Theor Chem Acc (1998) 99:224–230
DOI 10.1007/s0021498000m3

Theoretical
Chemistry Accounts

Regular article

Subduction of Q-conjugacy representations and characteristic monomials for combinatorial enumeration

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Received: 10 October 1997 / Accepted: 13 February 1998 / Published online: 17 June 1998

Abstract. A new method of combinatorial enumeration is presented. The subduction of **Q**-conjugacy representations gives a characteristic subduction table and a characteristic monomial table. A cycle index is defined on the basis of such monomials and used for combinatorial enumeration of isomers.

Key words: **Q**-conjugacy character table – Characteristic subduction table – Characteristic monomial table – isomer enumeration

1 Introduction

Group-theoretical problems in chemistry have mainly been discussed by means of linear representations that are analysed in terms of irreducible representations [1]. Thus, approaches using irreducible characters are familiar to most chemists, where character tables play an important role as tools of such analysis [2–9]. In contrast, such problems as combinatorial enumeration of isomers have been investigated in the light of permutation representations and coset representations [10–22]. In the latter type of approaches, marks and mark tables are used as versatile tools [19].

A series of articles has been devoted to integrating the two types of approaches [23, 24]. Thus, **Q**-conjugacy character tables derived from character tables in the first type of approach have been shown to be closely related to markaracter tables derived from mark tables in the second type of approach [25]. As a result, there is the possibility of applying the first approach to combinatorial enumeration which was originally unrelated. Hence, the aim of the present paper is to develop a new method of combinatorial enumeration on the basis of the first approach, in which characteristic subduction tables and characteristic monomial tables are proposed as versatile tools.

2 Characteristic subductions and characteristic monomials

2.1 Markaracters as rational characters

A markaracter that contains non-negative integers as elements has been shown in Eqs. (69) and (70) of Ref. [24] to be a linear combination of dominant markaracters (based on permutation representations).

On the other hand, a markaracter that contains integers as elements has been recognized as a rational character, which is a linear combination of characters induced by characters of cyclic subgroups in the light of Artin's theorem [1]. Although the latter characters are based on linear representations, they are equivalent to the dominant markaracters.

In both cases, the coefficients of the linear combinations are shown to be rational numbers. Thus, the formulation described in Sect. 3.3 in Ref. [24] can be applied to both of the cases, in which a markaracter table $\widetilde{M} = (m_{ij})$ (or its inverse $\widetilde{M}^{-1} = (\overline{m}_{ji})$) is a key to calculate such coefficients. Moreover, the sum of each row of $\widetilde{M}^{-1}$, i.e.

$$N_j = \sum_{i=1}^{s} \overline{m}_{ji} \ , \quad (1)$$

has a significant role in combinatorial enumeration. The sum N_j is equal to $|\mathbf{K}_j|/|\mathbf{G}|$, where each $|\mathbf{K}_j|$ denotes the size of the dominant class $\mathbf{K}_j$ corresponding to the subgroup $\mathbf{G}_j$.

The subduction of each dominant representation $\mathbf{G}(/\mathbf{G}_i)$ into each subgroup ($\mathbf{G}_j$) is regarded as a linear combination of dominant representations of $\mathbf{G}_j$. Thereby, the coefficient $\beta_k^{(ij)}$ of the linear combination is calculated using an inverse markaracter table for the subgroup $\mathbf{G}_j$, as shown in Eq. (48) of Ref. [24]:

$$\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j = \sum_{k=1}^{r} \beta_k^{(ij)} \mathbf{G}_j(/\mathbf{G}_k^{(j)}) \ . \quad (2)$$

These data are collected to form a dominant subduction table for $\mathbf{G}$.

Let us now consider a dummy variable $s_{d_{jk}}$, the subscript of which is the size of each orbit. Then we define a dominant unit subduced cycle index (USCI) as follows:

$$Z(\mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j; s_{d_{jk}}) = \prod_{k=1}^{r} s_{d_{jk}}^{\beta_k^{(ij)}} \quad , \tag{3}$$

where $d_{jk} = |\mathbf{G}_j|/|\mathbf{G}_k^{(j)}|$. These data are collected to form a dominant USCI table for $\mathbf{G}$.

2.1. Example 1

Let us examine the point group $\mathbf{T}$ of order 12. The matrix $\widetilde{M}_{\mathbf{T}}$ denotes the markaracter table of $\mathbf{T}$ [24], which is obtained from the corresponding mark table (Appendix A in Ref. [19]) by collecting the terms associated with a non-redundant set of cyclic subgroups.

$$\widetilde{M}_{\mathbf{T}} = \begin{array}{c} \\ \mathbf{T}(/\mathbf{C}_1) \\ \mathbf{T}(/\mathbf{C}_2) \\ \mathbf{T}(/\mathbf{C}_3) \end{array} \begin{array}{c} \begin{array}{ccc} \downarrow \mathbf{C}_1 & \downarrow \mathbf{C}_2 & \downarrow \mathbf{C}_3 \end{array} \\ \begin{pmatrix} 12 & 0 & 0 \\ 6 & 2 & 0 \\ 4 & 0 & 1 \end{pmatrix} \end{array} \tag{4}$$

The matrix $\widetilde{M}_{\mathbf{T}}^{-1}$ denotes the inverse matrix of $\widetilde{M}_{\mathbf{T}}$ [24], which is calculated directly from $\widetilde{M}_{\mathbf{T}}$ or alternatively obtained from the inverse mark table (Appendix B in Ref. [19]). The sum (N_j) of each row is shown after dotted lines:

$$\widetilde{M}_{\mathbf{T}}^{-1} = \begin{pmatrix} \frac{1}{12} & 0 & 0 \\ -\frac{1}{4} & \frac{1}{2} & 0 \\ -\frac{1}{3} & 0 & 1 \end{pmatrix} \begin{array}{c} \cdots \\ \cdots \\ \cdots \end{array} \begin{array}{c} N_j \\ \frac{1}{12} \\ \frac{1}{4} \\ \frac{2}{3} \end{array} \quad . \tag{5}$$

The subduction of each dominant representation of $\mathbf{T}$ is calculated by extracting a dominant subduction table from the markaracter table of $\widetilde{M}_{\mathbf{T}}$. For example, the subduction into $\mathbf{C}_2$ uses the columns $\downarrow \mathbf{C}_1$ and $\downarrow \mathbf{C}_2$ of $\widetilde{M}_{\mathbf{T}}$ to form a 3×2 matrix (a dominant subduction table) as shown in Eq. (6):

$$\begin{array}{c} \\ \mathbf{T}(/\mathbf{C}_1) \\ \mathbf{T}(/\mathbf{C}_2) \\ \mathbf{T}(/\mathbf{C}_3) \end{array} \begin{array}{c} \begin{array}{cc} \downarrow \mathbf{C}_1 & \downarrow \mathbf{C}_2 \end{array} \\ \begin{pmatrix} 12 & 0 \\ 6 & 2 \\ 4 & 0 \end{pmatrix} \end{array} \times \begin{array}{c} \widetilde{M}_{\mathbf{C}_2}^{-1} \\ \begin{pmatrix} \frac{1}{2} & 0 \\ -\frac{1}{2} & 1 \end{pmatrix} \end{array} = \begin{array}{c} \begin{array}{cc} \downarrow \mathbf{C}_1 & \downarrow \mathbf{C}_2 \end{array} \\ \begin{pmatrix} 6 & 0 \\ 2 & 2 \\ 2 & 0 \end{pmatrix} \end{array} \quad . \tag{6}$$

The resulting matrix is multiplied by $\widetilde{M}_{\mathbf{C}_2}^{-1}$ (the inverse of the markaracter table for $\mathbf{C}_2$) to form a 3×2 matrix, in which the elements of each row represent the multiplicities of the dominant representations of $\mathbf{C}_2$ for the corresponding dominant representation of $\mathbf{T}$. For example, the second row of the resulting matrix of Eq. (6) represents

$$\mathbf{T}(/\mathbf{C}_2) \downarrow \mathbf{C}_2 = 2\mathbf{C}_2(/\mathbf{C}_1) + 2\mathbf{C}_2(/\mathbf{C}_2) \quad , \tag{7}$$

which corresponds to Eq. (2) applied to the present case. These results are collected to form Table 1 as a dominant subduction table for $\mathbf{T}$.

Since the orbits corresponding to the right-hand side of Eq. (7) have the sizes $|\mathbf{C}_2|/|\mathbf{C}_1| = 2$ and $|\mathbf{C}_2|/|\mathbf{C}_2| = 1$, we use respective dummy variables s_2 and s_1. Thereby, we obtain a dominant USCI for $\mathbf{T}(/\mathbf{C}_2) \downarrow \mathbf{C}_2$, i.e. $s_1^2 s_2^2$, in which the powers are the coefficients appearing in Eq. (7). Thus, the data collected in Table 1 give the corresponding dominant USCIs, which are listed in Table 2 as a dominant USCI table for $\mathbf{T}$.

The sums listed in the last side of Eq. (5) are shown in the bottom row of this table.

2.2 Markaracters as matured characters

By means of the concept of $\mathbf{Q}$-conjugacy characters [25], a markaracter that contains integers as elements (i.e. a matured character [25]) is concluded to be a linear combination of $\mathbf{Q}$-conjugacy characters, in which the coefficients of the linear combination are integers [25]. Each of $\mathbf{Q}$-conjugacy characters $\widehat{\theta}_\ell$ ($\ell = 1, 2, \ldots, s$) can be regarded as a markaracter (a rational character). Hence, we obtain the following equation to describe the present case [25]:

$$\widehat{\theta}_\ell = \sum_{i=1}^{s} \alpha_{\ell i} \mathbf{G}(/\mathbf{G}_i) \qquad (\ell = 1, 2, \ldots, s), \tag{8}$$

where the symbol $\mathbf{G}(/\mathbf{G}_i)$ is used in order to designate the dominant markaracter (as a row vector) corresponding to the coset representation $\mathbf{G}(/\mathbf{G}_i)$ for the sake of simplicity. Although the same symbol is used, no confusions occur according to contexts.

Let us now consider the subduction of $\mathbf{Q}$-conjugacy representation $\widehat{\Theta}_\ell$ into $\mathbf{G}_j$, which is associated with the subduction of the $\mathbf{Q}$-conjugacy character $\widehat{\theta}_\ell$ into $\mathbf{G}_j$. By starting from Eq. (8) and using Eq. (2), we have

Table 1. Dominant subduction table for **T**

	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_2$	$\downarrow \mathbf{C}_3$
$\mathbf{T}(/\mathbf{C}_1)$	$12\mathbf{C}_1(/\mathbf{C}_1)$	$6\mathbf{C}_2(/\mathbf{C}_1)$	$4\mathbf{C}_3(/\mathbf{C}_1)$
$\mathbf{T}(/\mathbf{C}_2)$	$6\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_1) + 2\mathbf{C}_2(/\mathbf{C}_2)$	$2\mathbf{C}_3(/\mathbf{C}_1)$
$\mathbf{T}(/\mathbf{C}_2)$	$4\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_1)$	$\mathbf{C}_3(/\mathbf{C}_1) + \mathbf{C}_3(/\mathbf{C}_3)$

Table 2. Dominant USCI table for **T**

	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_3$
$\mathbf{T}(/\mathbf{C}_1)$	s_1^{12}	s_2^6	s_3^4
$\mathbf{T}(/\mathbf{C}_2)$	s_1^6	$s_1^2 s_2^2$	s_3^2
$\mathbf{T}(/\mathbf{C}_2)$	s_1^4	s_2^2	$s_1 s_3$
N_j	$\frac{1}{12}$	$\frac{1}{4}$	$\frac{2}{3}$

$$\begin{aligned}\widehat{\theta}_\ell \downarrow \mathbf{G}_j &= \sum_{i=1}^{s} \alpha_{\ell i} \mathbf{G}(/\mathbf{G}_i) \downarrow \mathbf{G}_j \\ &= \sum_{i=1}^{s} \alpha_{\ell i} \sum_{k=1}^{r} \beta_k^{(ij)} \mathbf{G}_j(/\mathbf{G}_k^{(j)}) \\ &= \sum_{k=1}^{r} \left(\sum_{i=1}^{s} \alpha_{\ell i} \beta_k^{(ij)} \right) \mathbf{G}_j(/\mathbf{G}_k^{(j)}) \\ &= \sum_{k=1}^{r} \chi_{\ell k}^{(j)} \mathbf{G}_j(/\mathbf{G}_k^{(j)}) \end{aligned} \tag{9}$$

for $\ell = 1, 2, \ldots, s$, where the last side is obtained by placing

$$\chi_{\ell k}^{(j)} = \sum_{i=1}^{s} \alpha_{\ell i} \beta_k^{(ij)} \ . \tag{10}$$

The resulting data are collected to give a characteristic subduction table for $\mathbf{G}$. Note that the value of Eq. (10) becomes independent of $\mathbf{G}_i$. Each value $\chi_{\ell k}^{(j)}$ is presumed to be an integer to our knowledge, though it remains to be proved in the future. It should be noted that the coefficients $\chi_{\ell r}^{(j)}$ of every one-membered orbit (governed by $\mathbf{G}_j(/\mathbf{G}_r^{(j)}) = \mathbf{G}_j(/\mathbf{G}_j)$) are collected to give a $\mathbf{Q}$-conjugacy character table.

Let us now consider a dummy variable $s_{d_{jk}}$, the subscript of which is the size of each orbit. Then, we define a monomial by the following equation. We call this monomial a *characteristic monomial*.

$$Z(\widehat{\theta}_\ell \downarrow \mathbf{G}_j; s_{d_{jk}}) = \prod_{k=1}^{r} s_{d_{jk}}^{\sum_{i=1}^{s} \alpha_{\ell i} \beta_k^{(ij)}} = \prod_{k=1}^{r} s_{d_{jk}}^{\chi_{\ell k}^{(j)}} \ , \tag{11}$$

where $d_{jk} = |\mathbf{G}_j|/|\mathbf{G}_k^{(j)}|$. The resulting data are collected to give a characteristic monomial table for $\mathbf{G}$. It should be noted that the collection of the powers of every s_1 variable gives the original $\mathbf{Q}$-conjugacy character table.

2.2.1. Example 2

Let us next examine the $\mathbf{Q}$-conjugacy character table of $\mathbf{T}$, which is constructed from the character table of $\mathbf{T}$ [25]. The $\mathbf{Q}$-conjugacy character table is expressed as a matrix form:

$$D_{\mathbf{T}} = \begin{array}{c} \\ A \\ E \\ T \end{array} \begin{array}{c} \begin{array}{ccc} \downarrow \mathbf{C}_1 & \downarrow \mathbf{C}_2 & \downarrow \mathbf{C}_3 \end{array} \\ \left(\begin{array}{ccc} 1 & 1 & 1 \\ 2 & 2 & -1 \\ 3 & -1 & 0 \end{array} \right) \end{array} \ . \tag{12}$$

The $\mathbf{Q}$-conjugacy character appearing in each row of $D_{\mathbf{T}}$ is regarded as a markaracter (rational character), which is expressed by a linear combination of dominant markaracters. The coefficients of the linear combination are calculated by $D_{\mathbf{T}}\widetilde{M}_{\mathbf{T}}^{-1}$ as follows:

$$D_{\mathbf{T}}\widetilde{M}_{\mathbf{T}}^{-1} = \begin{array}{c} \\ \widetilde{A} \\ \widetilde{E} \\ \widetilde{T} \end{array} \begin{array}{c} \begin{array}{ccc} \mathbf{T}(/\mathbf{C}_1) & \mathbf{T}(/\mathbf{C}_2) & \mathbf{T}(/\mathbf{C}_3) \end{array} \\ \left(\begin{array}{ccc} -\frac{1}{2} & \frac{1}{2} & 1 \\ 0 & 1 & -1 \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{array} \right) \end{array} \ . \tag{13}$$

Each row of the resulting matrix (Eq. 13) is regarded as a row vector ($\widetilde{A}$, $\widetilde{E}$, or $\widetilde{T}$), which is called a multiplicity vector. Thus, such a multiplicity vector is meaningful in the unmatured case ($\mathbf{T}$) as well as in a matured case (e.g. $\mathbf{T}_d$) described in Ref. [23].

In the next step, we shall calculate the characteristic subduction concerning each multiplicity vector. For example, let us consider the $\widetilde{A}$ vector:

$$\widetilde{A} = \left(-\tfrac{1}{2}, \tfrac{1}{2}, 1\right) \ , \tag{14}$$

the respective elements (rational numbers) of which represent the multiplicities of $\mathbf{T}(/\mathbf{C}_1)$, $\mathbf{T}(/\mathbf{C}_2)$ and $\mathbf{T}(/\mathbf{C}_3)$. Suppose that the $\downarrow \mathbf{C}_2$ column of the dominant subduction table for $\mathbf{T}$ (Table 1) is, for example, denoted as $[\mathbf{T} \downarrow \mathbf{C}_2]$:

$$\begin{aligned}[\mathbf{T} \downarrow \mathbf{C}_2]^T = (&6\mathbf{C}_2(/\mathbf{C}_1), 2\mathbf{C}_2(/\mathbf{C}_1) \\ &+ 2\mathbf{C}_2(/\mathbf{C}_2), 2\mathbf{C}_2(/\mathbf{C}_1)) \ . \end{aligned} \tag{15}$$

Then, the characteristic subduction for the A representation is calculated by multiplying $\widetilde{A}$ with $[\mathbf{T} \downarrow \mathbf{C}_2]$:

$$\begin{aligned}\widetilde{A} \times [\mathbf{T} \downarrow \mathbf{C}_2] &= -\tfrac{1}{2} \times 6\mathbf{C}_2(/\mathbf{C}_1) \\ &\quad + \tfrac{1}{2} \times (2\mathbf{C}_2(/\mathbf{C}_1) + 2\mathbf{C}_2(/\mathbf{C}_2)) \\ &\quad + 2\mathbf{C}_2(/\mathbf{C}_1) \\ &= \ \mathbf{C}_2(/\mathbf{C}_2) \ . \end{aligned} \tag{16}$$

The results for this and the other representations are collected to give the characteristic subduction table for $\mathbf{T}$ (Table 3).

Since the orbit corresponding to the right-hand side of Eq. (16) has the size $|\mathbf{C}_2|/|\mathbf{C}_2| = 1$, we use a dummy variable s_1. Thereby, we obtain a characteristic monomial for the A representation to be s_1, in which the power is a unit according to the coefficient of the right-hand side of Eq. (16). Thus, the data collected in Table 3 give the corresponding characteristic monomials, which are listed to give Table 4 as a characteristic monomial table for $\mathbf{T}$.

The sums listed in the last side of Eq. (5) are shown in the bottom row of this table. The collection of the powers of every s_1 variable in Table 4 gives the original $\mathbf{Q}$-conjugacy character table $D_{\mathbf{T}}$ (Eq. 12).

An alternative method of calculating characteristic monomials uses a dominant USCI table such as Table 2. For example, the multiplicity vector $\widetilde{A}$ (Eq. 14) treated by every column in Table 2 gives

$$\begin{aligned} s_1^{12\times(-1/2)} s_1^{6\times(1/2)} s_1^{4\times 1} &= s_1 \ , \\ s_2^{2\times(-1/2)} (s_1^2 s_2^2)^{1/2} s_2^{2\times 1} &= s_1 \ , \\ s_3^{4\times(-1/2)} s_3^{2\times(1/2)} (s_1 s_3)^{1\times 1} &= s_1 \ , \end{aligned}$$

Table 3. Characteristic subduction table for **T**

	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_2$	$\downarrow \mathbf{C}_3$
A	$\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}_3(/\mathbf{C}_3)$
E	$2\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}_3(/\mathbf{C}_1) - \mathbf{C}_3(/\mathbf{C}_3)$
T	$3\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_1) - \mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}_3(/\mathbf{C}_1)$

which are equal to the first row of Table 4. The other rows of Table 4 can be obtained in a similar way.

2.2.2 Example 3

Since the point group $\mathbf{T}_d$ is matured, its **Q**-conjugacy character table is identical to the usual character table. The character table regarded as a **Q**-conjugacy character table gives a set of multiplicity vectors as reported in Eq. (91) of Ref. [23]:

$$\begin{aligned}\widetilde{A}_1 &= \left(-\tfrac{1}{2}, 0, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right) \ , \\ \widetilde{A}_2 &= \left(0, \tfrac{1}{2}, -\tfrac{1}{2}, \tfrac{1}{2}, -\tfrac{1}{2}\right) \ , \\ \widetilde{E} &= \left(0, \tfrac{1}{2}, 0, -\tfrac{1}{2}, 0\right) \ , \\ \widetilde{T}_1 &= \left(\tfrac{1}{2}, -\tfrac{1}{2}, -\tfrac{1}{2}, 0, \tfrac{1}{2}\right) \ , \\ \widetilde{T}_2 &= \left(0, 0, \tfrac{1}{2}, 0, -\tfrac{1}{2}\right) \ .\end{aligned}$$

The $\downarrow \mathbf{C}_2$ column of the dominant subduction table for $\mathbf{T}_d$ (Table 1 of Ref. [24]) is denoted as $[\mathbf{T}_d \downarrow \mathbf{C}_2]$:

$$\begin{aligned}[\mathbf{T}_d \downarrow \mathbf{C}_2]^T = (&6\mathbf{C}_2(/\mathbf{C}_1), 4\mathbf{C}_2(/\mathbf{C}_1) + 4\mathbf{C}_2(/\mathbf{C}_2), 6\mathbf{C}_2(/\mathbf{C}_1), \\ &4\mathbf{C}_2(/\mathbf{C}_1), 2\mathbf{C}_2(/\mathbf{C}_1) + 2\mathbf{C}_2(/\mathbf{C}_2)) \ . \end{aligned} \tag{17}$$

The characteristic subduction for the T_2 representation is calculated in the light of Eq. (9). Thus, the vector $\widetilde{T}_2$ multiplied with $[\mathbf{T}_d \downarrow \mathbf{C}_2]$ gives

$$\begin{aligned}\widetilde{T}_2 \times [\mathbf{T}_d \downarrow \mathbf{C}_2] &= \tfrac{1}{2} \times 6\mathbf{C}_2(/\mathbf{C}_1) - \tfrac{1}{2} \times (2\mathbf{C}_2(/\mathbf{C}_1) \\ &\quad + 2\mathbf{C}_2(/\mathbf{C}_2)) \\ &= 2\mathbf{C}_2(/\mathbf{C}_1) - \mathbf{C}_2(/\mathbf{C}_2) \ , \end{aligned} \tag{18}$$

which gives a characteristic monomial, $s_1^{-1}s_2^2$. The same monomial can be obtained by using Eq. (11). The set of USCIs appearing in the corresponding column of the dominant USCI table for $\mathbf{T}_d$ (Table 2 of Ref. [24]) gives

$$s_2^{6\times(1/2)} \times (s_1^2 s_2^2)^{-(1/2)} = s_1^{-1} s_2^2 \ . \tag{19}$$

The data calculated by the two methods are collected to give a characteristic monomial table for $\mathbf{T}_d$ (Table 5).

The sums listed in the bottom row of this table are obtained from the inverse markaracter table of $\mathbf{T}_d$.

Table 4. Characteristic monomial table for **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
N_j	$\frac{1}{12}$	$\frac{1}{4}$	$\frac{2}{3}$

Table 5. Characteristic monomial table for $\mathbf{T}_d$

	$\downarrow \mathbf{C}_1$	$\downarrow \mathbf{C}_S$	$\downarrow \mathbf{C}_S$	$\downarrow \mathbf{C}_3$	$\downarrow \mathbf{S}_4$
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	$s_1^{-1}s_2$
E	s_1^2	s_1^2	s_2	$s_1^{-1}s_3$	s_2
T_1	s_1^3	$s_1^{-1}s_2^2$	$s_1^{-1}s_2^2$	s_3	$s_1s_2^{-1}s_4$
T_2	s_1^3	$s_1^{-1}s_2^2$	s_1s_2	s_3	$s_1^{-1}s_4$
N_j	$\frac{1}{24}$	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{4}$

3 Combinatorial enumeration

Combinatorial enumeration of isomers is formulated to be a problem in which an appropriate set of ligands are placed on the positions of a skeleton. Let us consider a skeleton with n positions. Suppose that the skeleton is controlled by point group $\mathbf{G}$, which has a non-redundant set of dominant subgroups,

$$SCSG_{\mathbf{G}} = \{\mathbf{G}_1, \mathbf{G}_2, \ldots, \mathbf{G}_s\} \ . \tag{20}$$

The positions of the skeleton are characterized by a permutation representation, $\mathbf{P}$, which affords a markaracter represented by

$$\widetilde{\mathbf{P}} = (\delta_1, \delta_2, \ldots, \delta_s) \ . \tag{21}$$

Let D be the **Q**-conjugacy character table of **G**,

$$D^T = (\widehat{\theta}_1, \widehat{\theta}_2, \ldots, \widehat{\theta}_s) \ , \tag{22}$$

in which each of the **Q**-conjugacy characters is regarded as a row vector, $\widehat{\theta}_\ell$ ($\ell = 1, 2, \ldots, s$). Each **Q**-conjugacy character $\widehat{\theta}_\ell$ corresponds to a **Q**-conjugacy representation $\widehat{\Theta}_\ell$. Suppose that the permutation representation **P** is transformed into a matrix representation. Then, the latter representation is a linear combination of **Q**-conjugacy representations, i.e.

$$\mathbf{P} = \sum_{\ell=1}^{s} a_\ell \widehat{\Theta}_\ell \ . \tag{23}$$

The coefficients are collected to give a multiplicity vector,

$$\widetilde{\mathbf{A}} = (a_1, a_2, \ldots, a_s) \ , \tag{24}$$

which is obtained by solving a set of linear equations,

$$\widetilde{A} = \widetilde{P} D^{-1} \ . \tag{25}$$

The coefficients obtained here are used to define a cycle index:

$$\begin{aligned}\mathrm{CI}(\mathbf{G}; s_{jk}) &= \sum_{j=1}^{s} \left(\left(\sum_{i=1}^{s} \overline{m}_{ji} \right) \prod_{\ell=1}^{s} \left(Z(\widehat{\theta}_\ell \downarrow \mathbf{G}_j; s_{d_{jk}}) \right)^{a_\ell} \right) \\ &= \sum_{j=1}^{s} \left(N_j \prod_{\ell=1}^{s} \left(\prod_{k=1}^{r} s_{d_{jk}}^{\chi_{\ell k}^{(j)}} \right)^{a_\ell} \right) \\ &= \sum_{j=1}^{s} \left(N_j \prod_{k=1}^{r} s_{d_{jk}}^{\chi_k^{(j)}} \right), \end{aligned} \tag{26}$$

where N_j is given in Eq. (1) and the power $\chi_k^{(j)}$ is represented by

$$\chi_k^{(j)} = \sum_{\ell=1}^{s} a_\ell \chi_{\ell k}^{(j)} \quad . \tag{27}$$

The cycle index defined by Eq. (26) is equivalent to the one defined by an alternative formulation (Sect. 3.3 of Ref. [24]). This fact can be easily proven by tracing both of the formulations. Moreover, the latter one [24] was shown to be equivalent to the counterpart described in definition 16.2 in Ref. [19], which was in turn shown to be equivalent to Polya's cycle index [26].

Suppose that η_i of ligands X_i $(i = 1, 2, \ldots, v)$ are selected from a set of ligands represented by

$$\mathbf{X} = \{X_1, X_2, \ldots, X_v\} \quad , \tag{28}$$

where we have a partition:

$$[\eta] = \sum_{i=1}^{v} \eta_i = n \quad . \tag{29}$$

They are placed on the positions of the skeleton to give isomers with the formula,

$$W_\eta = \prod_{i=1}^{v} X_i^{\eta_i} \quad . \tag{30}$$

The number (A_η) of isomers with the formula (Eq. 30) is enumerated by the following theorem.

3.1 Theorem 1.9

The number (A_η) of isomers with W_η is calculated by a generating function,

$$\sum_{[\eta]} A_\eta W_\eta = \mathrm{CI}(\mathbf{G}; s_{jk}) \quad , \tag{31}$$

where the cycle index (Eq. 27) in the right-hand side is substituted by ligand inventories,

$$s_{d_{jk}} = \sum_{\ell=1}^{v} X_\ell^{d_{jk}} \quad . \tag{32}$$

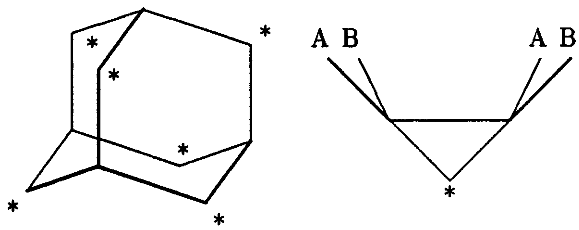
The following example is concerned with the point group **T**. Because the group **T** is unmatured, its **Q**-conjugacy character table is different from its character table.

3.1.1 Example 4

Let us examine an adamantane skeleton (Fig. 1a) of the point group **T** in which a chiral cyclopropane (Fig. 1b) is substituted on each bridge position (*) in a spiro manner.

We consider an appropriate enantiomer of Fig. 1a in which we take account of four bridgehead and six bridge positions. Suppose that these positions are replaced by C or Si to produce polysila-adamantane derivatives. Our problem is to count such polysila-adamantane derivatives.

Let us first obtain the inverse of the **Q**-conjugacy character table for **T**. From Eq. (12), we have



a b

Fig 1

$$D_{\mathbf{T}}^{-1} = \begin{pmatrix} \frac{1}{12} & \frac{1}{12} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & -\frac{1}{4} \\ \frac{2}{3} & -\frac{1}{3} & 0 \end{pmatrix} \quad . \tag{33}$$

The method described in Ref. [24] is applied to categorize the ten positions. The positions are characterized by a markaracter $(10, 2, 1)$, which is multiplied by the inverse $(D_{\mathbf{T}}^{-1})$, i.e.

$$(10, 2, 1)D_{\mathbf{T}}^{-1} = (2, 1, 2) \quad . \tag{34}$$

The vector in the right-hand side of Eq. (34) means that the positions are categorized into $2A + E + 2T$.

This result can be obtained alternatively by considering four bridgehead positions (governed by $\mathbf{T}(/\mathbf{C}_3)$) and six bridge positions [governed by $\mathbf{T}(/\mathbf{C}_2)$] separately. Thus, their markaracters are multiplied by the inverse $(D_{\mathbf{T}}^{-1})$, i.e.

$$(4, 0, 1)D_{\mathbf{T}}^{-1} = (1, 0, 1) \quad \text{for bridgehead positions} \ , \tag{35}$$

$$(6, 2, 0)D_{\mathbf{T}}^{-1} = (1, 1, 1) \quad \text{for bridge positions} \ . \tag{36}$$

It follows that

$$\mathbf{T}(/\mathbf{C}_3) = A + T \qquad \text{for bridgehead positions} \ , \tag{37}$$

$$\mathbf{T}(/\mathbf{C}_2) = A + E + T \quad \text{for bridge positions} \ , \tag{38}$$

where the results shown in the right-hand sides are summed up to give $2A + E + 2T$. By using the data of Table 4, the cycle index (Eq. 26) for this case is

$$\begin{aligned} f &= \mathrm{CI}(\mathbf{T}; s_d) \\ &= \tfrac{1}{12}(s_1)^2(s_1^2)(s_1^3)^2 + \tfrac{1}{4}(s_1)^2(s_1^2)(s_1^{-1}s_2^2)^2 \\ &\quad + \tfrac{2}{3}(s_1)^2(s_1^{-1}s_3)(s_3)^2 \\ &= \tfrac{1}{12}s_1^{10} + \tfrac{1}{4}s_1^2 s_2^4 + \tfrac{2}{3}s_1 s_3^3 \quad . \end{aligned} \tag{39}$$

A ligand inventory for this case is represented by

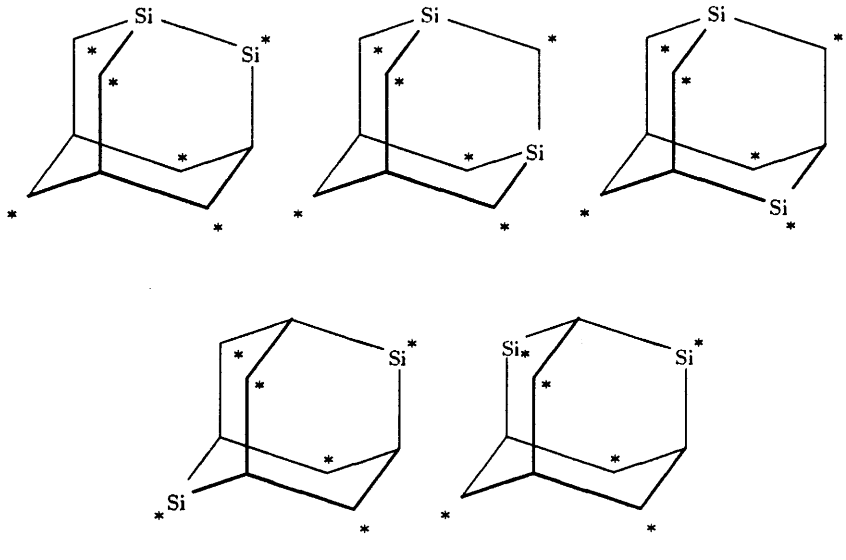
$$s_d = 1 + X^d \quad , \tag{40}$$

which is introduced into Eq. 39 in the light of Theorem 1. Thereby, we obtain

$$\begin{aligned} f &= \tfrac{1}{12}(1+X)^{10} + \tfrac{1}{4}(1+X)^2(1+X^2)^4 \\ &\quad + \tfrac{2}{3}(1+X)(1+X^3)^3 \\ &= 1 + 2X + 5X^2 + 14X^3 + 22X^4 + 24X^5 \\ &\qquad + 22X^6 + 14X^7 + 5X^8 + 2X^9 + X^{10} \quad , \end{aligned} \tag{41}$$

where the coefficient of the term X^x indicates the number of isomers with x of Si atoms. For illustrating the result

Fig 2



corresponding to the term $5X^2$ in Eq. (41), Fig. 2 shows five disila-adamantanes with substituents.

For comparison, we next deal with a matured group, in which its **Q**-conjugacy character table is identical to its character table [25]. We revisit the problem of example 7 of Ref. [24].

3.1.2 Example 5

According to example 7 of Ref. [24], let us consider adamantane itself as a skeleton ($\mathbf{T}_d$), in which we take account of four bridgehead and six bridge positions. These positions are replaced by C or N to produce polyaza-adamantane derivatives. Since the group $\mathbf{T}_d$ is matured, the **Q**-conjugacy character table for $\mathbf{T}_d$ is identical to the usual character table, as shown in a matrix form:

$$D_{\mathbf{T}_d} = \begin{matrix} \\ A_1 \\ A_2 \\ E \\ T_1 \\ T_2 \end{matrix} \begin{matrix} \downarrow \mathbf{C}_1 & \downarrow \mathbf{C}_2 & \downarrow \mathbf{C}_s & \downarrow \mathbf{C}_3 & \downarrow \mathbf{S}_4 \\ \end{matrix} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ 2 & 2 & 0 & -1 & 0 \\ 3 & -1 & -1 & 0 & 1 \\ 3 & -1 & 1 & 0 & -1 \end{pmatrix} , \quad (42)$$

which affords its inverse matrix:

$$D_{\mathbf{T}_d}^{-1} = \begin{pmatrix} \frac{1}{24} & \frac{1}{24} & \frac{1}{12} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & \frac{1}{4} & -\frac{1}{8} & -\frac{1}{8} \\ \frac{1}{4} & -\frac{1}{4} & 0 & -\frac{1}{4} & \frac{1}{4} \\ \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} & 0 & 0 \\ \frac{1}{4} & -\frac{1}{4} & 0 & \frac{1}{4} & -\frac{1}{4} \end{pmatrix} . \quad (43)$$

The ten positions are characterized by a markaracter $(10, 2, 4, 1, 0)$, the elements of which indicate the number of fixed points for $\mathbf{C}_1$, $\mathbf{C}_2$, $\mathbf{C}_s$, $\mathbf{C}_3$ and $\mathbf{S}_4$, respectively. The method described in Ref. [24] is applied to categorize the ten positions, where the markaracter is multiplied by the inverse ($D_{\mathbf{T}_d}^{-1}$), i.e.

$$(10, 2, 4, 1, 0)D_{\mathbf{T}_d}^{-1} = (2, 0, 1, 0, 2) . \quad (44)$$

It follows that the positions are categorized into $2A_1 + E + 2T_2$.

This result can be obtained alternatively by considering four bridgehead positions (governed by $\mathbf{T}_d(/\mathbf{C}_{3v})$) and six bridge positions (governed by $\mathbf{T}_d(/\mathbf{C}_{2v})$) separately [26]:

$$\mathbf{T}_d(/\mathbf{C}_{3v}) = A_1 + T_2 \quad \text{for bridgehead positions} , \quad (45)$$

$$\mathbf{T}_d(/\mathbf{C}_{2v}) = A_1 + E + T_2 \text{ for bridge positions} , \quad (46)$$

where the results shown on the right-hand sides are summed up to give $2A_1 + E + 2T_2$.

By using the data from Table 5, the cycle index (Eq. 26) for this case is

$$\begin{aligned} f &= \mathrm{CI}(\mathbf{T}_d; s_d) \\ &= \tfrac{1}{24}(s_1)^2(s_1^2)(s_1^3)^2 + \tfrac{1}{8}(s_1)^2(s_1^2)(s_1^{-1}s_2^2)^2 \\ &\quad + \tfrac{1}{4}(s_1)^2(s_2^2)(s_1s_2)^2 \\ &\quad + \tfrac{1}{3}(s_1)^2(s_1^{-1}s_3)(s_3)^2 + \tfrac{1}{4}(s_1)^2(s_2)(s_1^{-1}s_4)^2 \\ &= \tfrac{1}{24}s_1^{10} + \tfrac{1}{8}s_1^2s_2^4 + \tfrac{1}{4}s_1^4s_2^3 + \tfrac{1}{3}s_1s_3^3 + \tfrac{1}{4}s_2s_4^2 . \end{aligned} \quad (47)$$

The resulting cycle index is identical to the one obtained in example 7 of Ref. [24].

4 Conclusions

A method of combinatorial enumeration is presented, in which another definition of cycle indices other than Polya's definition [27] is proposed on the basis of several new concepts:

1. **Q**-conjugacy character tables and their inverse matrices,
2. The subduction of **Q**-conjugacy representations and characteristic subduction tables,
3. Characteristic monomials and characteristic monomial tables.

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