gamma) \ , \tag{37}$$

where the weight $w_{i\alpha}(X_\gamma)$ is assigned to each orbit ($\Delta_{i\alpha}$); the symbol v in the last product is effective if X_γ is placed on the orbit $\Delta_{i\alpha}$; and $w_{i0}(X_\gamma) = 1$. A generating function for the total number A_η of isomers with the weight W_η is represented by

$$\sum_{\eta} A_\eta W_\eta = CI(\mathbf{G}; s_{d_{jk}}^{(i\alpha)}) \ , \tag{38}$$

into which the inventories,

$$s_{d_{jk}}^{(i\alpha)} = \sum_{\gamma=1}^{v} w_{i\alpha}(X_\gamma)^{d_{jk}} \ , \tag{39}$$

are introduced.

In a special case in which the weight $w_{i\alpha}(X_\gamma)$ is constant over all the ligands, we can place $w_{i\alpha}(X_\gamma) = X_\gamma$. This means that the weight W_η [Eq. (37)] can be regarded as the molecular formula of an isomer. Hence, we obtain a corollary.

Corollary 1: *Suppose η_γ of ligands X_γ ($\gamma = 1, 2, \ldots, v$) are selected from a set of ligands represented by Eq.* (35), *where we have a partition represented by Eq.* (36). *They are placed on n of the positions in a skeleton to give isomers with the weight* (*molecular formula*)

$$W_\eta = \prod_{\gamma=1}^{v} X_\gamma^{\eta_\gamma} \tag{40}$$

A generating function for the total number A_η of isomers with the weight W_η is represented by

$$\sum_{\eta} A_\eta W_\eta = CI(\mathbf{G}; s_{d_{jk}}), \tag{41}$$

where

$$s_{d_{jk}} = \sum_{\gamma=1}^{v} X_\gamma^{d_{jk}}. \tag{42}$$

This corollary is equivalent to Pólya's theorem, though its definition of CI is different from that of Pólya's theorem.

Example 3: Let us consider adamantane-2,6-dione as a skeleton, where the carbon atom of each position is replaced by a carbon, a nitrogen, or an oxygen atom. This example has once been discussed with a different method using USCIs in Chap. 15 of Ref. [21]. Obviously, the two carbonyl carbons can be ommitted from our consideration, since they cannot be replaced by N or O. Hence, we take acount of the four bridge positions (the orbit $\Delta^{(a)}$) to be replaced by C, N or O and the four bridgehead positions (the orbit $\Delta^{(b)}$) to be replaced by C or N. The orbit $\Delta^{(a)}$ is governed by the coset representation $\mathbf{D}_{2d}(/\mathbf{C}_2')$, while $\Delta^{(b)}$ is governed by $\mathbf{D}_{2d}(/\mathbf{C}_s)$. The coset representation $\mathbf{D}_{2d}(/\mathbf{C}_2')$ has a fixed-point vector: FPV $=$ $(4, 0, 2, 0, 0, 0)$. This row vector is multiplied by the inverse matrix of $D_{\mathbf{D}_{2d}}$ (Eq. 25) to give

$$(4,0,2,0,0,0) \times \begin{array}{c} \\ \downarrow \mathbf{C}_1 \\ \downarrow \mathbf{C}_2 \\ \downarrow \mathbf{C}_2' \\ \downarrow \mathbf{C}_s \\ \downarrow \mathbf{S}_4 \end{array} \begin{array}{c} \begin{array}{ccccc} A_1 & A_2 & B_1 & B_2 & E \end{array} \\ \begin{pmatrix} \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{4} \\ \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & -\frac{1}{4} \\ \frac{1}{4} & -\frac{1}{4} & \frac{1}{4} & -\frac{1}{4} & 0 \\ \frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{1}{4} & 0 \\ \frac{1}{4} & \frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & 0 \end{pmatrix} \end{array}$$
$$= (1,0,1,0,1) \ . \tag{43}$$

The row vector in the right-hand side indicates $A_1 + B_1 + E$. Thus, the coset representations are reduced into **Q**-conjugacy representations as follows:

$$\mathbf{D}_{2d}(/\mathbf{C}_2') = A_1 + B_1 + E$$
$$\mathbf{D}_{2d}(/\mathbf{C}_s) = A_1 + B_2 + E$$

These results are apparently equal to the ones obtained for irreducible representaions [31], since the group $\mathbf{D}_{2d}$ is matured. However, the symbols A_1 etc. used in the present paper represent **Q**-conjugacy representations, while the counterparts used in Ref. [31] express irreducible representations.

From the characteristic monomials collected in Table 2, we obtain SCIs for each orbit by using Eq. (32):

orbit	reduction	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_2$	$\downarrow \mathbf{C}_2'$	$\downarrow \mathbf{C}_s$	$\downarrow \mathbf{S}_4$
$\Delta^{(a)}$	$\mathbf{D}_{2d}(/\mathbf{C}_2') = A_1 + B_1 + E$	s_1^4	s_2^2	$s_1^2 s_2$	s_2^2	s_4
$\Delta^{(b)}$	$\mathbf{D}_{2d}(/\mathbf{C}_s) = A_1 + B_2 + E$	s_1^4	s_2^2	s_2^2	$s_1^2 s_2$	s_4
	N_j	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$

These SCIs are equal to the USCIs obtained with a different method [32]. For relevant results using USCIs, see Chap. 15 of Ref. [21].

Thereby, the CI (Eq. 33) for the present enumeration is obtained to be

$$\begin{aligned} f &= CI(D_{2d}; s_{d_{jk}}) \\ &= \tfrac{1}{8}(s_1^4)^{(a)}(s_1^4)^{(b)} + \tfrac{1}{8}(s_2^2)^{(a)}(s_2^2)^{(b)} + \tfrac{1}{4}(s_1^2 s_2)^{(a)}(s_2^2)^{(b)} \\ &\quad + \tfrac{1}{4}(s_2^2)^{(a)}(s_1^2 s_2)^{(b)} + \tfrac{1}{4}(s_4)^{(a)}(s_4)^{(b)} \ , \end{aligned} \tag{44}$$

where the superscripts (a) and (b) designate correspondence to the orbits $\Delta^{(a)}$ and $\Delta^{(b)}$.

The ligand inventories [Eq. (39)] for this case are obtained as follows.

$$s_d^{(a)} = C^d + N^d + O^d \qquad \text{for } \Delta^{(a)} \tag{45}$$

$$s_d^{(b)} = C^d + N^d \qquad \text{for } \Delta^{(b)} \tag{46}$$

The former inventory is free from the restriction due to the OMV (=2) of the bridge positions, since the valencies of C, N and O are equal to or greater than 2. On the other hand, the latter inventory indicates the restriction due to the OMV (=3) of the bridgehead positions. They are introduced into Eq. (44) of Theorem 3 and expanded to give a generating function:

$$\begin{aligned} f &= C^8 \\ &\quad + 2C^7N + C^7O \\ &\quad + 6C^6N^2 + 4C^6NO + 2C^6O^2 \\ &\quad + 10C^5N^3 + 12C^5N^2O + 6C^5NO^2 + C^5O^3 \\ &\quad + 13C^4N^4 + 19C^4N^3O + 15C^4N^2O^2 + 3C^4NO^3 \\ &\quad + C^4O^4 \\ &\quad + 10C^3N^5 + 19C^3N^4O + 18C^3N^3O^2 + 6C^3N^2O^3 \\ &\quad + C^3NO^4 \\ &\quad + 6C^2N^6 + 12C^2N^5O + 15C^2N^4O^2 + 6C^2N^3O^3 \\ &\quad + 2C^2N^2O^4 \\ &\quad + 2CN^7 + 4CN^6O + 6CN^5O^2 + 3CN^4O^3 + CN^3O^4 \\ &\quad + N^8 + N^7O + 2N^6O^2 + N^5O^3 + N^4O^4 \end{aligned} \tag{47}$$

where the coefficient of the term $C^\ell N^m O^n$ is the number of isomers with the formula $\mathrm{C}_\ell \mathrm{N}_m \mathrm{O}_n$.

To illustrate this enumeration six diaza derivatives that correspond to the coefficient of the term C^6N^2 in Eq. (47) are shown in Fig. 7. These derivatives are free from the restriction due to the OMV. It should be noted that the present enumeration regarded a pair of enantiomers as one isomer, if the isomer is chiral. Hence, Fig. 1 illustrates an arbitrary enantiomer selected from each pair of enantiomers.

On the other hand, the coefficient of the term C^6O^2 indicates the existence of two dioxa derivatives, as illustrated in Fig. 2. This case shows the OMV restriction, where O is incapable of substituting for the bridgehead positions of the skeleton. This result stems from the use of the ligand inventory represented by eq. (46).

In additon, Fig. 3 shows an intermediate case concerning the term C^6NO. Note that C and N are free from OMV while O is incapable of substituting for any bridgehead positions. Hence, the number of resulting

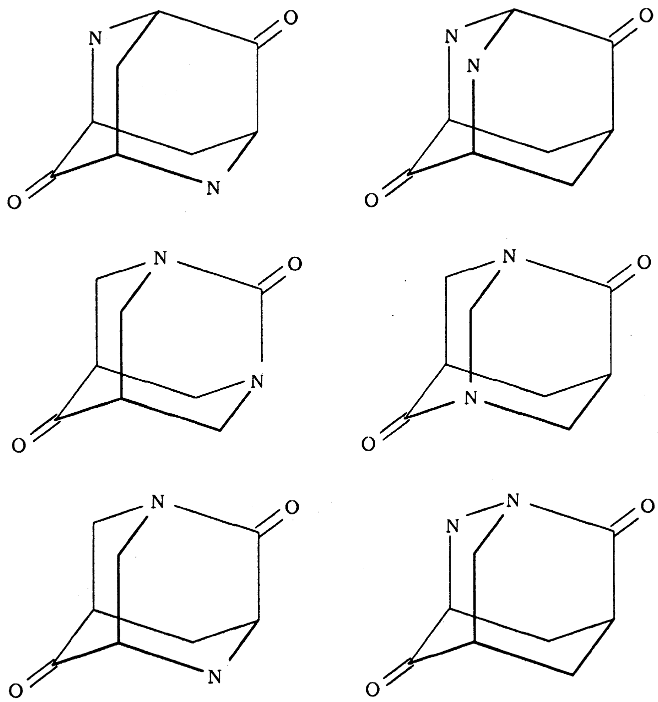

Fig. 1. Diaza derivatives. For a chiral isomer, an arbitrary enantiomer is depicted

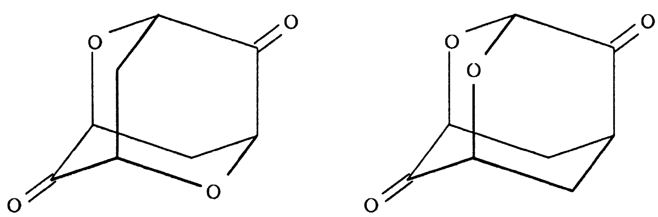

Fig. 2. Dioxa derivatives. For a chiral isomer, an arbitrary enantiomer is depicted

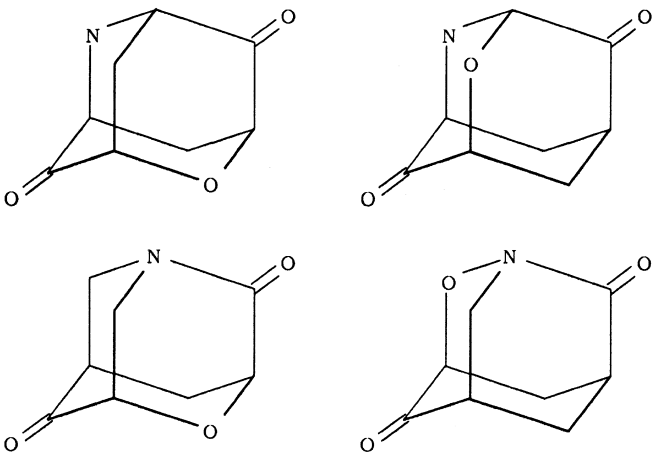

Fig. 3. Azoxa derivatives. For a chiral isomer, an arbitrary enantiomer is depicted

azoxa derivatives is four, which appears as the coefficent of the term C^6NO in Eq. (47).

Figures 1–3 correspond to the third row of Eq. (47). Since each row of Eq. (47) contains terms having the same power on C, the coefficients of these terms indicate the effects of OMV restriction. The present enumeration agrees with the previously itemized enumeration [21].

4 Conclusion

Characteristic monomials for a group **G** are obtained by direct subductions of **Q**-conjugate representations:

1. The restriction of a **Q**-conjugacy character table of the group **G** into subgroup $\mathbf{G}_j$ to give $D_{\mathbf{G}\downarrow\mathbf{G}_j}$
2. The multiplication of $D_{\mathbf{G}\downarrow\mathbf{G}_j}$ by the inverse of the dominant markaracter table of $\mathbf{G}_j$ to give a multiplicity matrix $X_{\mathbf{G}_j}$
3. The construction of a characteristic monomial on the basis of the multiplicities appearing as a row of the matirix $X_{\mathbf{G}_j}$.

The resulting characteristic monomials are shown to give a generating function that is capable of solving enumeration problems.

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