The unit-subduced-cycle-index methods and the characteristic-monomial method. Their relationship as group-theoretical tools for chemical combinatorics *

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Dedicated to the 80th birthday of Professor Frank Harary

Among the four methods of the unit-subduced-cycle-index (USCI) approach, the subduced-cycle-index (SCI) method and the partial-cycle-index (PCI) method have been discussed by using adamantane of $\mathbf{T}_d$-symmetry as a probe for enumeration problems, where USCIs are derived on the basis of permutaion representations, coset representations (CRs) and marks. After the examination of the SCIs and PCIs, Pólya's theorem that is a standard method of chemical combinatorics has been derived from the USCI approach. As another approach, a new method called the characteristic-monomial (CM) method has been developed by virtue of charactereistic monomials (CMs). The CMs have been derived from $\mathbf{Q}$-conjugacy representations and $\mathbf{Q}$-conjugacy characters, which have been related to irreducible representations and irreducible characters of the standard repertoire of chemical group theory. The two approaches have been compared to discuss group-theoretical tools for chemical combinatorics on a common basis.

KEY WORDS: group theory, chemical combinatorics, isomer enumeration

1.   Introduction

Two disciplines of chemical group theory.   Chemical combinatorics is one of the major chemical fields that heavily depend on group-theoretical tools, where its discrete nature has been treeted with permutation groups. Pólya's theorem [1–5] has widely used in chemical combinatorics, the results of which have been summarized in excellent reviews [6–8] and books [9–11]. Redfield's method [12–14] and related tools [15–17] have been reported, but less familiar to chemists as well as to mathematicians than Pólya's theorem. Later, a method based on double cosets has been reported [18,19]. The three

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types of methods have been applied to the enumeration of rigid isomers [20–22] as well as to that of non-rigid isomers [23,24]. But, it should be emphasized here that isomers counted by these methods are itemized with respect to molecular formulas only. In other words, their results are not concerned with the symmetries of isomers.

Combinatorial enumeration concerning both molecular formulas and symmetries has later been investigated by many authors [25–30]. In order to take account of isomer symmetries, mark tables introduced by Burnside [31] or framework groups introduced by Pople [32] has been combined with permutation groups.

We have pointed out the importance of coset representations (CRs) in order to systematize combinatorial enumeration [33] as well as to comprehend stereochemical phenomena [34]. In particular, we have proposed a new concept, "the subduction of coset representations (CRs)", which is a key to link stereochemistry with chemical combinatorics [33–35]. From the data of the subduction of CRs, we have introduced unit subduced cycle indices (USCIs). Thereby, we have developed four methods for combinatorial enumeration concerning both molecular formulas and symmetries, i.e., the subduced-cycle-index (SCI) method [33], the partial-cycle index (PCI) method [36], the elementary-superposition method [37], and the partial-superposition method [37]. They are collectively called "the USCI approach", since they start from unit subduced cycle indices (USCIs) obtained by the subduction of CRs.

By virtue of the formulation of the USCI approach, all of the methods described above are clarified to be based on permutation groups or permutation representations. More precisely speaking, they are based on permutation representations, coset representations (CRs) as transitive permutation representations, and marks as invariants. Pólya's theorem, which was originally formulated on the basis of permutation groups, has been alternatively derived from the USCI approach [38]. In addition, the Pólya's theorem has been shown to stem from dominant representations and dominant markaracters (mark-character) that have been defined as the CRs and the marks for cyclic subgroups [39,40].

In contrast, other chemical fields that treat problems of continuous nature have employed another type of group-theoretical tools: linear representations, irreducible representations and characters for point groups. These tools have been widely and successfully used in quantum chemistry [41], molecular spectroscopy [42], and related fields [43], where they meet the continuous nature of the problems. Many textbooks have been published to describe the details of them [44–50].

As clarified by the discussion in the preceding paragaraphs, chemical group theory has been developed on the basis of different disciplines: one discipline due to permutation representations and the related concepts vs. the other discipline due to linear representations and the related concepts. Although these two disciplines have found their own applications in the respective fields in chemistry and in mathematics, the common basis between them should be developed to obtain a further insight into chemical group theory.

Integration of the two disciplines.   The crux for integrating the two desciplines is the parallelism between a set of permutation representations, dominant representations, and

dominant markaracters and another set of linear representations, irreducible representations and characters. If we develop a system of combinatorial enumeration by starting from the latter set, we can find a clue for integrating the two desciplines.

According to this guideline, we have recently developed the characteristic-monomial (CM) method for combinatorial enumeration by starting from another type of representations, i.e., **Q**-conjugacy representations [51–53]. The **Q**-conjugacy representations have been shown to mediate between dominant representations and irreducible representations; as well as between dominant markaracters and irreducible characters. In other word, they have been found to be a clue for integrating the two desciplines.

The short history described in the preceding paragraphs shows that it is not so an easy task to grasp the point of the integration, because the relationships between the items discussed in the respective papers are entangled with each other. Hence, the goal of the present paper is to give a comprehensive perspective on the two desciplines of chemical group theory and to grasp the point of their integration. To arrive at this goal, the USCI methods based on the one descipline and the CM method based on the other descipline will be compared by using a common enumeration problem as a probe for testing such integration.

2. Orbits and coset representations

Let us consider the ten carbons of an adamantane skeleton (figure 1). Generally speaking, any set of equivalent objects is called an orbit, which is an equivalence class from the mathematical point of view. Thus, the six bridge carbons shown by solid circles are equivalent to each other and construct a six-membered orbit. On the other hand, the four bridgehead carbons construct another orbit, as shown by open circles. Now, our problem is how to characterize these orbits.

To do this task, we take account of the global symmetry of the adamantane skeleton and the local symmetry of each carbon [35,54]. For example, any one of the bridge carbons has the local symmetry of C_{2v}. Hence, we combine the local symmetry with the
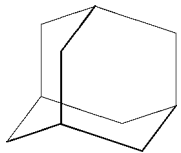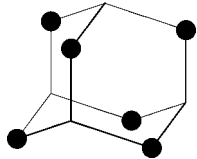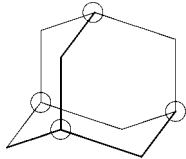
Ten carbons of Adamantane	Six bridgeheads	Four bridges
Global Symmetry	T_d	T_d
Local Symmetry	C_{2v}	C_{3v}
Coset Representation	$T_d(/C_{2v})$	$T_d(/C_{3v})$
Orbit Size	$\lvert T_d \rvert / \lvert C_{2v} \rvert = 24/4 = 6$	$\lvert T_d \rvert / \lvert C_{3v} \rvert = 24/6 = 4$
USCI	s_6	s_4

Figure 1. Orbits for adamantane.

Table 1
Mark table of $\mathbf{T}_d$.

	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_3$	$\mathbf{S}_4$	$\mathbf{D}_2$	$\mathbf{C}_{2v}$	$\mathbf{C}_{3v}$	$\mathbf{D}_{2d}$	$\mathbf{T}$	$\mathbf{T}_d$
$\mathbf{T}_d(/\mathbf{C}_1)$	24	0	0	0	0	0	0	0	0	0	0
$\mathbf{T}_d(/\mathbf{C}_2)$	12	4	0	0	0	0	0	0	0	0	0
$\mathbf{T}_d(/\mathbf{C}_s)$	12	0	2	0	0	0	0	0	0	0	0
$\mathbf{T}_d(/\mathbf{C}_3)$	8	0	0	2	0	0	0	0	0	0	0
$\mathbf{T}_d(/\mathbf{S}_4)$	6	2	0	0	2	0	0	0	0	0	0
$\mathbf{T}_d(/\mathbf{D}_2)$	6	6	0	0	0	6	0	0	0	0	0
$\mathbf{T}_d(/\mathbf{C}_{2v})$	6	2	2	0	0	0	2	0	0	0	0
$\mathbf{T}_d(/\mathbf{C}_{3v})$	4	0	2	1	0	0	0	1	0	0	0
$\mathbf{T}_d(/\mathbf{D}_{2d})$	3	3	1	0	1	3	1	0	1	0	0
$\mathbf{T}_d(/\mathbf{T})$	2	2	0	2	0	2	0	0	0	2	0
$\mathbf{T}_d(/\mathbf{T}_d)$	1	1	1	1	1	1	1	1	1	1	1

global symmetry of $\mathbf{T}_d$ so as to coin a new symbol $\mathbf{T}_d(/\mathbf{C}_{2v})$, as shown in the row of CR. To characterize the orbit of bridgeheads, we use a new symbol $\mathbf{T}_d(/\mathbf{C}_{3v})$ in accord with the local symmetry of $\mathbf{C}_{3v}$.

This procedure, however, has a qualitative meaning only. The next problem is how to add a quantitative meaning to these symbols, $\mathbf{T}_d(/\mathbf{C}_{2v})$ and $\mathbf{T}_d(/\mathbf{C}_{3v})$. For this purpose, we should note that the transformation of the members of an orbit is ascribed to that of the corresponding cosets. Hence, we can ascribe the symbol $\mathbf{T}_d(/\mathbf{C}_{2v})$ to a permutation representation of degree 6, though we do not show the concrete form of the permutation representation. Similarly, we can ascribe the symbol $\mathbf{T}_d(/\mathbf{C}_{3v})$ to a permutation representation of degree 4. The degrees of such CRs can be calculated by dividing the order of global symmetry with the order of the local symmetry, as shown in the "orbit size" row of figure 1 [35].

Mathematically speaking, the assignment of a coset representation to an orbit is conducted by counting fixed points during the desymmetrization to the local symmetry. We take account of a nonredundant set of subgroups (SSG) in order to avoid duplicated consideration:

$$\text{SSG} = \{\mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_s, \mathbf{C}_3, \mathbf{S}_4, \mathbf{D}_2, \mathbf{C}_{2v}, \mathbf{C}_{3v}, \mathbf{D}_{2d}, \mathbf{T}, \mathbf{T}_d\}. \tag{1}$$

Thus, we can obtain a fixed point vector (FPV) by arranging such numbers of fixed points in the order of the SSG. The FPV obtained in this procedure is compared with the rows of a mark table (table 1), so that the identical row indicates the corresponding CR:

$$6\bullet \Longrightarrow \text{FPV} = (6, 2, 2, 0, 0, 0, 2, 0, 0, 0, 0) \xrightarrow[\text{(table 1)}]{\text{Mark table}} \mathbf{T}_d(/\mathbf{C}_{2v}),$$

$$4\circ \Longrightarrow \text{FPV} = (4, 0, 2, 1, 0, 0, 0, 1, 0, 0, 0) \xrightarrow[\text{(table 1)}]{\text{Mark table}} \mathbf{T}_d(/\mathbf{C}_{3v}).$$

Table 2
The inverse of the mark table of $\mathbf{T}_d$.

	$\mathbf{T}_d$ $(/\mathbf{C}_1)$	$\mathbf{T}_d$ $(/\mathbf{C}_2)$	$\mathbf{T}_d$ $(/\mathbf{C}_s)$	$\mathbf{T}_d$ $(/\mathbf{C}_3)$	$\mathbf{T}_d$ $(/\mathbf{S}_4)$	$\mathbf{T}_d$ $(/\mathbf{D}_2)$	$\mathbf{T}_d$ $(/\mathbf{C}_{2v})$	$\mathbf{T}_d$ $(/\mathbf{C}_{3v})$	$\mathbf{T}_d$ $(/\mathbf{D}_{2d})$	$\mathbf{T}_d$ $(/\mathbf{T})$	$\mathbf{T}_d$ $(/\mathbf{T}_d)$	Sum
$\mathbf{C}_1$	$\frac{1}{24}$	0	0	0	0	0	0	0	0	0	0	$\frac{1}{24}$
$\mathbf{C}_2$	$-\frac{1}{8}$	$\frac{1}{4}$	0	0	0	0	0	0	0	0	0	$\frac{1}{8}$
$\mathbf{C}_s$	$-\frac{1}{4}$	0	$\frac{1}{2}$	0	0	0	0	0	0	0	0	$\frac{1}{4}$
$\mathbf{C}_3$	$-\frac{1}{6}$	0	0	$\frac{1}{2}$	0	0	0	0	0	0	0	$\frac{1}{3}$
$\mathbf{S}_4$	0	$-\frac{1}{4}$	0	0	$\frac{1}{2}$	0	0	0	0	0	0	$\frac{1}{4}$
$\mathbf{D}_2$	$\frac{1}{12}$	$-\frac{1}{4}$	0	0	0	$\frac{1}{6}$	0	0	0	0	0	0
$\mathbf{C}_{2v}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{2}$	0	0	0	$\frac{1}{2}$	0	0	0	0	0
$\mathbf{C}_{3v}$	$\frac{1}{2}$	0	-1	$-\frac{1}{2}$	0	0	0	1	0	0	0	0
$\mathbf{D}_{2d}$	0	$\frac{1}{2}$	0	0	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	0	1	0	0	0
$\mathbf{T}$	$\frac{1}{6}$	0	0	$-\frac{1}{2}$	0	$-\frac{1}{6}$	0	0	0	$\frac{1}{2}$	0	0
$\mathbf{T}_d$	$-\frac{1}{2}$	0	1	$\frac{1}{2}$	0	$\frac{1}{2}$	0	-1	-1	$-\frac{1}{2}$	1	0

Table 1 shows the mark table of $\mathbf{T}_d$, which has been computationally calculated [35]. The FPVs obtained in the above procedure are found in the rows of the corresponding CRs, which are undelined for emphasis.

A mark table (M) such as table 1 is regarded as a square matrix. The inverse (M^{-1}) of the mark table is more useful to do the task of assignment. Table 2 shows the inverse mark table of $\mathbf{T}_d$, which has been computationally calculated [35].

The FPVs obtained in the above procedure are multiplied by the inverse mark table (M^{-1}) to give the multiplicity of each CR:

$$\mathbf{T}_d(/\mathbf{C}_{2v})\text{: } (6, 2, 2, 0, 0, 0, 2, 0, 0, 0, 0)M^{-1} = (0, 0, 0, 0, 0, 0, \overset{\mathbf{C}_{2v}}{1}, 0, 0, 0, 0),$$

$$\mathbf{T}_d(/\mathbf{C}_{3v})\text{: } (4, 0, 2, 1, 0, 0, 0, 1, 0, 0, 0)M^{-1} = (0, 0, 0, 0, 0, 0, 0, \overset{\mathbf{C}_{3v}}{1}, 0, 0, 0).$$
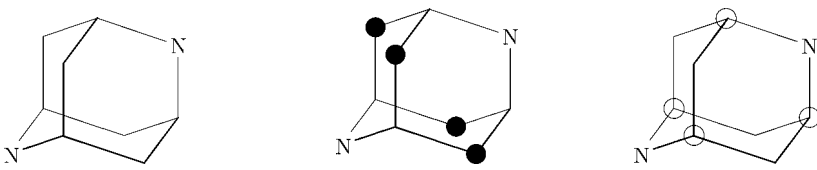
It should be noted that we can assure the appearance of $\mathbf{T}_d(/\mathbf{C}_{2v})$ and $\mathbf{T}_d(/\mathbf{C}_{3v})$ from the data of the total FPV for the ten carbons of the adamantane skeleton:

$$\text{Total: } (10, 2, 4, 1, 0, 0, 2, 1, 0, 0, 0)M^{-1} = (0, 0, 0, 0, 0, 0, \overset{\mathbf{C}_{2v}}{1}, \overset{\mathbf{C}_{3v}}{1}, 0, 0, 0).$$

Each sum collected in the right most column of table 2 is the summation of each row. It should be noted here that the summation for a cyclic subgroup is a positive rational number, while the one for a non-cyclic subgroup vanishes to zero. This has been proved in general [35].

3. Subduction of coset representations and unit subduced cycle indices (USCI)

Let us now cosider the process of converting the adamantane skeleton into a diazaadamantane skeleton, which belongs to the symmetry $\mathbf{D}_{2d}$ (figure 2). This desym-

C_8N_2	Four bridgeheads	NN	Four bridges
Global Symmetry	$\mathbf{D}_{2d}$	$\mathbf{D}_{2d}$	$\mathbf{D}_{2d}$
Local Symmetry	$\mathbf{C}_2'$	$\mathbf{C}_{2v}$	$\mathbf{C}_s$
Coset Representation	$\mathbf{D}_{2d}(/\mathbf{C}_2')$	$\mathbf{D}_{2d}(/\mathbf{C}_{2v})$	$\mathbf{D}_{2d}(/\mathbf{C}_{3v})$
Orbit Size	$\|\mathbf{D}_{2d}\|/\|\mathbf{C}_2'\|$ $= 8/2 = 4$	$\|\mathbf{D}_{2d}\|/\|\mathbf{C}_{2v}\|$ $= 8/4 = 2$	$\|\mathbf{D}_{2d}\|/\|\mathbf{C}_s\|$ $= 8/2 = 4$
USCI		$s_2 s_4$	s_4

Figure 2. Orbits for diazaadamantane.

$$\mathbf{D}_{2d}\begin{cases} I & \sim (1)(2)(3)(4) \,|(5)(6) \\ C_{2(1)} \sim \quad (12)(34) \,|(5)(6) \\ C_{2(2)} \sim \quad (12)(3)(4) \,| (56) \\ C_{2(3)} \sim \quad (1)(2)(34) \,| (56) \\ \sigma_{d(2)} \sim \quad (13)(24) \,|(5)(6) \\ \sigma_{d(4)} \sim \quad (14)(23) \,|(5)(6) \\ S_{4(1)} \sim \quad (1324) \,| (56) \\ S_{4(1)}^3 \sim \quad (1423) \,| (56) \end{cases}$$

$$\underbrace{\qquad\qquad}_{\mathbf{D}_{2d}(/\mathbf{C}_2')} \overbrace{\qquad}^{\mathbf{D}_{2d}(/\mathbf{C}_{2v})}$$

Figure 3. Subduction of coset representations. Example of concrete permutations.

metization causes the division of the six-membered orbit of bridge carbons to produce a four-membered orbit of carbons and a two-membered orbit of nitrogens. In contrast, the four-membered orbit of bridgehead carbons does not divided during the desymmetrization. By considering the global symmetry and local symmetries, we can assign a CR to each of these orbits divided.

These desymmetrization processes are ascribed to the division of an original representation for a group into several permutation representations for a subgroup. For example, figure 3 shows the behavior of the CR $\mathbf{T}_d(/\mathbf{C}_{2v})$ during the desymmetrization from the group $\mathbf{T}_d$ to the subgroup $\mathbf{D}_{2d}$, where the six-membered orbit of bridge carbons are divided into two parts. Thus, we select the eight permutations corresponding to the subgroup $\mathbf{D}_{2d}$ (figure 3) from the CR of the six-membered $\mathbf{T}_d(/\mathbf{C}_{2v})$-orbit. The resulting set of the permutations is a permutation representation of the $\mathbf{D}_{2d}$.

The inspection of the permutations collected in figure 3 provides us with the division into a set of permutations of degree 4 and another set of permutations of degree 2.

Hence, the division is formally expressed by the following equation:

$$\mathbf{T}_d(/\mathbf{C}_{2v}) \downarrow \mathbf{D}_{2d} = \mathbf{D}_{2d}(/\mathbf{C}_2') + \mathbf{D}_{2d}(/\mathbf{C}_{2v}),$$

$$\frac{|\mathbf{D}_{2d}|}{|\mathbf{C}_2'|} = 4, \qquad \frac{|\mathbf{D}_{2d}|}{|\mathbf{C}_{2v}|} = 2.$$

$$\text{USCI} \qquad \underbrace{\qquad\qquad\qquad\qquad}_{s_2 s_4}$$

The size of each resulting orbit is calculated by starting from the orders of the participating groups. Thereby, we obtain a unit subduced cycle index (USCI) of $s_2 s_4$, which corresponds to the sizes of the resulting orbits. The pictorial treatment illustrated by figures 2 and 3 can be assured algebraically by using the mark table and its inverse for the $\mathbf{D}_{2d}$-group, as formally expressed by the equations of subductions:

$$\mathbf{T}_d(/\mathbf{C}_{2v}) \downarrow \mathbf{D}_{2d} = \mathbf{D}_{2d}(/\mathbf{C}_2') + \mathbf{D}_{2d}(/\mathbf{C}_{2v}), \qquad (2)$$

$$\mathbf{T}_d(/\mathbf{C}_{3v}) \downarrow \mathbf{D}_{2d} = \mathbf{D}_{2d}(/\mathbf{C}_s). \qquad (3)$$

Table 3
Subduction table of $\mathbf{T}_d$ (left half).

	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{S}_4$	$\downarrow\mathbf{D}_2$
$\mathbf{T}_d(/\mathbf{C}_1)$	$24\mathbf{C}_1(/\mathbf{C}_1)$	$12\mathbf{C}_2(/\mathbf{C}_1)$	$12\mathbf{C}_s(/\mathbf{C}_1)$	$8\mathbf{C}_3(/\mathbf{C}_1)$	$6\mathbf{S}_4(/\mathbf{C}_1)$	$6\mathbf{D}_2(/\mathbf{C}_1)$
$\mathbf{T}_d(/\mathbf{C}_2)$	$12\mathbf{C}_1(/\mathbf{C}_1)$	$4\mathbf{C}_2(/\mathbf{C}_1)$ $+4\mathbf{C}_2(/\mathbf{C}_2)$	$6\mathbf{C}_s(/\mathbf{C}_1)$	$4\mathbf{C}_3(/\mathbf{C}_1)$	$2\mathbf{S}_4(/\mathbf{C}_1)$ $+2\mathbf{S}_4(/\mathbf{C}_2)$	$2\mathbf{D}_2(/\mathbf{C}_2)$ $+2\mathbf{D}_2(/\mathbf{C}_2')$ $+2\mathbf{D}_2(/\mathbf{C}_2'')$
$\mathbf{T}_d(/\mathbf{C}_s)$	$12\mathbf{C}_1(/\mathbf{C}_1)$	$6\mathbf{C}_2(/\mathbf{C}_1)$	$5\mathbf{C}_s(/\mathbf{C}_1)$ $+2\mathbf{C}_s(/\mathbf{C}_s)$	$4\mathbf{C}_3(/\mathbf{C}_1)$	$3\mathbf{S}_4(/\mathbf{C}_1)$	$3\mathbf{D}_2(/\mathbf{C}_1)$
$\mathbf{T}_d(/\mathbf{C}_3)$	$8\mathbf{C}_1(/\mathbf{C}_1)$	$4\mathbf{C}_2(/\mathbf{C}_1)$	$4\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_1)$ $+2\mathbf{C}_3(/\mathbf{C}_3)$	$2\mathbf{S}_4(/\mathbf{C}_1)$	$2\mathbf{D}_2(/\mathbf{C}_1)$
$\mathbf{T}_d(/\mathbf{S}_4)$	$6\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_1)$ $+2\mathbf{C}_2(/\mathbf{C}_2)$	$3\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{S}_4(/\mathbf{C}_1)$ $+2\mathbf{S}_4(/\mathbf{S}_4)$	$\mathbf{D}_2(/\mathbf{C}_2)$ $+\mathbf{D}_2(/\mathbf{C}_2')$ $+\mathbf{D}_2(/\mathbf{C}_2'')$
$\mathbf{T}_d(/\mathbf{D}_2)$	$6\mathbf{C}_1(/\mathbf{C}_1)$	$6\mathbf{C}_2(/\mathbf{C}_2)$ $+2\mathbf{C}_2(/\mathbf{C}_2)$	$3\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_1)$	$3\mathbf{S}_4(/\mathbf{C}_2)$ $+2\mathbf{S}_4(/\mathbf{S}_4)$	$6\mathbf{D}_2(/\mathbf{D}_2)$ $+\mathbf{D}_2(/\mathbf{C}_2')$
$\mathbf{T}_d(/\mathbf{C}_{2v})$	$6\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_1)$ $+2\mathbf{C}_2(/\mathbf{C}_2)$	$2\mathbf{C}_s(/\mathbf{C}_1)$ $+2\mathbf{C}_s(/\mathbf{C}_s)$	$2\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{S}_4(/\mathbf{C}_1)$ $+\mathbf{S}_4(/\mathbf{C}_2)$	$\mathbf{D}_2(/\mathbf{C}_2)$ $+\mathbf{D}_2(/\mathbf{C}_2')$ $+\mathbf{D}_2(/\mathbf{C}_2'')$
$\mathbf{T}_d(/\mathbf{C}_{3v})$	$4\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_1)$	$\mathbf{C}_s(/\mathbf{C}_1)$ $+2\mathbf{C}_s(/\mathbf{C}_s)$	$\mathbf{C}_3(/\mathbf{C}_1)$ $+\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{S}_4(/\mathbf{C}_1)$	$\mathbf{D}_2(/\mathbf{C}_1)$
$\mathbf{T}_d(/\mathbf{D}_{2d})$	$3\mathbf{C}_1(/\mathbf{C}_1)$	$3\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}_s(/\mathbf{C}_1)$ $+\mathbf{C}_s(/\mathbf{C}_s)$	$\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{S}_4(/\mathbf{C}_2)$ $+\mathbf{S}_4(/\mathbf{S}_4)$	$3\mathbf{D}_2(/\mathbf{C}_2)$
$\mathbf{T}_d(/\mathbf{T})$	$2\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{S}_4(/\mathbf{C}_2)$	$2\mathbf{D}_2(/\mathbf{C}_2)$
$\mathbf{T}_d(/\mathbf{T}_d)$	$\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}_s(/\mathbf{C}_s)$	$\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{S}_4(/\mathbf{S}_4)$	$\mathbf{D}_2(/\mathbf{D}_2)$

Table 4
Subduction table of $\mathbf{T}_d$ (right half).

	$\downarrow\mathbf{C}_{2v}$	$\downarrow\mathbf{C}_{3v}$	$\downarrow\mathbf{D}_{2d}$	$\downarrow\mathbf{T}$	$\downarrow\mathbf{T}_d$
$\mathbf{T}_d(/\mathbf{C}_1)$	$6\mathbf{C}_{2v}(/\mathbf{C}_1)$	$4\mathbf{C}_{3v}(/\mathbf{C}_1)$	$3\mathbf{D}_{2d}(/\mathbf{C}_1)$	$2\mathbf{T}(/\mathbf{C}_1)$	$\mathbf{T}_d(/\mathbf{C}_1)$
$\mathbf{T}_d(/\mathbf{C}_2)$	$2\mathbf{C}_{2v}(/\mathbf{C}_1)$ $+2\mathbf{C}_{2v}(/\mathbf{C}_2)$	$2\mathbf{C}_{3v}(/\mathbf{C}_1)$	$\mathbf{D}_{2d}(/\mathbf{C}_2)$ $+2\mathbf{D}_{2d}(/\mathbf{C}_2')$	$2\mathbf{T}(/\mathbf{C}_2)$	$\mathbf{T}_d(/\mathbf{C}_2)$
$\mathbf{T}_d(/\mathbf{C}_s)$	$2\mathbf{C}_{2v}(/\mathbf{C}_1)$ $+\mathbf{C}_{2v}(/\mathbf{C}_s)$ $+\mathbf{C}_{2v}(/\mathbf{C}_s')$	$\mathbf{C}_{3v}(/\mathbf{C}_1)$ $+2\mathbf{C}_{3v}(/\mathbf{C}_s)$	$\mathbf{D}_{2d}(/\mathbf{C}_1)$ $+2\mathbf{D}_{2d}(/\mathbf{C}_s)$	$\mathbf{T}(/\mathbf{C}_1)$	$\mathbf{T}_d(/\mathbf{C}_s)$
$\mathbf{T}_d(/\mathbf{C}_3)$	$2\mathbf{C}_{2v}(/\mathbf{C}_1)$	$\mathbf{C}_{3v}(/\mathbf{C}_1)$ $+\mathbf{C}_{3v}(/\mathbf{C}_3)$	$\mathbf{D}_{2d}(/\mathbf{C}_1)$	$2\mathbf{T}(/\mathbf{C}_3)$	$\mathbf{T}_d(/\mathbf{C}_3)$
$\mathbf{T}_d(/\mathbf{S}_4)$	$\mathbf{C}_{2v}(/\mathbf{C}_1)$ $+\mathbf{C}_{2v}(/\mathbf{C}_s)$	$\mathbf{C}_{3v}(/\mathbf{C}_1)$	$\mathbf{D}_{2d}(/\mathbf{C}_2')$ $+2\mathbf{D}_{2d}(/\mathbf{S}_4)$	$\mathbf{T}(/\mathbf{C}_2)$	$\mathbf{T}_d(/\mathbf{S}_4)$
$\mathbf{T}_d(/\mathbf{D}_2)$	$3\mathbf{C}_{2v}(/\mathbf{C}_s)$ $+\mathbf{C}_{2v}(/\mathbf{C}_s)$	$\mathbf{C}_{3v}(/\mathbf{C}_1)$	$3\mathbf{D}_{2d}(/\mathbf{D}_2)$ $+2\mathbf{D}_{2d}(/\mathbf{S}_4)$	$2\mathbf{T}(/\mathbf{D}_2)$	$\mathbf{T}_d(/\mathbf{D}_2)$
$\mathbf{T}_d(/\mathbf{C}_{2v})$	$\mathbf{C}_{2v}(/\mathbf{C}_1)$ $+2\mathbf{C}_{2v}(/\mathbf{C}_{2v})$	$2\mathbf{C}_{3v}(/\mathbf{C}_s)$	$\mathbf{D}_{2d}(/\mathbf{C}_2')$ $+2\mathbf{D}_{2d}(/\mathbf{C}_{2v})$	$\mathbf{T}(/\mathbf{C}_2)$	$\mathbf{T}_d(/\mathbf{C}_{2v})$
$\mathbf{T}_d(/\mathbf{C}_{3v})$	$\mathbf{C}_{2v}(/\mathbf{C}_s)$ $+\mathbf{C}_{2v}(/\mathbf{C}_s')$	$\mathbf{C}_{3v}(/\mathbf{C}_s)$ $+\mathbf{C}_{3v}(/\mathbf{C}_{3v})$	$\mathbf{D}_{2d}(/\mathbf{C}_s)$	$\mathbf{T}(/\mathbf{C}_3)$	$\mathbf{T}_d(/\mathbf{C}_{3v})$
$\mathbf{T}_d(/\mathbf{D}_{2d})$	$\mathbf{C}_{2v}(/\mathbf{C}_2)$ $+\mathbf{C}_{2v}(/\mathbf{C}_{2v})$	$\mathbf{C}_{3v}(/\mathbf{C}_s)$	$\mathbf{D}_{2d}(/\mathbf{D}_2)$ $+\mathbf{D}_{2d}(/\mathbf{D}_{2d})$	$\mathbf{T}(/\mathbf{D}_2)$	$\mathbf{T}_d(/\mathbf{D}_{2d})$
$\mathbf{T}_d(/\mathbf{T})$	$\mathbf{C}_{2v}(/\mathbf{C}_2)$	$\mathbf{C}_{3v}(/\mathbf{C}_3)$	$\mathbf{D}_{2d}(/\mathbf{D}_2)$	$2\mathbf{T}(/\mathbf{T})$	$\mathbf{T}_d(/\mathbf{T})$
$\mathbf{T}_d(/\mathbf{T}_d)$	$\mathbf{C}_{2v}(/\mathbf{C}_{2v})$	$\mathbf{C}_{3v}(/\mathbf{C}_{3v})$	$\mathbf{D}_{2d}(/\mathbf{D}_{2d})$	$\mathbf{T}(/\mathbf{T})$	$\mathbf{T}_d(/\mathbf{T}_d)$

In general, such a subduction of a given CR into each subgroup can be computationally calculated by starting from mark tables and inverse mark tables. The results are summarized as a subduction table, as shown in tables 3 and 4, although the concrete procedure is abbreviated [35].

From the data of the subduction table (tables 3 and 4), we can obtain the corresponding USCI table (table 5).

4. The USCI approach

4.1. Four methods of the USCI approach

On the basis of the USCIs, we have developed four methods. They are collectively called "the USCI approach", since they start from unit subduced cycle indices (USCIs) obtained by the subduction of CRs.

(1) The SCI method [33] is a generating-function method based on subduced cycle indices (SCIs) and mark tables, the former of which are derived from the subduction of CRs.

Table 5
USCI table of $\mathbf{T}_d$.

	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{S}_4$	$\downarrow\mathbf{D}_2$	$\downarrow\mathbf{C}_{2v}$	$\downarrow\mathbf{C}_{3v}$	$\downarrow\mathbf{D}_{2d}$	$\downarrow\mathbf{T}$	$\downarrow\mathbf{T}_d$
$\mathbf{T}_d(/\mathbf{C}_1)$	s_1^{24}	s_2^{12}	s_2^{12}	s_3^{8}	s_4^{6}	s_4^{6}	s_4^{6}	s_6^{4}	s_6^{3}	s_{12}^{2}	s_{24}
$\mathbf{T}_d(/\mathbf{C}_2)$	s_1^{12}	$s_1^{4}s_2^{4}$	s_2^{6}	s_3^{4}	$s_2^{2}s_4^{2}$	s_2^{6}	$s_2^{2}s_4^{2}$	s_6^{2}	s_4^{3}	s_6^{2}	s_{12}
$\mathbf{T}_d(/\mathbf{C}_s)$	s_1^{12}	s_2^{6}	$s_1^{2}s_2^{5}$	s_3^{4}	s_4^{3}	s_4^{3}	$s_2^{2}s_4^{2}$	$s_3^{2}s_6$	$s_4 s_8$	s_{12}	s_{12}
$\mathbf{T}_d(/\mathbf{C}_3)$	s_1^{8}	s_2^{4}	s_2^{4}	$s_1^{2}s_3^{2}$	s_4^{2}	s_4^{2}	s_4^{2}	$s_2 s_6$	s_8	s_4^{2}	s_8
$\mathbf{T}_d(/\mathbf{S}_4)$	s_1^{6}	$s_1^{2}s_2^{2}$	s_2^{3}	s_3^{2}	$s_1^{2}s_4$	s_2^{3}	$s_2 s_4$	s_6	$s_2 s_4$	s_6	s_6
$\mathbf{T}_d(/\mathbf{D}_2)$	s_1^{6}	s_1^{6}	s_2^{3}	s_3^{2}	s_2^{3}	s_1^{6}	s_2^{3}	s_6	s_2^{3}	s_3^{2}	s_6
$\mathbf{T}_d(/\mathbf{C}_{2v})$	s_1^{6}	$s_1^{2}s_2^{2}$	$s_1^{2}s_2^{2}$	s_3^{2}	$s_2 s_4$	s_2^{3}	$s_1^{2}s_4$	s_3^{2}	$s_2 s_4$	s_6	s_6
$\mathbf{T}_d(/\mathbf{C}_{3v})$	s_1^{4}	s_2^{2}	$s_1^{2}s_2$	$s_1 s_3$	s_4	s_4	s_2^{2}	$s_1 s_3$	s_4	s_4	s_4
$\mathbf{T}_d(/\mathbf{D}_{2d})$	s_1^{3}	s_1^{3}	$s_1 s_2$	s_3	$s_1 s_2$	s_1^{3}	$s_1 s_2$	s_3	$s_1 s_2$	s_3	s_3
$\mathbf{T}_d(/\mathbf{T})$	s_1^{2}	s_1^{2}	s_2	s_1^{2}	s_2	s_1^{2}	s_2	s_2	s_2	s_1^{2}	s_2
$\mathbf{T}_d(/\mathbf{T}_d)$	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1	s_1
Sum	1/24	1/8	1/4	1/3	1/4	0	0	0	0	0	0

(2) The PCI method [36] is also a generating-function method using partial cycle indices (PCIs), which are also derived from the subduction of CRs.

(3) The elementary-superposition method [37] is based on the concept of the elemental superposition, which has been proposed to discuss desymmetrization processes and has been applied to SCIs.

(4) The partial-superposition method [37] is also based on the elemental superposition, which is applied to PCIs.

Among the four methods, we here mention the SCI method and the PCI method.

An SCI represened by the symbol $\mathrm{ZI}(\mathbf{G}_j; s_{d_{jk}}^{(\alpha)})$ is calculated for a subgroup $\mathbf{G}_j$ from the data of USCIs, which are multiplied in accord with participating orbits:

$$\mathrm{ZI}(\mathbf{G}_j; s_{d_{jk}}^{(\alpha)}) = \prod_{i=1}^{s}\prod_{\alpha=0}^{\alpha_i}\prod_{k=1}^{\nu}\left(s_{d_{jk}}^{(\alpha)}\right)^{\beta_k^{(ij)}}. \tag{4}$$

Although the meanings of the symbols are not explained for the sake of simplicity, the use of equation (4) is straightforward because each USCI represened by the inner product $(\prod_{k=1}^{\nu}(s_{d_{jk}}^{(\alpha)})^{\beta_k^{(ij)}})$ is collected in the $\mathbf{G}_j$-column of a USCI table (e.g., table 5). Note that the participant orbits ($\mathbf{G}(/\mathbf{G}_i)$) are distinguished by the superscript (α) so that they are ascribed to respective ligand inventories described below. Each of the monomials (equation (4)) produces a generating function for calculating intermediate numbers ($\rho_{\theta j}$) of isomers with various formulas W_θ and the fixed symmetry $\mathbf{G}_j$:

$$\sum_{\theta}\rho_{\theta j}W_\theta = \mathrm{ZI}\left(\mathbf{G}_j; s_{d_{jk}}^{(\alpha)}\right), \tag{5}$$

where we use ligand-inventories:

$$s_{d_{jk}}^{(\alpha)} = \sum_r w_{i\alpha}(X_r)^{d_{jk}}. \tag{6}$$

The intermediate numbers ($\rho_{\theta j}$) construct the $\mathbf{G}_j$-column of an intermediate matrix (equation (7)). The resulting matrix is multiplied by the inverse mark table (M^{-1}), providing the numbers ($A_{\theta j}$) of isomers with a given formula and a given symmetry, as shown in the matrix of the right-hand side of equation (7).

$$\begin{pmatrix} \rho_{11} & \rho_{12} & \cdots & \rho_{1s} \\ \rho_{21} & \rho_{22} & \cdots & \rho_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{|\theta|1} & \rho_{|\theta|2} & \cdots & \rho_{|\theta|s} \end{pmatrix} M^{-1} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1s} \\ A_{21} & A_{22} & \cdots & A_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ A_{|\theta|1} & A_{|\theta|2} & \cdots & A_{|\theta|s} \end{pmatrix}. \tag{7}$$

The data of SCIs are aligned in the order of SSG to give a row vector of SCIs. The row vector of SCIs is multiplied by the column vector of the inverse mark table (M^{-1}) to give a PCI for a subgroup $\mathbf{G}_i$:

$$\text{PCI}\big(\mathbf{G}_i; s_{d_{jk}}^{(\alpha)}\big) = \sum_{j=1}^s \overline{m}_{ji} \text{ZI}\big(\mathbf{G}_j; s_{d_{jk}}^{(\alpha)}\big), \tag{8}$$

where the SCI $\text{ZI}(\mathbf{G}_j; s_{d_{jk}}^{(\alpha)})$ is given by equation (4) and the symbol $\overline{m}_{ji}$ represents the jth element in the ith column of the inverse mark table (M^{-1}).

The PCI for a fixed subgroup $\mathbf{G}_i$ (equation (8)) is a polynomial, which gives a generating function for calculating the numbers $A_{\theta j}$ of isomers with various formulas (W_θ) and the fixed symmetry $\mathbf{G}_i$:

$$\sum_\theta A_{\theta i} W_\theta = \text{PCI}\big(\mathbf{G}_i; s_{d_{jk}}^{(\alpha)}\big), \tag{9}$$

where we use ligand-inventories represented by equation (6).

4.2. Isomer enumeration by the SCI method

Let us now enumerate adamantane isomers, where the bridges and bridgeheads of an adamantane skeleton are replaced by carbons, nitrogens and oxygens (figure 4). To do this enumeration, we shoud take account of the obligatory minimum valency (OMV) of each position [35]. That is to say, each bridge position is able to accomodate carbons, nitrogens and oxygens, while each bridgehead cannot take oxygen atoms. We can treat the OMV by using two kinds of ligand inventories.

Since the bridges and the bridgeheads belong to $\mathbf{T}_d(/\mathbf{C}_{2v})$ and $\mathbf{T}_d(/\mathbf{C}_{3v})$, respectively, we obtain the SCIs from the data of the USCI table. For example, the SCI for $\mathbf{C}_{3v}$ is calculated to be $(s_3^2)^{(1)} \times (s_1 s^3)^{(2)}$, where the superscripts (1) and (2) represent the $\mathbf{T}_d(/\mathbf{C}_{2v})$-orbit and $\mathbf{T}_d(/\mathbf{C}_{3v})$-orbit, respectively. Then, the ligand inventories shown in figure 4 are introduced into the resulting SCIs. The resulting equations are expanded
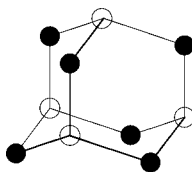
•Orbits and OMV (Obligatory minimum valency)

Bridges $\mathbf{T}_d(/\mathbf{C}_{2v})$: C, N, O $\implies$ Ligand Inventory:
$$s_d = x^d + y^d + z^d$$

Bridgeheads $\mathbf{T}_d(/\mathbf{C}_{3v})$: C, N (no O) $\implies$ Ligand Inventory:
$$s_d = x^d + y^d$$

•SCIs for Every Subgroups

	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_3$	$\mathbf{S}_4$	$\mathbf{D}_2$	$\mathbf{C}_{2v}$	$\mathbf{C}_{3v}$	$\mathbf{D}_{2d}$	$\mathbf{T}$	$\mathbf{T}_d$
$\mathbf{T}_d(/\mathbf{C}_{2v})$	s_1^6	$s_1^2 s_2^2$	$s_1^2 s_2^2$	s_3^2	$s_2 s_4$	s_2^3	$s_1^2 s_4$	s_3^2	$s_2 s_4$	s_6	s_6
	$\times$	$\times$	$\times$	$\times$	$\times$	$\times$	$\times$	$\times$	$\times$	$\times$	$\times$
$\mathbf{T}_d(/\mathbf{C}_{3v})$	s_1^4	s_2^2	$s_1^2 s_2$	$s_1 s_3$	s_4	s_4	s_2^2	$s_1 s_3$	s_4	s_4	s_4

Figure 4. Isomer enumeration by the SCI method.

to give generating functions for ρ-values. As an example, the expansion process for the subgroup $\mathbf{C}_{3v}$ is shown as follows:

$$\begin{aligned}
&\left(x^3 + y^3 + z^3\right)^2 (x + y)\left(x^3 + y^3\right) \\
&= x^{10} + x^9 y + 3x^7 y^3 + 3x^6 y^4 + 3x^4 y^6 + 3x^3 y^7 + xy^9 + y^{10} \\
&\quad + 2x^7 z^3 + x^4 z^6 + 2y^7 z^3 + y^4 z^6 \\
&\quad + 2x^6 yz^3 + x^3 yz^6 + 2xy^6 z^3 + xy^3 z^6.
\end{aligned} \tag{10}$$

The coefficients appearing in each of the expanded generating functions are collected to construct the corresponding column of an intermediate matrix in accord with equation (7), as shown in the first matrix of figure 5. For example, the coefficients in the right-hand side of equation (10) are listed in the $\mathbf{C}_{3v}$-row of the first matrix of figure 5. Then, the resulting matrix is multiplied by the inverse mark table (M^{-1}) for $\mathbf{T}_d$ to give a matrix collecting isomer numbers, as shown in the second matrix of figure 5.

To illustrate the results of enumeration, we depict isomers of $x^8 y^2$ and $x^8 z^2$, which corespond to diaza- and dioxa-adamantanes (figure 6). As for diaza-adamantane isomers, there are three $\mathbf{C}_s$-isomers, one $\mathbf{C}_{2v}$-isomer, and one $\mathbf{D}_{2d}$-isomer. On the other hand, there are one $\mathbf{C}_s$-dioxa isomer and one $\mathbf{D}_{2d}$-isomer. Our SCI method gives us isomer numbers with itemized symmetries. It should be noted here that Pólya's theorem gives value 5 for diaza- isomers and value 2 for dioxa- isomers, where itemization concerning symmetries is not taken into consideration.

$(\rho_{\theta j})$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_3$	$\mathbf{S}_4$	$\mathbf{D}_2$	$\mathbf{C}_{2v}$	$\mathbf{C}_{3v}$	$\mathbf{D}_{2d}$	$\mathbf{T}$	$\mathbf{T}_d$
x^{10}	1	1	1	1	1	1	1	1	1	1	1
x^9y	10	2	4	1	0	0	2	1	0	0	0
x^9z	6	2	2	0	0	0	2	0	0	0	0
x^8y^2	45	5	9	0	1	3	3	0	1	0	0
x^8z^2	15	3	3	0	1	3	1	0	1	0	0
x^8yz	54	2	6	0	0	0	2	0	0	0	0
x^7y^3	120	8	16	3	0	0	4	3	0	0	0
x^7z^3	20	4	4	2	0	0	0	2	0	0	0
x^7y^2z	216	8	12	0	0	0	4	0	0	0	0
x^7yz^2	120	4	10	0	0	0	0	0	0	0	0

M^{-1}

$(A_{\theta j})$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_3$	$\mathbf{S}_4$	$\mathbf{D}_2$	$\mathbf{C}_{2v}$	$\mathbf{C}_{3v}$	$\mathbf{D}_{2d}$	$\mathbf{T}$	$\mathbf{T}_d$
x^{10}	0	0	0	0	0	0	0	0	0	0	1
x^9y	0	0	0	0	0	0	1	1	0	0	0
x^9z	0	0	0	0	0	0	1	0	0	0	0
$\mathbf{x^8y^2}$	0	0	3	0	0	0	1	0	1	0	0
$\mathbf{x^8z^2}$	0	0	1	0	0	0	0	0	1	0	0
x^8yz	1	0	2	0	0	0	1	0	0	0	0
x^7y^3	2	1	3	0	0	0	2	3	0	0	0
x^7z^3	0	1	0	0	0	0	0	2	0	0	0
x^7y^2z	6	1	4	0	0	0	2	0	0	0	0
x^7yz^2	2	1	5	0	0	0	0	0	0	0	0

(with leading $=$ sign before the matrix)

Figure 5. Isomer enumeration by the SCI method.

4.3. Isomer enumeration by the PCI method

The PCI method gives equivalent results. For example, we have a PCI for $\mathbf{C}_{3v}$ as follows:

$$\text{PCI} = \left(s_3^2\right)^{(1)}(s_1 s_3)^{(2)} - (s_6)^{(1)}(s_4)^{(2)}, \tag{11}$$

where the superscripts (1) and (2) represent the $\mathbf{T}_d(/\mathbf{C}_{2v})$- and $\mathbf{T}_d(/\mathbf{C}_{3v})$-orbits. Note that the coefficients of equation (11) are picked up from the $\mathbf{T}_d(/\mathbf{C}_{3v})$-column of the inverse of the mark table of $\mathbf{T}_d$ (table 2), where the elements at the intersections with $\mathbf{C}_{3v}$- and $\mathbf{T}_d$-rows in the column are non-zero and the remaining values are equal to zero. The ligand inventories shown in figure 4 are introduced into the PCI (equation (11)), which is expanded to give the numbers of $\mathbf{C}_{3v}$-isomers as the coefficients of a generating functions:

$$\left(x^3 + y^3 + z^3\right)^2(x + y)\left(x^3 + y^3\right) - \left(x^6 + y^6 + z^6\right)\left(x^4 + y^4\right)$$
$$= x^9y + 3x^7y^3 + 2x^6y^4 + 2x^4y^6 + 3x^3y^7 + xy^9$$
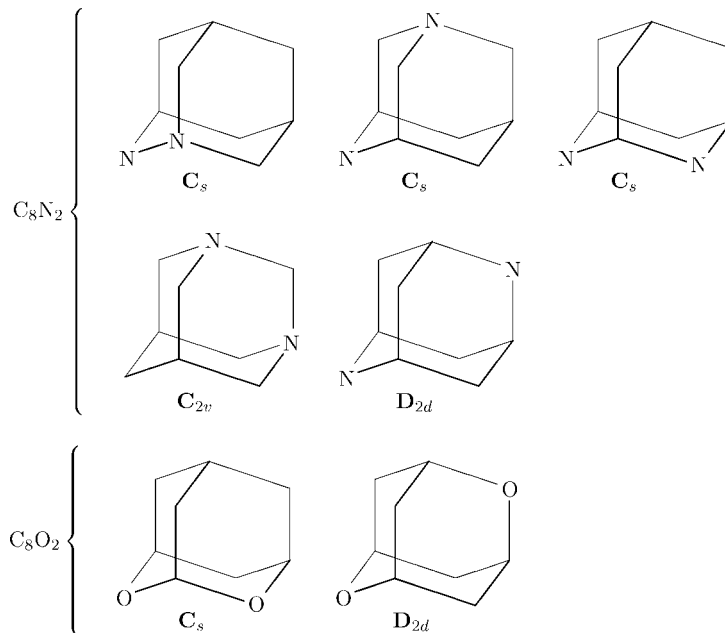$$+ 2x^7z^3 + 2y^7z^3 + 2x^6yz^3 + x^3yz^6 + 2xy^6z^3 + xy^3z^6. \tag{12}$$

Figure 6. Diaza- and dioxa-adamantane isomers.

The values are in agreement with the $\mathbf{C}_{3v}$-column of the matrix obtained by the SCI method shown in figure 5. The PCIs for the other subgroups and the corresponding generating functions can be obtained similarly.

4.4. Pólya's theorem derived from USCI approach

We have derived Pólya's theorem by starting from the USCI approach, where we have correlated USCIs with Pólya's cycle indices [38]. Thereby, a new formulation of a cycle index (CI) is represented by starting from SCIs as follows:

$$\text{CI}\big(\mathbf{G}; s_{d_{jk}}^{(\alpha)}\big) = \sum_{j=1}^{s} \left(\sum_{i=1}^{s} \overline{m}_{ji} \right) \text{ZI}\big(\mathbf{G}_j; s_{d_{jk}}^{(\alpha)}\big), \tag{13}$$

where the SCIs ($\text{ZI}(\mathbf{G}_j; s_{d_{jk}}^{(\alpha)})$) are represented by equation (4). By using the newly-defined CI (equation (13)), a generating function for enumeration of isomers with formula W_θ is obtained:

$$\sum_{\theta} A_\theta W_\theta = \text{CI}\big(\mathbf{G}; s_{d_{jk}}^{(\alpha)}\big) \tag{14}$$

where we use ligand-inventories represented by equation (6). This equation means that we have another formulation of Pólya's theorem on the basis of our USCI approach. The inner summation ($\sum_{i=1}^{s} \overline{m}_{ji}$) appearing in the definition of the CI (equation (13)) is the sum described in the inverse mark table (table 2).

Let us reexamine the enumeration of adamantane isomers by the CI method of the USCI approach. Under the tabulation of the SCIs for every subgroups, the inner summations are collected. Remember that each sum is a rational number for each cyclic subgroup, but vanishes for each non-cyclic subgroup. From the data collected in figure 4, we obtain the CI for this case:

$$CI = \frac{1}{24}\left(s_1^6\right)^{(1)}\left(s_1^4\right)^{(2)} + \frac{1}{8}\left(s_1^2 s_2^2\right)^{(1)}\left(s_2^2\right)^{(2)} + \frac{1}{4}\left(s_1^2 s_2^2\right)^{(1)}\left(s_1^2 s_2\right)^{(2)}$$
$$+ \frac{1}{3}\left(s_3^2\right)^{(1)}(s_1 s_3)^{(2)} + \frac{1}{4}(s_2 s_4)^{(1)}(s_4)^{(2)}. \tag{15}$$

After the ligand inventories shown in figure 4 are introduced, the resulting equation is expanded to give a generating function:

$$\sum_\theta A_\theta W_\theta = \frac{1}{24}(x + y + z)^6 (x + y)^4$$
$$+ \frac{1}{8}(x + y + z)^2\left(x^2 + y^2 + z^2\right)^2\left(x^2 + y^2\right)^2 + \cdots$$
$$= x^{10} + 2x^9 y + x^9 z + \underline{5x^8 y^2} + 4x^8 yz + \underline{2x^8 y^2} + \cdots. \tag{16}$$

As found easily, the CI defined here contains terms for cyclic subgroups, but does not contain terms for non-cyclic subgroups. Thereby, we reach an important conclusion: *Pólya's theorem takes account of cyclic subgroups only*! More precisely speaking, Pólya's theorem has been found to take account of conjugacy classes that are related to cyclic subgroups.

5. Restriction to cyclic subgroups

5.1. Markaracter tables, dominant subduction tables and dominant USCI tables

The conclusion described in the last section implies that we can select rows and columns for cyclic groups from the data of a mark table. For example, we select the upperleft part of the mark table of $\mathbf{T}_d$ (table 1) to produce a markaracter table (table 6) [39,40]. The term "markaracter" has been coined by us to discuss marks for permutation representations and characters for linear representations in a common basis. A dominant markaracter for a cyclic subgroup is here defined a row vector appearing in the resulting markaracter table.

On the same line as described on markaracters, subduction tables such as tables 3 and 4 can be restricted to treat cyclic subgroups only. The resulting tables (e.g., table 7) are called dominant subduction tables.

On the same line, USCI tables such as table 5 can be restricted to treat cyclic subgroups only. The resulting tables (e.g., table 8) are called dominant USCI tables. Obviously, the power of the variable s_1 in each dominant USCI (e.g., table 8) is equal to the corresponding character collected in the markaracter table (e.g., table 6).

Table 6
Markaracter table of $\mathbf{T}_d$ ($\widetilde{M}$).

	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_3$	$\mathbf{S}_4$
$\mathbf{T}_d(/\mathbf{C}_1)$	24	0	0	0	0
$\mathbf{T}_d(/\mathbf{C}_2)$	12	4	0	0	0
$\mathbf{T}_d(/\mathbf{C}_s)$	12	0	2	0	0
$\mathbf{T}_d(/\mathbf{C}_3)$	8	0	0	2	0
$\mathbf{T}_d(/\mathbf{S}_4)$	6	2	0	0	2

Table 7
Dominant subduction table of $\mathbf{T}_d$.

	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{S}_4$
$\mathbf{T}_d(/\mathbf{C}_1)$	$24\mathbf{C}_1(/\mathbf{C}_1)$	$12\mathbf{C}_2(/\mathbf{C}_1)$	$12\mathbf{C}_s(/\mathbf{C}_1)$	$8\mathbf{C}_3(/\mathbf{C}_1)$	$6\mathbf{S}_4(/\mathbf{C}_1)$
$\mathbf{T}_d(/\mathbf{C}_2)$	$12\mathbf{C}_1(/\mathbf{C}_1)$	$4\mathbf{C}_2(/\mathbf{C}_1)$ $+4\mathbf{C}_2(/\mathbf{C}_2)$	$6\mathbf{C}_s(/\mathbf{C}_1)$	$4\mathbf{C}_3(/\mathbf{C}_1)$	$2\mathbf{S}_4(/\mathbf{C}_1)$ $+2\mathbf{S}_4(/\mathbf{C}_2)$
$\mathbf{T}_d(/\mathbf{C}_s)$	$12\mathbf{C}_1(/\mathbf{C}_1)$	$6\mathbf{C}_2(/\mathbf{C}_1)$	$5\mathbf{C}_s(/\mathbf{C}_1)$ $+2\mathbf{C}_s(/\mathbf{C}_s)$	$4\mathbf{C}_3(/\mathbf{C}_1)$	$3\mathbf{S}_4(/\mathbf{C}_1)$
$\mathbf{T}_d(/\mathbf{C}_3)$	$8\mathbf{C}_1(/\mathbf{C}_1)$	$4\mathbf{C}_2(/\mathbf{C}_1)$	$4\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_1)$ $+2\mathbf{C}_3(/\mathbf{C}_3)$	$2\mathbf{S}_4(/\mathbf{C}_1)$
$\mathbf{T}_d(/\mathbf{S}_4)$	$6\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_1)$ $+2\mathbf{C}_2(/\mathbf{C}_2)$	$3\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{S}_4(/\mathbf{C}_1)$ $+2\mathbf{S}_4(/\mathbf{S}_4)$

Table 8
Dominant USCI table of $\mathbf{T}_d$.

	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{S}_4$
$\mathbf{T}_d(/\mathbf{C}_1)$	s_1^{24}	s_2^{12}	s_2^{12}	s_3^8	s_4^6
$\mathbf{T}_d(/\mathbf{C}_2)$	s_1^{12}	$s_1^4 s_2^4$	s_2^6	s_3^4	$s_2^2 s_4^2$
$\mathbf{T}_d(/\mathbf{C}_s)$	s_1^{12}	s_2^6	$s_1^2 s_2^5$	s_3^4	s_4^3
$\mathbf{T}_d(/\mathbf{C}_3)$	s_1^8	s_2^4	s_2^4	$s_1^2 s_3^2$	s_4^2
$\mathbf{T}_d(/\mathbf{S}_4)$	s_1^6	$s_1^2 s_2^2$	s_2^3	s_3^2	$s_1^2 s_4$
Sum	1/24	1/8	1/4	1/3	1/4

5.2. *Markaracters, subductions, and USCIs for non-cyclic subgroups*

Let us examine now markaracters for CRs concerning non-cyclic subgroups [39]. For example, the markaracter of $\mathbf{T}_d(/\mathbf{C}_{3v})$ is shown as follows:

$$\mathbf{T}_d(/\mathbf{C}_{3v}) = \begin{pmatrix} \mathbf{C}_1 & \mathbf{C}_2 & \mathbf{C}_s & \mathbf{C}_3 & \mathbf{S}_4 \\ 4 & 0 & 2 & 1 & 0 \end{pmatrix}.$$

This markaracter is calculated by a linear combination of dominant markaracters, which are concerned with the cyclic subgroups:

$$
\begin{array}{lcccccc}
-\frac{1}{2}\mathbf{T}_d(/\mathbf{C}_1) & = & -24 \times \frac{1}{2} & 0 & 0 & 0 & 0 \\
+\mathbf{T}_d(/\mathbf{C}_s) & = & 12 & 0 & 2 & 0 & 0 \\
+\frac{1}{2}\mathbf{T}_d(/\mathbf{C}_3) & = & 8 \times \frac{1}{2} & 0 & 0 & 2 \times \frac{1}{2} & 0 \\
\hline
\text{Total} & & 4 & 0 & 2 & 1 & 0
\end{array}
$$

The coefficients appearing in this linear combination are rational numbers, i.e., $-1/2$, $+1$ and $+1/2$. Markaracters of the present paper are equivalent to rational characters of the standard terminology and that this linear combination is equivalent to the calculation due to Artin's theorem on rational characters. It should be noted that the concept of markaracters stems from the concept of marks that are defined on the basis of permutation representatins, while the concept of rational characters comes from the concept of linear representations. The result is formally represented by using the symbols of CRs:

$$\mathbf{T}_d(/\mathbf{C}_{3v}) = -\frac{1}{2}\mathbf{T}_d(/\mathbf{C}_1) + \mathbf{T}_d(/\mathbf{C}_s) + \frac{1}{2}\mathbf{T}_d(/\mathbf{C}_3). \tag{17}$$

The subduction of the both sides of this equation is conducted formally so that the subduction concerning non-cyclic subgroups is represented by the subductions concerning cyclic subgroups:

$$\mathbf{T}_d(/\mathbf{C}_{3v}) \downarrow \mathbf{G}_i = -\frac{1}{2}\mathbf{T}_d(/\mathbf{C}_1) \downarrow \mathbf{G}_i + \mathbf{T}_d(/\mathbf{C}_s) \downarrow \mathbf{G}_i + \frac{1}{2}\mathbf{T}_d(/\mathbf{C}_3) \downarrow \mathbf{G}_i. \tag{18}$$

The formal subduction represented by equation (18) gives the subduction of non-dominant CRs from the data for cyclic subgroups [40]. For example, we have the CR $\mathbf{T}_d(/\mathbf{C}_{3v})$ subduced into $\mathbf{C}_s$ as follows:

$$
\begin{aligned}
\mathbf{T}_d(/\mathbf{C}_{3v}) \downarrow \mathbf{C}_s &= -\frac{1}{2}\mathbf{T}_d(/\mathbf{C}_1) \downarrow \mathbf{C}_s + \mathbf{T}_d(/\mathbf{C}_s) \downarrow \mathbf{C}_s + \frac{1}{2}\mathbf{T}_d(/\mathbf{C}_3) \downarrow \mathbf{C}_2 \\
&= -\frac{1}{2}\bigl(12\mathbf{C}_s(/\mathbf{C}_1)\bigr) + \bigl(5\mathbf{C}_s(/\mathbf{C}_1) + 2\mathbf{C}_s(/\mathbf{C}_s)\bigr) + \frac{1}{2}\bigl(4\mathbf{C}_s(/\mathbf{C}_1)\bigr) \\
&= \mathbf{C}_s(/\mathbf{C}_1) + 2\mathbf{C}_s(/\mathbf{C}_s). \tag{19}
\end{aligned}
$$

This result has already appeared in the left part of the subduction table of $\mathbf{T}_d$ (table 3).

The result represented by equation (18) also gives a useful result about the USCIs for CRs concerning non-cyclic subgroups [40]. Thus we obtain USCIs for non-dominant CRs for $\mathbf{T}_d(/\mathbf{C}_{3v})$:

$$
\begin{aligned}
\mathbf{C}_1 &: s_1^{24 \times (-1/2)} \times s_1^{12} \times s_1^{8 \times (1/2)} = s_1^4, \\
\mathbf{C}_2 &: s_2^{12 \times (-1/2)} \times s_2^6 \times s_2^{4 \times (1/2)} = s_2^2, \\
\mathbf{C}_s &: s_2^{12 \times (-1/2)} \times s_1^2 s_2^5 \times s_2^{4 \times (1/2)} = s_1^2 s_2, \\
\mathbf{C}_3 &: s_3^{8 \times (-1/2)} \times s_3^4 \times s_1^{2 \times (1/2)} s_3^{2 \times (1/2)} = s_1 s_3, \\
\mathbf{S}_4 &: s_4^{6 \times (-1/2)} \times s_4^3 \times s_4^{1 \times (1/2)} = s_4.
\end{aligned}
$$

These USCIs have already appeared in the lower left part of the USCI table of $\mathbf{T}_d$ (table 5).

6. Q-conjugacy and characteristic monomials

6.1. Markaracter tables, character tables, and Q-conjugacy character tables

Now, we are ready to discuss the relationship between markaracter tables and character tables [51,55]. Remember that chemical applications of the group theory, such as quantum chemistry and spectroscopic analyses, are based on character tables, whereas combinatorial eneumeration discussed here is based on markaracter tables.

Let us now compare the markaracter table of $\mathbf{T}_d$ and the corresoponding character table (table 9). As found easily, they have the same numbers of rows and the same numbers of columns. When we do, however, take the columns of these tables into consideration, we shoud mention that the markaracter table is itemized with respect to conjugate cyclic subgroups, while the character table is itemized with respect to conjugacy classes. Note also that the rows of the markaracter table are itemized with respect to CRs (more precisely dominant coset representations), while the rows of the character table are itemized with respect to irreducible representations. Thus, it is rather an accidental case that they have the same numbers of rows and the same numbers of columns. We call such a case as $\mathbf{T}_d$ "a matured case" [56]. This means that a character table is identi-

Table 9

(a) markaracter table ($\widetilde{M}$) and (b) (Q-conjugacy) character table of $\mathbf{T}_d$.

$\widetilde{M}$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_3$	$\mathbf{S}_4$
$\mathbf{T}_d(/\mathbf{C}_1)$	24	0	0	0	0
$\mathbf{T}_d(/\mathbf{C}_2)$	12	4	0	0	0
$\mathbf{T}_d(/\mathbf{C}_s)$	12	0	2	0	0
$\mathbf{T}_d(/\mathbf{C}_3)$	8	0	0	2	0
$\mathbf{T}_d(/\mathbf{S}_4)$	6	2	0	0	2

(a)

(D, Q)	$\mathbf{C}_1$ I	$\mathbf{C}_2$ $3C_2$	$\mathbf{C}_s$ $6\sigma_d$	$\mathbf{C}_3$ $8C_3$	$\mathbf{S}_4$ $6S_4$
A_1	1	1	1	1	1
A_2	1	1	−1	1	−1
E	2	2	0	−1	0
T_1	3	−1	−1	0	1
T_2	3	−1	1	0	−1

(b)

Table 10

(a) markaracter table ($\widetilde{M}$), (b) character table (D), and (c) Q-conjugacy character table (Q) of $\mathbf{T}$.

$\widetilde{M}$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_3$
$\mathbf{T}(/\mathbf{C}_1)$	12	0	0
$\mathbf{T}(/\mathbf{C}_2)$	6	2	0
$\mathbf{T}_d(/\mathbf{C}_3)$	4	0	1

(a)

(D)	I	$3C_2$	$4C_3$	$4C_3^2$
A_1	1	1	1	1
E_a	1	1	ω	ω^2
E_b	1	1	ω^2	ω
T	3	−1	0	0

(b)

(Q)	$\mathbf{C}_1$ I	$\mathbf{C}_2$ $3C_2$	$\mathbf{C}_3$ $\{4C_3, 4C_3^2\}$
A_1	1	1	1
E	2	2	−1
T	3	−1	0

(c)

Note: $\omega + \omega^2 = -1$.

cal with a **Q**-conjugacy character table, as clarified later by the discussion on unmatured cases.

In the case of **T** group, on the other hand, the markaracter table is different to the character table (table 10). We call this case "an unmatured case" [56,57]. In place of conjugacy classes based on conjugates operations, we use **Q**-conjugacy classes based on conjugate cyclic subgroups. Although a proof is abbreviated, we can add the E_1-row to E_2-row of the character table (table 10), where the results for the rightmost two columns are equal to each other, which are now called "**Q**-conjugacy characters". As a result, we obtain the **Q**-conjugacy character table. It should be noted here that this treatment is not a simple addition of a pair of conjugate complex characters, which is a standard treatment of chemical group theory [44].

In general, markaracter tables and **Q**-conjugacy character tables are interconvertible by appropriate transformation matrices, although a proof is abbreviated here. The interconvertibility between them has been proved by means of the Möbius function [53]. It is well known that irreducible characters are orthnormal; i.e., any two of them are orthogonal to each other and each irreducible character is normalized. In contrast, each **Q**-conjugacy character is not always normalized while two **Q**-conjugacy characters are orthoganal [58]. The present treatment represents a markaracter as a linear combination of **Q**-conjugacy characters with coefficients of integers [58], whereas Artin's theorem represents a markaracter (or a rational character) as a linear combination of dominant markaracters with coefficients of rational numbers [59].

6.2. Characteristic monomial tables and the characteristic-monomial method

The discussion on **Q**-conjugacy character tables enables us to construct a characteristic monomial (CM) table (e.g., table 11), which corresponds to a dominant USCI table described above (e.g., table 8). Note that the power of each dummy variable for the former table can be a minus integer, whereas the counterpart for the latter table is a plus integer [53]. Obviously, the power of the variable s_1 in each dominant CM (e.g., table 11) is equal to the corresponding character collected in the **Q**-conjugacy character table (e.g., table 9). This is parallel to the relashionship between markaracter tables and dominant USCI tables (e.g., table 9 vs. table 8).

Table 11
Characteristic monomial table for $\mathbf{T}_d$.

	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{S}_4$
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	$\frac{1}{24}$	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{4}$

From the data of a characteristic monomial (CM) table, we can construct a cycle index [52,60]:

$$\mathrm{CI}(\mathbf{G}; s_d') = \sum_{j=1} N_j \prod_i \left[Z(\Gamma_i \downarrow \mathbf{C}_j; s_d') \right]^{\alpha_i}. \qquad (20)$$

Although the general formula of the characteristic monomial $Z(\Gamma_i \downarrow \mathbf{C}_j; s_d')$ is not shown for the sake of simplicity, the use of equation (20) is straightforward by means of a CM table (e.g., table 11). Thereby, we can obtain a generating function for enumeration of isomers with formula W_θ:

$$\sum_\theta A_\theta W_\theta = \mathrm{CI}(\mathbf{G}; s_d') \qquad (21)$$

where we use ligand-inventories represented by equation (6). This is a further formulation equivalent to Pólya's theorem.

Let us reexamine the enumeration of adamantane isomers (figure 4) by means of the characteristic-monomial (CM) method. For example, the markaracter for $\mathbf{T}_d(/\mathbf{C}_{2v})$ is reduced into dominant markaracter A_1, E, and T_2 as follows:

$$\mathbf{T}_d(/\mathbf{C}_{2v}) = A_1 + E + T_2,$$
$$\mathbf{T}_d(/\mathbf{C}_{3v}) = A_1 + T_2.$$

According to this reduction, we can calculate the corresponding SCIs from the data of the characteristic monomial table of $\mathbf{T}_d$ (table 11). The CMs for $\mathbf{T}_d(/\mathbf{C}_{2v})$ are found in table 11 as follows:

$\mathbf{T}_d(/\mathbf{C}_{2v})$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_3$	$\mathbf{S}_4$
A_1	s_1	s_1	s_1	s_1	s_1
E	s_1^2	s_1^2	s_2	$s_1^{-1}s_3$	s_2
T_2	s_1^3	$s_1^{-1}s_2^2$	$s_1 s_2$	s_3	$s_1^{-1}s_4$

which are respectively multiplied by the CMs for $\mathbf{T}_d(/\mathbf{C}_{3v})$ taken also from table 11:

$\mathbf{T}_d(/\mathbf{C}_{3v})$	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_3$	$\mathbf{S}_4$
A_1	s_1	s_1	s_1	s_1	s_1
T_2	s_1^3	$s_1^{-1}s_2^2$	$s_1 s_2$	s_3	$s_1^{-1}s_4$
N_j	1/24	1/8	1/4	1/3	1/4

By introducing these SCIs into equation (20), we obtain a cycle index for this case:

$$\mathrm{CI} = \frac{1}{24}\left(s_1^6\right)^{(1)}\left(s_1^4\right)^{(2)} + \frac{1}{8}\left(s_1^2 s_2^2\right)^{(1)}\left(s_2^2\right)^{(2)} + \frac{1}{4}\left(s_1^2 s_2^2\right)^{(1)}\left(s_1^2 s_2\right)^{(2)}$$
$$+ \frac{1}{3}\left(s_3^2\right)^{(1)}(s_1 s_3)^{(2)} + \frac{1}{4}(s_2 s_4)^{(1)}(s_4)^{(2)}. \qquad (22)$$

The CI is identical with equation (15) obtained by the CI method of the USCI approach. By introducing the ligand inventories shown in figure 4, we can obtain a generating func-

Permutation Representation	Linear Representation

Marks – Markaracters — Q-Conjugacy characters — Characters
USCI – Dominant USCIs — Characteristic Monomials
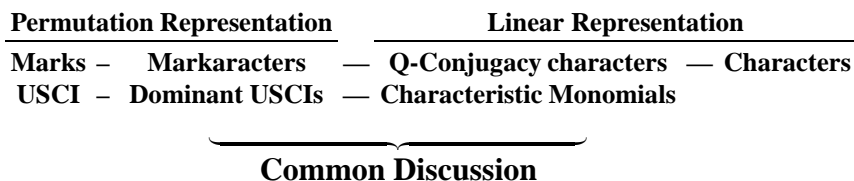
Common Discussion

Figure 7. Basis for common discussion.

tion, which is identical with the counterpart (equation (16)) derived by the CI method of the USCI approach.

7. Conclusion

Chemical applications of the group theory have two major fields, as shown in Introduction. Chemical combinatorics is based on permutation representations, which are characterized by means of "marks" as basic invariants, as shown in the left part of figure 7. On the other hand, applications to quantum chemistry etc. are linked to linear representations, which are charactereized by means of "characters" as basic invariants, as shown in the right part of figure 7. In this paper, we have derived markaracters from marks, while we derive **Q**-conjugacy characters from characters. Thereby, we have shown that the markaracters and the **Q**-conjugacy characters are interconvertible so as to be discussed in a common basis.

In agreement of this interconvertibility, dominant USCIs derived from USCIs have a common basis with characteristic monomials. Although the characteristic-monomial method have less advantage than the USCI method as a tool of chemical combinatorics, the common basis accompanied with the formulation of characteristic monomials are useful to comprehend group-theoretical applications.

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