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Systematic Classification of Molecular Symmetry by Subductions of Coset Representations

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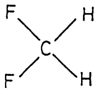
The notation based on the subduction of coset representations (the SCR notation) is presented for the systematic characterization of molecular symmetry. The positions of a parent skeleton are divided into orbits on which the corresponding coset representations (CRs) act. Each of the CRs is then subduced to the subsymmetry that characterizes a molecule derived from the skeleton. The resulting subduced representations are further reduced into CRs, which provide a basis of the SCR notation. The SCR notation is more discriminative than the point-group notation as well as than the framework-group notation. A new concept "unit subduced cycle index" is introduced in order to determine which subsymmetry is realized if we begin with a parent skeleton of a given symmetry.

Although point groups have long been used to classify molecular symmetry,[1)] they are frequently incomplete to afford full symmetry information about a molecule. For the purpose of remedying the incompleteness, Pople has proposed an elegant concept "framework group."[2)] This method provides more specific description of the symmetry information than do point groups. For example, molecules **1** and **2**, both of which have the same $\mathbf{C}_{2v}$ symmetry in the point-group approach, can be distinguished into $\mathbf{C}_{2v}[C_2(C), \sigma_v(F_2H_2)]$ and $\mathbf{C}_{2v}[C_2(C), \sigma_v(F_2), \sigma_v'(H_2)]$ in terms of the framework group.



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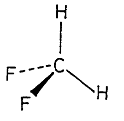

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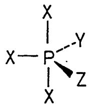
Recently, Brocas has pointed out that three isomers (**3**, **4**, and **5**), all of which are derived from a trigonal bipyramid ($\mathbf{D}_{3h}$) skeleton, have the same framework group, namely, $\mathbf{C}_s[\sigma(PXYZ), X(X_2)]$.[3)] Brocas has discussed in detail the necessity of discriminating these isomers. For this purpose, Brocas has proposed modified Schönflies symbols. Thus, the isomer (**3**) belongs to $\mathbf{C}_{sh}$, and isomers **4** and **5** are of $\mathbf{C}_{sv}$ symmetry.



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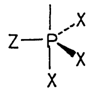

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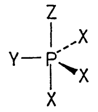

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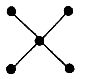
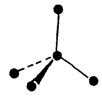
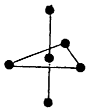
The two improved approaches are different in the perspectives from which they view molecular symmetry. The formulation of a framework group stems from the view that five atoms (CH_2F_2) directly occupy appropriate positions of a space to give a $\mathbf{C}_{2v}$ molecule. On the other hand, the modified Schönflies symbols imply the presence of a parent skeleton, so that a molecule is considered to be a derivative of the skeleton. Thus, the $\mathbf{C}_{sh}$ molecule (**3**) and the $\mathbf{C}_{sv}$ ones (**4** and **5**) are implicitly regarded as derivatives of the $\mathbf{D}_{3h}$ skeleton (**8**). The latter point of view has been widely adopted, especially for the enumeration of chemical structures.[3—5)] For example, Prelog's lecture for the Nobel Prize in Chemistry presented this methodology.[1a)] The $\mathbf{C}_{2v}$ compounds (**1** and **2**) can thus be considered to be derived by the respective CH_2F_2 substitutions on square ($\mathbf{D}_{4h}$) and tetrahedron ($\mathbf{T}_d$) skeleton (**6** and **7**).[1a,5)]


6 (D_{4h})


7 (T_d)


8 (D_{3h})

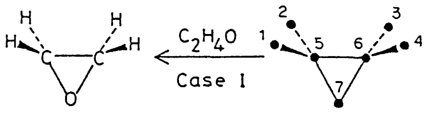
The incorporation of the modified Schönflies symbols into the framework group may provide a more effective tool for describing molecular symmetry. However, the modified Schönflies symbols still have some disadvantages, so that the symbol ($\mathbf{C}_{sv}$) is incapable of differentiating between **4** and **5**, though the pair of Y and Z in **4** is different from that in **5**). This drawback comes from the fact that the approach has never taken the transitivity of a skeleton into explicit consideration.

The above discussions show that a more discriminating method is neccessary for a systematic identification of molecular symmetry. We have reported the subduction of coset representations, which is a key to the enumeration of chemical structures.[6)] Subduction provides a detailed classification of the positions of a given structure in accord with its symmetry. In the present paper, we indicate that the subduction of coset representations is also a key concept for the classification or molecular symmetry. We thereby present the notation based on the subduction of coset representations (the SCR notation).

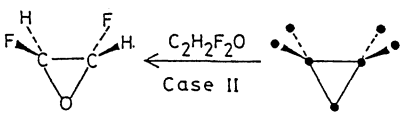
I. Molecules Based on a Parent Skeleton

We start from the standpoint that a molecule is regarded as being a derivative of a given skeleton. The skeleton is defined as a three-dimensional body that has a finite number of nodes (or positions) connected by bonds. Any molecule can be constructed by replacing the positions with appropriate atoms or ligands.

Let us first examine an oxirane molecule (**9**). This molecule can be considered to be a derivative of a parent skeleton (**10**) with C_2H_4O. In this case, both the molecule (**9**) and the skeleton (**10**) have the same $\mathbf{C}_{2v}$ symmetry. In other words, the substitution with C_2H_4O provides no change of symmetry. On the other hand, in case of compound **11**, a substitution with $C_2H_2F_2O$ on the skeleton (**10**) reduces the original $\mathbf{C}_{2v}$ symmetry into $\mathbf{C}_2$ symmetry.

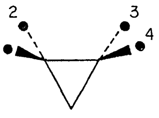


9 (C_{2v}) 10 (C_{2v})



11 (C_2) 10 (C_{2v})

Skeleton (**10**) has three types of equivalent positions (nodes), which are represented by heavy dots in **12**, **13**, and **14**. Each set of equivalent positions are called an *orbit*. Two cases (**9** and **11**) are different regarding their modes of packing such orbits. Molecule (**9**) has four hydrogens on orbit (**12**), two carbons on **13**, and one oxygen on **14**. Thus, the same kind of atoms fulfill the respective orbit in molecule (**9**). On the other hand, the corresponding positions (**12**) in molecule **11** are occupied by two hydrogens and two fluorines so as to create a $\mathbf{C}_2$ subsymmetry.



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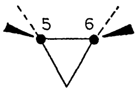

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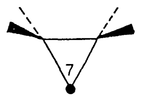

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In general, there are two cases in the substitution of a skeleton. The first case (Case I) affords a molecule of which the symmetry is the same as that of a parent skeleton, as shown in the case of **9**. Another case (Case II) creates a molecule that has a lower symmetry than that of the skeleton, as exemplified by **11**. Our target is a detailed specification of symmetry which is effective in Case I as well as in Case II. Case I can be described by the concept of coset representations. Case II requires a novel concept *subduction of coset representations*.

II. Coset Representations and Transitivity of a Parent Skeleton

Although the concept of coset representations is well-known in mathematics,[7,8] its application to chemical problems has been limited. We have reported the definition of the coset representations and provide them with chemical meaning.[6,9]

Let **G** be a finite group. Suppose that **H** is a subgroup of **G**. We then consider a coset decompostion,

$$\mathbf{G}=\mathbf{H}g_1+\mathbf{H}g_2+\cdots+\mathbf{H}g_m, \tag{1}$$

where $g_1=I$ (identity) and $g_j \in \mathbf{G}$ (for $j=1, 2,\cdots, m$). The set of the elements $(g_1, g_2, \cdots, g_m)$ is called a transversal. In accord with this decomposition we construct a coset representation (CR) which is designated by the symbol $\mathbf{G}(/\mathbf{H})$. The CR that is originally a permutation group on a set of cosets can be regarded as a permutation group on a set of positions of a skeleton.[10] This fact is important to the chemical application of CRs.

A set of subgroups (SSG) of **G** is defined as an irredundant set that contains a representative of each set of conjugate subgroups,

$$\mathrm{SSG}=\{\mathbf{G}_1, \mathbf{G}_2, \cdots, \mathbf{G}_s\}, \tag{2}$$

in ascending order of their orders, where $\mathbf{G}_1=\mathbf{C}_1$ (an identity group) and $\mathbf{G}_s=\mathbf{G}$. The set of corresponding CRs,

$$\mathrm{SCR}=\{\mathbf{G}(/\mathbf{G}_1), \mathbf{G}(/\mathbf{G}_2), \cdots, \mathbf{G}(/\mathbf{G}_s)\}, \tag{3}$$

has been proved to be a complete set of different transitive representations of **G**.[11] Obviously, $\mathbf{G}(/\mathbf{G}_1)$ is a regular representation and $\mathbf{G}(/\mathbf{G}_s)$ is homomorphic to an identity group.

Suppose that **G** acts on

$$\Delta=\{\delta_1, \delta_2,\cdots, \delta_{|\Delta|}\} \tag{4}$$

in the form of a permutation representation $\mathbf{P}_\mathbf{G}$ on Δ. In this case, Δ may contain one or more orbits on the action of **G**. Chemically, Δ corresponds to a set of positions contained in a given skeleton and **G** may be the point group of the skeleton. The following theorem holds for any $\mathbf{P}_\mathbf{G}$.[11]

Theorem 1. The permutation representation $\mathbf{P}_\mathbf{G}$ can be reduced into transitive CRs in terms of

$$\mathbf{P}_\mathbf{G}=\sum_{i=1}^{s}\alpha_i\mathbf{G}(/\mathbf{G}_i), \tag{5}$$

where each α_i is a non-negative integer. The multiplicities α_i $(i=1, 2, \cdots, s)$ are obtained by

$$\mu_j=\sum_{i=1}^{s}\alpha_i m_j^{(i)} \qquad (j=1, 2, \cdots, s), \tag{6}$$

where μ_j is the mark (the number of fixed points) of $\mathbf{G}_j$ in $\mathbf{P}_\mathbf{G}$ and $m_j^{(i)}$ is the mark of $\mathbf{G}_j$ in $\mathbf{G}(/\mathbf{G}_i)$.[12]

The matrix of $m_j^{(i)}$'s is called a table of marks (or a mark table), which has been introduced by Burnside.[7,13] Equation 6 can be rewritten as follows by using the inverse of the mark table,

$$\alpha_i=\sum_{j=1}^{s}\mu_j\overline{m}_j^{(i)} \qquad \text{for } i=1, 2, \cdots, s. \tag{7}$$

We then define two vectors for further discussions, i.e.,

$$\text{a fixed-point vector (FPV), } (\mu_1\mu_2\cdots\mu_s), \tag{8}$$

and

$$\text{a multiplicity vector (MV), } (\alpha_1\alpha_2\cdots\alpha_s). \tag{9}$$

The MV is a descriptor of the symmetry of a skeleton.

Table 1 collects the coset representations of $\mathbf{C}_{2v}$ group, where each permutation is represented as the product of cycles. The corresponding table of marks (Table 2) can be derived from the data of Table 1. Table 3 shows the inverse of the mark table. Tables 4—6 contain the counterparts of the $\mathbf{D}_{3h}$ group. Table 7 collects the inverse of the mark table of the $\mathbf{T}_d$ group.

Equation 5 (Theorem 1) determines the mode of action of $\mathbf{G}$ on the $\mathbf{G}$-set (Δ), which is divided into a set of orbits:

$$\left\{\begin{array}{l} \Delta_{11}, \Delta_{12}, \cdots, \Delta_{1\alpha_1}, \text{ each of which } \mathbf{G}(/\mathbf{G}_1) \text{ acts on;} \\ \Delta_{21}, \Delta_{22}, \cdots, \Delta_{2\alpha_2}, \text{ each of which } \mathbf{G}(/\mathbf{G}_2) \text{ acts on;} \\ \qquad \cdots \\ \text{and} \\ \Delta_{s1}, \Delta_{s2}, \cdots, \Delta_{s\alpha_s}, \text{ each of which } \mathbf{G}(/\mathbf{G}_s) \text{ acts on.} \end{array}\right. \tag{10}$$

In a chemical sense, Eq. 10 indicates the transitivitity of a parent skeleton. Suppose that the $\mathbf{G}$-set (Δ) denotes a set of the positions of the skeleton. Then, each orbit $\Delta_{i\alpha}$ represented by Eq. 10 is a set of equivalent positions contained in the skeleton. It should be noted that a coset representation on $\Delta_{i\alpha}(\alpha=1, 2,\cdots, \alpha_i)$, is determined only by $\mathbf{G}$ and $\mathbf{G}_i$.

Example 1. The positions of the skeleton (**10**) are numbered as 1, 2, ···, 7. Let the seven positions be a $\mathbf{C}_{2v}$-set. A permutation representation ($\mathbf{P}_{\mathbf{C}_{2v}}$) is obtained as follows:

I: (1)(2)(3)(4)(5)(6)(7),
C_2: (1 3)(2 4)(5 6)(7),
$\sigma_{v(1)}$: (1 4)(2 3)(5 6)(7),

Table 1. Coset Representations of $\mathbf{C}_{2v}$

$\mathbf{C}_{2v}$	$\mathbf{C}_{2v}(/\mathbf{C}_1)$	$\mathbf{C}_{2v}(/\mathbf{C}_2)$	$\mathbf{C}_{2v}(/\mathbf{C}_s)$	$\mathbf{C}_{2v}(\mathbf{C}_s')$	$\mathbf{C}_{2v}(\mathbf{C}_{2v})$
I	(1) (2) (3) (4)	(1) (2)	(1) (2)	(1) (2)	(1)
C_2	(1 2) (3 4)	(1) (2)	(1 2)	(1 2)	(1)
$\sigma_{v(1)}$	(1 3) (2 4)	(1 2)	(1) (2)	(1 2)	(1)
$\sigma_{v(2)}$	(1 4) (2 3)	(1 2)	(1 2)	(1) (2)	(1)

Table 2. The Mark Table of $\mathbf{C}_{2v}$

	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_s'$	$\mathbf{C}_{2v}$
$\mathbf{C}_{2v}(/\mathbf{C}_1)$	4	0	0	0	0
$\mathbf{C}_{2v}(/\mathbf{C}_2)$	2	2	0	0	0
$\mathbf{C}_{2v}(/\mathbf{C}_s)$	2	0	2	0	0
$\mathbf{C}_{2v}(/\mathbf{C}_s')$	2	0	0	2	0
$\mathbf{C}_{2v}(/\mathbf{C}_{2v})$	1	1	1	1	1

Table 3. The Inverse of the Mark Table of $\mathbf{C}_{2v}$

	$\mathbf{C}_{2v}(/\mathbf{C}_1)$	$\mathbf{C}_{2v}(/\mathbf{C}_2)$	$\mathbf{C}_{2v}(/\mathbf{C}_s)$	$\mathbf{C}_{2v}(/\mathbf{C}_s')$	$\mathbf{C}_{2v}(/\mathbf{C}_{2v})$
$\mathbf{C}_1$	1/4	0	0	0	0
$\mathbf{C}_2$	−1/4	1/2	0	0	0
$\mathbf{C}_s$	−1/4	0	1/2	0	0
$\mathbf{C}_s'$	−1/4	0	0	1/2	0
$\mathbf{C}_{2v}$	1/2	−1/2	−1/2	−1/2	1

Table 4. Coset Representations of $\mathbf{D}_{3h}$

$\mathbf{D}_{3h}$	$\mathbf{D}_{3h}(/\mathbf{C}_1)$	$\mathbf{D}_{3h}(/\mathbf{C}_2)$	$\mathbf{D}_{3h}(/\mathbf{C}_s)$	$\mathbf{D}_{3h}(/\mathbf{C}_s')$	$\mathbf{D}_{3h}(/\mathbf{C}_3)$	$\mathbf{D}_{3h}$ $(/\mathbf{C}_{2v})$	$\mathbf{D}_{3h}$ $(/\mathbf{C}_{3v})$	$\mathbf{D}_{3h}$ $(/\mathbf{C}_{3h})$	$\mathbf{D}_{3h}$ $(/\mathbf{D}_3)$	$\mathbf{D}_{3h}$ $(/\mathbf{D}_{3h})$
I	(1)(2)(3)(4)(5)(6)- (7)(8)(9)(10)(11)(12)	(1)(2)(3)- (4)(5)(6)	(1)(2)(3)- (4)(5)(6)	(1)(2)(3)- (4)(5)(6)	(1)(2)(3)(4)	(1)(2)(3)	(1)(2)	(1)(2)	(1)(2)	(1)
C_3	(1 2 3)(4 5 6)(7 8 9)- (10 12 11)	(1 2 3)- (4 5 6)	(1 2 3)- (4 6 5)	(1 2 3)- (4 6 5)	(1)(2)(3)(4)	(1 2 3)	(1)(2)	(1)(2)	(1)(2)	(1)
C_3^2	(1 3 2)(4 5 6)(7 9 8)- (10 11 12)	(1 3 2)- (4 6 5)	(1 3 2)- (4 5 6)	(1 3 2)- (4 5 6)	(1)(2)(3)(4)	(1 3 2)	(1)(2)	(1)(2)	(1)(2)	(1)
$C_{2(1)}$	(1 4)(2 5)(3 6)(7 10)- (8 11)(9 12)	(1)(2 3)(4)- (5 6)	(1 4)(2 5)- (3 6)	(1 4)(2 5)- (3 6)	(1 2)(3 4)	(1)(2 3)	(1 2)	(1 2)	(1)(2)	(1)
$C_{2(2)}$	(1 5)(2 6)(3 4)(7 11)- (8 12)(9 10)	(1 3)(2)- (4 6)(5)	(1 5)(2 6)- (3 4)	(1 5)(2 6)- (3 4)	(1 2)(3 4)	(1 3)(2)	(1 2)	(1 2)	(1)(2)	(1)
$C_{2(3)}$	(1 6)(2 4)(3 5)(7 12)- (8 10)(9 11)	(1 2)(3)- (4 5)(6)	(1 6)(3 5)- (2 4)	(1 6)(2 4)- (3 5)	(1 2)(3 4)	(1 2)(3)	(1 2)	(1 2)	(1)(2)	(1)
σ_h	(1 7)(2 8)(3 9)(4 10)- (5 11)(6 12)	(1 4)(2 5)- (3 6)	(1 4)(2 6)- (3 5)	(1)(2)(3)- (4)(5)(6)	(1 3)(2 4)	(1)(2)(3)	(1 2)	(1)(2)	(1 2)	(1)
S_3	(1 8 3 7 2 9)- (4 12 5 10 6 11)	(1 5 3 4 2 6)	(1 6 3 4 2 5)	(1 2 3)- (4 6 5)	(1 3)(2 4)	(1 2 3)	(1 2)	(1)(2)	(1 2)	(1)
S_3^5	(1 9 2 7 3 8)- (4 11 6 10 5 12)	(1 6 2 4 3 5)	(1 5 2 4 3 6)	(1 3 2)- (4 5 6)	(1 3)(2 4)	(1 3 2)	(1 2)	(1)(2)	(1 2)	(1)
$\sigma_{v(1)}$	(1 10)(2 11)(3 12)- (4 7)(5 8)(6 9)	(1 4)(2 6)- (3 5)	(1)(2 3)(4)- (5 6)	(1 4)(2 5)- (3 6)	(1 4)(2 3)	(1)(2 3)	(1)(2)	(1 2)	(1 2)	(1)
$\sigma_{v(2)}$	(1 11)(2 12)(3 10)- (4 9)(5 7)(6 8)	(1 6)(2 5)- (3 4)	(1 3)(2)- (4 5)(6)	(1 5)(2 6)- (3 4)	(1 4)(2 3)	(1 3)(2)	(1)(2)	(1 2)	(1 2)	(1)
$\sigma_{v(3)}$	(1 12)(2 10)(3 11)- (4 8)(5 9)(67)	(1 5)(2 4)- (3 6)	(1 2)(3)- (4 6)(5)	(1 6)(2 4)- (3 5)	(1 4)(2 3)	(1 2)(3)	(1)(2)	(1 2)	(1 2)	(1)

and

$$\sigma_{v(2)}\text{: } (1\ 2)(3\ 4)(5)(6)(7).$$

From these data, we obtain the marks of the subgroups in $\mathbf{P}_{\mathbf{C}_{2v}}$:

$$\mu_{\mathbf{C}_1}=7,\ \mu_{\mathbf{C}_2}=1,\ \mu_{\mathbf{C}_s}=1,\ \mu_{\mathbf{C}_s'}=3, \text{ and } \mu_{\mathbf{C}_{2v}}=1.$$

This affords an FPV=(7 1 1 3 1), the elements of which are aligned in the order of SSG={$\mathbf{C}_1$, $\mathbf{C}_2$, $\mathbf{C}_s$, $\mathbf{C}_s'$, $\mathbf{C}_{2v}$}. Then, the FPV is introduced into Eq. 7 to yield

$$\text{MV}=(7\ 1\ 1\ 3\ 1)\text{IMT}=(1\ 0\ 0\ 1\ 1), \tag{11}$$

where IMT is the inverse of the mark table of $\mathbf{C}_{2v}$ found in Table 3. The MV=(1 0 0 1 1) corresponds to a reduction,

$$\mathbf{P}_{\mathbf{C}_{2v}}=\mathbf{C}_{2v}(/\mathbf{C}_1)+\mathbf{C}_{2v}(/\mathbf{C}_s')+\mathbf{C}_{2v}(/\mathbf{C}_{2v}), \tag{12}$$

since SCR={$\mathbf{C}_{2v}(/\mathbf{C}_1)$, $\mathbf{C}_{2v}(/\mathbf{C}_2)$, $\mathbf{C}_{2v}(/\mathbf{C}_s)$, $\mathbf{C}_{2v}(/\mathbf{C}_{s'})$, $\mathbf{C}_{2v}(/\mathbf{C}_{2v})$}.

Table 5. The Mark Table of $\mathbf{D}_{3h}$

	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_s$	$\mathbf{C}_s'$	$\mathbf{C}_3$	$\mathbf{C}_{2v}$	$\mathbf{C}_{3v}$	$\mathbf{C}_{3h}$	$\mathbf{D}_3$	$\mathbf{D}_{3h}$
$\mathbf{D}_{3h}(/\mathbf{C}_1)$	12	0	0	0	0	0	0	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_2)$	6	2	0	0	0	0	0	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_s)$	6	0	2	0	0	0	0	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_s')$	6	0	0	6	0	0	0	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_3)$	4	0	0	0	4	0	0	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_{2v})$	3	1	1	3	0	1	0	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_{3v})$	2	0	2	0	2	0	2	0	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_{3h})$	2	0	0	2	2	0	0	2	0	0
$\mathbf{D}_{3h}(/\mathbf{C}_3)$	2	2	0	0	2	0	0	0	2	0
$\mathbf{D}_{3h}(/\mathbf{C}_{3h})$	1	1	1	1	1	1	1	1	1	1

The concrete forms of the CRs appearing in the right-hand side are found in Table 1. Note that the numbering of Table 1 is different from the present one. The CR, $\mathbf{C}_{2v}(/\mathbf{C}_1)$, is a permutation group on Δ_1={1,2,3,4}, the orbits of which are illustrated in **12**. The second CR, $\mathbf{C}_{2v}(/\mathbf{C}_s')$, is concerned with Δ_2={5,6} (**13**). The third CR, $\mathbf{C}_{2v}(/\mathbf{C}_{2v})$, acts on Δ_3={1} (**14**). Thus, the actions of CRs can be graphically verified.

III. The SCR Notation for Case I

The discussions given in Section II provide a basis for describing the symmetry of a molecule or Case I, in which the full symmetry of a given skeleton is conserved during the process of atom substitution. Suppose that the positions of the skeleton are divided into orbits by Eq. 5. In order to realize the full symmetry, all of the positions of each orbit ($\Delta_{i\alpha}$), on which $\mathbf{G}(/\mathbf{G}_i)$ acts (Eq. 10), should be fully occupied by r of the same kind of atoms $\mathrm{A}^{(i)}$, where $r=|\Delta_{i\alpha}|=|\mathbf{G}|/|\mathbf{G}_i|$. This situation is denoted as

$$\mathbf{G}[\cdots;/\mathbf{G}_i(\mathrm{A}_r^{(i)});\cdots] \tag{13}$$

by using each term of Eq. 5, where all the terms that appear in Eq. 5 are listed sequentially to show the

Table 6. The Inverse of the Mark Table of $\mathbf{D}_{3h}$[a)]

	$/\mathbf{C}_1$	$/\mathbf{C}_2$	$/\mathbf{C}_s$	$/\mathbf{C}_s'$	$/\mathbf{C}_3$	$/\mathbf{C}_{2v}$	$/\mathbf{C}_{3v}$	$/\mathbf{C}_{3h}$	$/\mathbf{D}_3$	$/\mathbf{D}_{3h}$
$\mathbf{C}_1$	1/12	0	0	0	0	0	0	0	0	0
$\mathbf{C}_2$	−1/4	1/2	0	0	0	0	0	0	0	0
$\mathbf{C}_s$	−1/4	0	1/2	0	0	0	0	0	0	0
$\mathbf{C}_s'$	−1/12	0	0	1/6	0	0	0	0	0	0
$\mathbf{C}_3$	−1/12	0	0	0	1/4	0	0	0	0	0
$\mathbf{C}_{2v}$	1/2	−1/2	−1/2	−1/2	0	1	0	0	0	0
$\mathbf{C}_{3v}$	1/4	0	−1/2	0	−1/4	0	1/2	0	0	0
$\mathbf{C}_{3h}$	1/12	0	0	−1/6	−1/4	0	0	1/2	0	0
$\mathbf{D}_3$	1/4	−1/2	0	0	−1/4	0	0	0	1/2	0
$\mathbf{D}_{3h}$	−1/2	1/2	1/2	1/2	1/2	−1	−1/2	−1/2	−1/2	1

a) The symbol $/\mathbf{G}_i$ is the abbreviated form of $\mathbf{G}(/\mathbf{G}_i)$.

Table 7. The Inverse ($\overline{\mathrm{M}}$) of the Mark Table of $\mathbf{T}_d$

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

symmetry of the Case I molecule. This SCR notation indicates how a set of equivalent atoms is transformed in itself by operations of **G**.

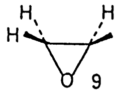
Any molecule of Case I can be specified in terms of Eq. 13. For example, the symmetry of oxirane **9** is represented by $\mathbf{C}_{2v}[/\mathbf{C}_1(H_4); /\mathbf{G}_s'(C_2); /\mathbf{C}_{2v}(O)]$, because the skeleton (**10**) is reduced by Eq. 12 (Example 1). This notation means that four hydrogen atoms (H_4) occupy the orbit Δ_1 (**12**) on which $\mathbf{C}_{2v}(/\mathbf{C}_1)$ acts, two carbons (C_2) fill Δ_2(**13**) on which $\mathbf{C}_{2v}(/\mathbf{C}_s')$ acts and one oxygen (O) takes Δ_3 (**14**) on which $\mathbf{C}_{2v}(/\mathbf{C}_{2v})$ acts.

Table 8 lists the SCR notations of several molecules of $\mathbf{C}_{2v}$ symmetry: phenanthrene (**15**), an iceanedione (**16**), noradamantane (**17**), norbornane (**18**), basketane (**19**), and water (**20**). The FPV of each compound is obtained by counting fixed points on the operations of respective subsymmetries. Each MV of Table 8 is then obtained by multiplying the FPV with the

Table 8. $\mathbf{C}_{2v}$ Molecules on $\mathbf{C}_{2v}$ Skeletons[a)]

Molecule	FPV	MV	SCR notation
9	(7 1 1 3 1)	(1 0 0 1 1)	$\mathbf{C}_{2v}[/\mathbf{C}_1(H_4); /\mathbf{C}_s'(C_2); /\mathbf{C}_{2v}(O)]$
15	(24 0 24 0 0)	(0 0 12 0 0)	$\mathbf{C}_{2v}[12/\mathbf{C}_s(7C_2, 5H_2)]$
16	(28 0 8 0 0)	(5 0 4 0 0)	$\mathbf{C}_{2v}[5/\mathbf{C}_1(2C_4, 3H_4); 4/\mathbf{C}_s(2C_2, H_2, O_2)]$
17	(23 1 7 5 1)	(3 0 3 2 1)	$\mathbf{C}_{2v}[3/\mathbf{C}_1(C_4, 2H_4); 3/\mathbf{C}_s(C_2, 2H_2); 2/\mathbf{C}_s'(C_2, H_2); /\mathbf{C}_{2v}(C)]$
18	(19 1 5 3 1)	(3 0 2 1 1)	$\mathbf{C}_{2v}[3/\mathbf{C}_1(C_4, 2H_4); 2/\mathbf{C}_s(C_2, H_2); /\mathbf{C}_s'(H_2); /\mathbf{C}_{2v}(C)]$
19	(22 0 10 0 0)	(3 0 5 0 0)	$\mathbf{C}_{2v}[3/\mathbf{C}_1(C_4, 2H_4); 5/\mathbf{C}_s(3C_2, 2H_2)]$
20	(3 1 3 1 1)	(0 0 1 0 1)	$\mathbf{C}_{2v}[/\mathbf{C}_s(H_2); /\mathbf{C}_{2v}(O)]$

a) SSG={$\mathbf{C}_1$, $\mathbf{C}_2$, $\mathbf{C}_s$, $\mathbf{C}_s'$, $\mathbf{C}_{2v}$} for $\mathbf{C}_{2v}$. See Eq. 7. The corresponding set of coset representations (SCR) is obtained in terms of Eq. 8. Each MV (multiplicity vector) denotes the respective multiplicities of the coset representations contained in the SCR. The MV is obtained by the multiplication of the corresponding fixed point vector (FPV) by the inverse of the mark table (Table 3). See Eq. 12.



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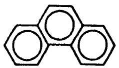
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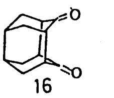

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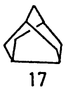
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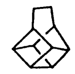
18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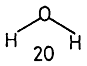
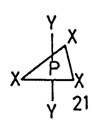


20

Table 9. $\mathbf{D}_{3h}$ Molecules on $\mathbf{D}_{3h}$ Skeletons[a)]

Molecule	FPV	MV	SCR notation
21	(6 2 4 4 3 2 3 1 1 1)	(0 0 0 0 0 1 1 0 0 1)	$\mathbf{D}_{3h}[/\mathbf{C}_{2v}(X_3); /\mathbf{C}_{3v}(Y_2); /\mathbf{D}_{3h}(P)]$
22	(9 1 3 3 0 1 0 0 0 0)	(0 0 1 0 0 1 0 0 0 0)	$\mathbf{D}_{3h}[/\mathbf{C}_s(H_6); /\mathbf{C}_{2v}(C_3)]$
23	(9 1 1 9 0 1 0 0 0 0)	(0 0 0 1 0 1 0 0 0 0)	$\mathbf{D}_{3h}[/\mathbf{C}_s'(H_6); /\mathbf{C}_{2v}(C_3)]$
24	(9 3 3 9 0 3 0 0 0 0)	(0 0 0 0 0 3 0 0 0 0)	$\mathbf{D}_{3h}[3/\mathbf{C}_{2v}(C_3, 2H_3)]$
25	(12 0 4 0 0 0 0 0 0 0)	(0 0 2 0 0 0 0 0 0 0)	$\mathbf{D}_{3h}[2/\mathbf{C}_s(C_6, H_6)]$
26	(34 0 14 0 4 0 4 0 0 0)	(0 0 5 0 0 0 2 0 0 0)	$\mathbf{D}_{3h}[5/\mathbf{C}_s(3C_6, 2H_6); 2/\mathbf{C}_{3v}(C_2, H_2)]$
27	(24 0 0 12 0 0 0 0 0 0)	(1 0 0 2 0 0 0 0 0 0)	$\mathbf{D}_{3h}[/\mathbf{C}_1(H_{12}); 2/\mathbf{C}_s'(2C_6)]$
28	(4 2 2 4 1 3 1 1 1 1)	(0 0 0 0 0 1 0 0 0 1)	$\mathbf{D}_{3h}[/\mathbf{C}_{2v}(F_3); /\mathbf{D}_{3h}(B)]$

a) SSG={$\mathbf{C}_1$, $\mathbf{C}_2$, $\mathbf{C}_s$, $\mathbf{C}_s'$, $\mathbf{C}_3$, $\mathbf{C}_{2v}$, $\mathbf{C}_{3v}$, $\mathbf{C}_{3h}$, $\mathbf{D}_3$, $\mathbf{D}_{3h}$} for $\mathbf{D}_{3h}$. See the footnote of Table 8. The inverse of the mark table of $\mathbf{D}_{3h}$ is found in Table 6.



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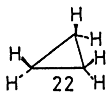

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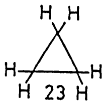

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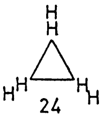

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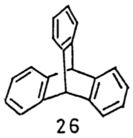
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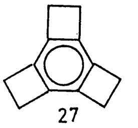
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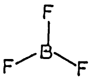

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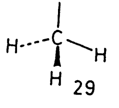
Table 10. $\mathbf{T}_d$ Molecules on $\mathbf{T}_d$ Skeletons[a)]

Molecule	FPV	MV	SCR notation
29	(5 1 3 2 1 1 1 2 1 1 1)	(0 0 0 0 0 0 0 1 0 0 1)	$\mathbf{T}_d[/\mathbf{C}_{3v}(H_4); /\mathbf{T}_d(C)]$
30	(8 0 4 2 0 0 0 2 0 0 0)	(0 0 0 0 0 0 0 2 0 0 0)	$\mathbf{T}_d[2/\mathbf{C}_{3v}(C_4, H_4)]$
31	(26 2 8 2 0 0 2 2 0 0 0)	(0 0 1 0 0 0 1 2 0 0 0)	$\mathbf{T}_d[/\mathbf{C}_s(H_{12}); /\mathbf{C}_{2v}(C_6); 2/\mathbf{C}_{3v}(C_4, H_4)]$

a) SSG={$\mathbf{C}_1$, $\mathbf{C}_2$, $\mathbf{C}_s$, $\mathbf{C}_3$, $\mathbf{S}_4$, $\mathbf{D}_2$, $\mathbf{C}_{2v}$, $\mathbf{C}_{3v}$, $\mathbf{D}_{2d}$, $\mathbf{T}$, $\mathbf{T}_d$} for $\mathbf{T}_d$. See the footnote of Table 8. The inverse of the mark table of $\mathbf{T}_d$ is found in Table 7.



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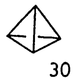
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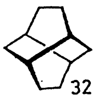
31

Table 11. Molecules on $\mathbf{D}_2$, $\mathbf{D}_{2d}$ and $\mathbf{D}_{2h}$ Skeletons[a)]

Molecule	FPV	MV	SCR notation
32	(26 0 0 2 0)	(6 0 0 1 0)	$\mathbf{D}_2[6/\mathbf{C}_1(2C_4, 4H_4); /\mathbf{C}_2'(C_2)]$
33	(7 3 1 5 1 3 1 1)	(0 0 0 1 0 1 0 1)	$\mathbf{D}_{2d}[/\mathbf{C}_s(H_4); /\mathbf{C}_{2v}(C_2); /\mathbf{D}_{2d}(C)]$
34	(13 1 1 3 1 1 1 1)	(1 0 0 1 0 0 0 1)	$\mathbf{D}_{2d}[/\mathbf{C}_1(H_8); /\mathbf{C}_s(C_4); /\mathbf{D}_{2d}(C)]$
35	(30 2 0 8 0 2 0 0)	(2 0 0 3 0 1 0 0)	$\mathbf{D}_{2d}[2/\mathbf{C}_1(C_8, H_8); 3/\mathbf{C}_s(C_4, 2H_4); /\mathbf{C}_{2v}(C_2)]$
36	(30 2 0 0 10 6 0 0 2 0 0 0 0 0 0 0)	(2 0 0 0 2 1 0 0 1 0 0 0 0 0 0 0)	$\mathbf{D}_{2h}[2/\mathbf{C}_1(C_8, H_8); 2/\mathbf{C}_2(C_4, H_4); /\mathbf{C}_s'(H_4); /\mathbf{C}_{2v}(C_2)]$

a) For $\mathbf{D}_2$, SSG=$\{\mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_2', \mathbf{C}_2'', \mathbf{D}_2\}$. For $\mathbf{D}_{2d}$, SSG=$\{\mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_2', \mathbf{C}_s, \mathbf{S}_4, \mathbf{C}_{2v}, \mathbf{D}_2, \mathbf{D}_{2d}\}$. For $\mathbf{D}_{2h}$, SSG=$\{\mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_2', \mathbf{C}_2'', \mathbf{C}_s, \mathbf{C}_s', \mathbf{C}_s'', \mathbf{C}_i, \mathbf{C}_{2v}, \mathbf{C}_{2v}', \mathbf{C}_{2v}'', \mathbf{C}_{2h}, \mathbf{C}_{2h}', \mathbf{C}_{2h}'', \mathbf{D}_2, \mathbf{D}_{2h}\}$. See the footnote of Table 8.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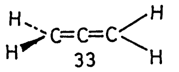

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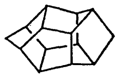
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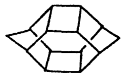

36

inverse of the mark table (Table 3). It should be emphasized that the SCR notations are capable of discriminating these $\mathbf{C}_{2v}$ molecules.

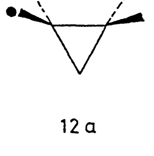
Compound **21** of $\mathbf{D}_{3h}$ symmetry (Table 9) is a derivative of the skeleton **8**. The mode of X_3Y_2 substitution is specified by the notation $\mathbf{D}_{3h}[/\mathbf{C}_{2v}(X_3), /\mathbf{C}_{3v}(Y_2), /\mathbf{D}_{3h}(P)]$. This symbol indicates that X_3 are subject to $\mathbf{D}_{3h}(/\mathbf{C}_{2v})$, Y_2 to $\mathbf{D}_{3h}(/\mathbf{C}_{3v})$, and P to $\mathbf{D}_{3h}(/\mathbf{D}_{3h})$.

Table 9 collects several molecules that are based on various skeletons having $\mathbf{D}_{3h}$ symmetry. Cyclopropane (**22**) and alternative $\mathbf{D}_{3h}$ planar forms **23** and **24** differ in their SCR notations. Prismane (**25**), triptycene (**26**) and other molecules **27** and **28** have the same $\mathbf{D}_{3h}$ symmetry, but can be characterized by the SCR notations.

Table 10 collects several molecules of $\mathbf{T}_d$ symmetry (methane (**29**), tetrahedrane (**30**), and adamantane (**31**)) and their SCR notations. Table 11 lists the SCR notations of $\mathbf{D}_2$ (for twistane (**32**)), $\mathbf{D}_{2d}$ (for allene (**33**), spiro[2.2]pentane (**34**), and isogarudane (**35**)) and $\mathbf{D}_{2h}$ molecules (garudane (**36**)).

IV. Subduction of a Coset Representation

As a foundation to a discussion of the notations for Case II, we introduce a subduction of the coset representation. The subsititution of a parent skeleton with a given set of atoms (or ligands) reduces the original symmetry of the skeleton into a subsymmetry. For example, the orbit (**12**) of the skeleton (**10**) is divided into two suborbits (**12a** and **12b**) in the process of a reduction of $\mathbf{C}_{2v}$ into $\mathbf{C}_2$ symmetry. One of the suborbits is then occupied by H_2 and the other by F_2 to give a $\mathbf{C}_2$ molecule (**11**). This intuitive explanation can be formulated by introducing a subduction of coset representations (CRs).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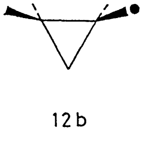

12 b

We extract all permutations of a subgroup $\mathbf{G}_j$ ($\leqslant\mathbf{G}$) from the permutations contained in $\mathbf{G}(/\mathbf{G}_i)$. The resulting set of permutations is denoted as $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$, which is called a *subduced representation* (SR). Let us select an irredundant set of conjugate subgroups of $\mathbf{G}_j$,

$$\mathrm{SSG}=\{\mathbf{H}_1, \mathbf{H}_2, \cdots, \mathbf{H}_v\}, \tag{14}$$

and the corresponding set of CRs as follows,

$$\mathrm{SCR}=\{\mathbf{G}_j(/\mathbf{H}_1), \mathbf{G}_j(/\mathbf{H}_2), \cdots, \mathbf{G}_j(/\mathbf{H}_v)\}, \tag{15}$$

in a similar way as above. Note that $\mathbf{H}_k$ is subject to $\mathbf{G}_j$ though, for simplicity of the following discussions, this fact is not denoted explicitly. The subduced representation $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$ is a permutation group on the orbit ($\Delta_{i\alpha}$) represented by Eq. 10. Hence, Theorem 1 is applicable to this case. We thus arrive at

Corollary 1-1. The subduced representation $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$ can be reduced into transitive CRs in terms of

$$\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j=\sum_{k=1}^{v}\beta_k^{(ij)}\mathbf{G}_j(/\mathbf{H}_k) \tag{16}$$

$$\text{for } i=1, 2, \cdots, s \quad \text{and for } j=1, 2, \cdots, s,$$

where each $\beta_k^{(ij)}$ is a non-negative integer. The multiplicities $\beta_k^{(ij)}$ ($k=1, 2, \cdots, v$) are obtained by

$$\nu_i=\sum_{k=1}^{v}\beta_k^{(ij)}m_i^{(k)} \tag{17}$$

$$\text{for } i=1, 2, \cdots, v,$$

where ν_i is the mark of $\mathbf{H}_i$ in $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$.

We now define a subduction vector (SV) as

$$\mathrm{SV}=(\beta_1^{(ij)}, \beta_2^{(ij)}, \cdots, \beta_v^{(ij)}). \tag{18}$$

A coset representation $\mathbf{G}(/\mathbf{G}_i)$ is determined only by $\mathbf{G}$ and $\mathbf{G}_i$ and, hence, is independent of any $\mathbf{G}$-set. As a result, the SV is constant if $\mathbf{G}_i$ and $\mathbf{G}_j$ are given. Compare this with the fact that MV is dependent upon the $\mathbf{G}$-set to be considered. These facts permit us to preestimate the subduction of $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$.[6,9)] Table 12 collects such subductions for $\mathbf{D}_{3h}$ group.

In terms of the Corollary 1-1, the orbit $\Delta_{i\alpha}$ on which

Table 12. Subduction of the Coset Representations of $\mathbf{D}_{3h}$

i	j									
	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{C}_s'$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{C}_{2v}$	$\downarrow\mathbf{C}_{3v}$	$\downarrow\mathbf{C}_{3h}$	$\downarrow\mathbf{D}_3$	$\downarrow\mathbf{D}_{3h}$
$\mathbf{D}_{3h}(/\mathbf{C}_1)$	$12\mathbf{C}_1(/\mathbf{C}_1)$	$6\mathbf{C}_2(/\mathbf{C}_1)$	$6\mathbf{C}_s(/\mathbf{C}_1)$	$6\mathbf{C}_s'(/\mathbf{C}_1)$	$4\mathbf{C}_3(/\mathbf{C}_1)$	$3\mathbf{C}_{2v}(/\mathbf{C}_1)$	$2\mathbf{C}_{3v}(/\mathbf{C}_1)$	$2\mathbf{C}_{3h}(/\mathbf{C}_1)$	$2\mathbf{D}_3(/\mathbf{C}_1)$	$\mathbf{D}_{3h}(/\mathbf{C}_1)$
$\mathbf{D}_{3h}(/\mathbf{C}_2)$	$6\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_1)$ $+2\mathbf{C}_2(/\mathbf{C}_2)$	$3\mathbf{C}_s(/\mathbf{C}_1)$	$3\mathbf{C}_s'(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{C}_{2v}(/\mathbf{C}_1)$ $+\mathbf{C}_{2v}(/\mathbf{C}_2)$	$\mathbf{C}_{3v}(/\mathbf{C}_1)$	$\mathbf{C}_{3h}(/\mathbf{C}_1)$	$2\mathbf{D}_3(/\mathbf{C}_2)$	$\mathbf{D}_{3h}(/\mathbf{C}_2)$
$\mathbf{D}_{3h}(/\mathbf{C}_s)$	$6\mathbf{C}_1(/\mathbf{C}_1)$	$3\mathbf{C}_2(/\mathbf{C}_1)$	$2\mathbf{C}_s(/\mathbf{C}_1)$ $+2\mathbf{C}_s(/\mathbf{C}_s)$	$3\mathbf{C}_s'(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{C}_{2v}(/\mathbf{C}_1)$ $+\mathbf{C}_{2v}(/\mathbf{C}_s)$	$2\mathbf{C}_{3v}(/\mathbf{C}_s)$	$\mathbf{C}_{3h}(/\mathbf{C}_1)$	$\mathbf{D}_3(/\mathbf{C}_1)$	$\mathbf{D}_{3h}(/\mathbf{C}_s)$
$\mathbf{D}_{3h}(/\mathbf{C}_s')$	$6\mathbf{C}_1(/\mathbf{C}_1)$	$3\mathbf{C}_2(/\mathbf{C}_1)$	$3\mathbf{C}_s(/\mathbf{C}_1)$	$6\mathbf{C}_s'(/\mathbf{C}_s')$	$2\mathbf{C}_3(/\mathbf{C}_1)$	$3\mathbf{C}_{2v}(/\mathbf{C}_s')$	$\mathbf{C}_{3v}(/\mathbf{C}_1)$	$2\mathbf{C}_{3h}(/\mathbf{C}_s')$	$\mathbf{D}_3(/\mathbf{C}_1)$	$\mathbf{D}_{3h}(/\mathbf{C}_s')$
$\mathbf{D}_{3h}(/\mathbf{C}_3)$	$4\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_1)$	$2\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{C}_s'(/\mathbf{C}_1)$	$4\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{C}_{2v}(/\mathbf{C}_1)$	$2\mathbf{C}_{3v}(/\mathbf{C}_3)$	$2\mathbf{C}_{3h}(/\mathbf{C}_3)$	$2\mathbf{D}_3(/\mathbf{C}_3)$	$\mathbf{D}_{3h}(/\mathbf{C}_3)$
$\mathbf{D}_{3h}(/\mathbf{C}_{2v})$	$3\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_2(/\mathbf{C}_1)$ $+\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}_s(/\mathbf{C}_1)$ $+\mathbf{C}_s(/\mathbf{C}_s)$	$3\mathbf{C}_s'(/\mathbf{C}_s')$	$\mathbf{C}_3(/\mathbf{C}_1)$	$\mathbf{C}_{2v}(/\mathbf{C}_s')$ $+\mathbf{C}_{2v}(/\mathbf{C}_{2v})$	$\mathbf{C}_{3v}(/\mathbf{C}_s)$	$\mathbf{C}_{3h}(/\mathbf{C}_s')$	$\mathbf{D}_3(/\mathbf{C}_2)$	$\mathbf{D}_{3h}(/\mathbf{C}_{2v})$
$\mathbf{D}_{3h}(/\mathbf{C}_{3v})$	$2\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_2(/\mathbf{C}_1)$	$2\mathbf{C}_s(/\mathbf{C}_s)$	$\mathbf{C}_s'(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{C}_{2v}(/\mathbf{C}_s)$	$2\mathbf{C}_{3v}(/\mathbf{C}_{3v})$	$\mathbf{C}_{3h}(/\mathbf{C}_3)$	$\mathbf{D}_3(/\mathbf{C}_3)$	$\mathbf{D}_{3h}(/\mathbf{C}_{3v})$
$\mathbf{D}_{3h}(/\mathbf{C}_{3h})$	$2\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_2(/\mathbf{C}_1)$	$\mathbf{C}_s(/\mathbf{C}_1)$	$2\mathbf{C}_s'(/\mathbf{C}_s')$	$2\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{C}_{2v}(/\mathbf{C}_s')$	$\mathbf{C}_{3v}(/\mathbf{C}_3)$	$2\mathbf{C}_{3h}(/\mathbf{C}_{3h})$	$\mathbf{D}_3(/\mathbf{C}_3)$	$\mathbf{D}_{3h}(/\mathbf{C}_{3h})$
$\mathbf{D}_{3h}(/\mathbf{D}_3)$	$2\mathbf{C}_1(/\mathbf{C}_1)$	$2\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}_s(/\mathbf{C}_1)$	$\mathbf{C}_s'(/\mathbf{C}_1)$	$2\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{C}_{2v}(/\mathbf{C}_2)$	$\mathbf{C}_{3v}(/\mathbf{C}_3)$	$\mathbf{C}_{3h}(/\mathbf{C}_3)$	$2\mathbf{D}_3(/\mathbf{D}_3)$	$\mathbf{D}_{3h}(/\mathbf{D}_3)$
$\mathbf{D}_{3h}(/\mathbf{D}_{3h})$	$\mathbf{C}_1(/\mathbf{C}_1)$	$\mathbf{C}_2(/\mathbf{C}_2)$	$\mathbf{C}_s(/\mathbf{C}_s)$	$\mathbf{C}_s'(/\mathbf{C}_s')$	$\mathbf{C}_3(/\mathbf{C}_3)$	$\mathbf{C}_{2v}(/\mathbf{C}_{2v})$	$\mathbf{C}_{3v}(/\mathbf{C}_{3v})$	$\mathbf{C}_{3h}(/\mathbf{C}_{3h})$	$\mathbf{D}_3(/\mathbf{D}_3)$	$\mathbf{D}_{3h}(/\mathbf{D}_{3h})$

$\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$ acts is subdivided into the corresponding suborbits,

$$\Delta^{(i\alpha)}_{k\beta}\ (k=1,2,\cdots,v;\ \beta=1,2,\cdots,\beta^{(ij)}_{k}), \tag{19}$$

on which $\mathbf{G}_j(/\mathbf{H}_k)$ acts. Figure 1 illustrates the process of the present work, i.e. a division by Eq. 5 and the subsequent subdivision by Eq. 16.

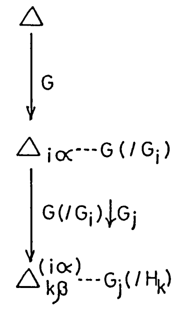


Fig. 1. Division and subdivision of the positions of a skeleton.

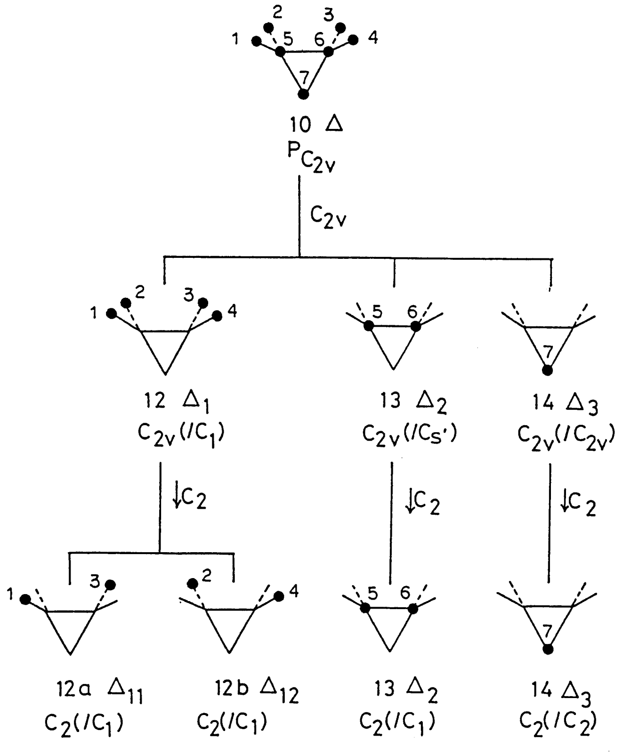


Fig. 2. Orbits and suborbits of the oxirane skeleton (**10**). Each set of positions with a heavy dot constitutes an orbit (or suborbit) that is subject to the coset representation cited.

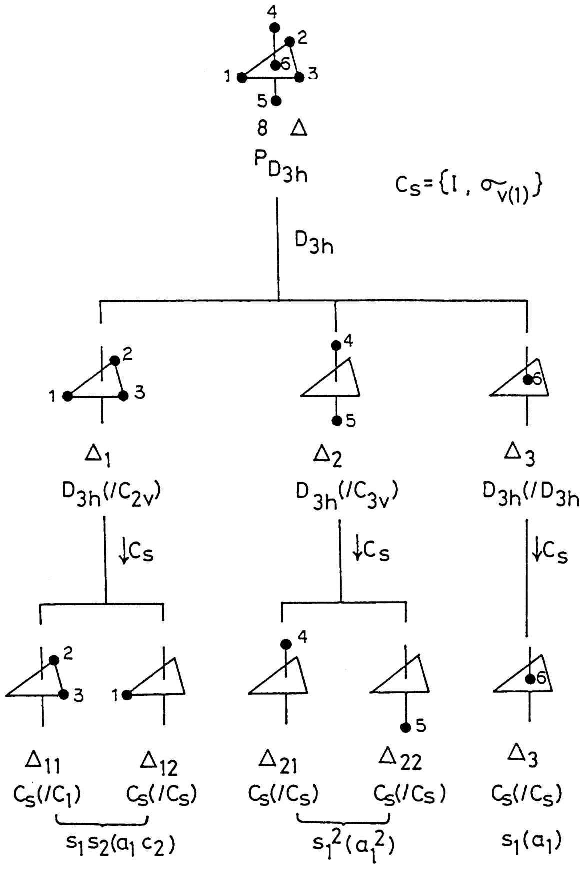


Fig. 3. Orbits and suborbits of the trigonal-bipyramid-plus-center skeleton (**8**) during the subduction into the $\mathbf{C}_s$ group. Each set of positions with a heavy dot constitutes an orbit (or suborbit) that is subject to the coset representation cited.

The following examples clarify the chemical meaning of the subduction of CRs represented by Eq. 16.

Example 2. We examine the subduction of the skeleton (**10**). Figure 2 illustrates the division and the subdivision of the seven positions of **10**. Since the positions are divided by Eq. 12 (Example 1), we examine each of the CRs contained in the right-hand side. The first CR, $\mathbf{C}_{2v}(/\mathbf{C}_1)$, has been shown to be reduced in terms of

$$\mathbf{C}_{2v}(/\mathbf{C}_1)\downarrow\mathbf{C}_2=2\mathbf{C}_2(/\mathbf{C}_1). \tag{20}$$

This equation indicates that $\Delta_1=\{1, 2, 3, 4\}$ (illustrated as **12**) is subdivided into $\Delta_{11}=\{1, 3\}$ and $\Delta_{12}=\{2\ 4\}$, both of which are subject to $\mathbf{C}_2(/\mathbf{C}_1)$. These suborbits corresponds to **12a** and **12b**. The 2nd and 3rd CRs of Eq. 12 are subduced by

$$\mathbf{C}_{2v}(/\mathbf{C}_2)\downarrow\mathbf{C}_2=\mathbf{C}_2(/\mathbf{C}_1) \tag{21}$$

and

$$\mathbf{C}_{2v}(/\mathbf{C}_{2v})\downarrow\mathbf{C}_2=\mathbf{C}_2(/\mathbf{C}_2). \tag{22}$$

These equations indicate that orbits $\Delta_2=\{5, 6\}$ (illustrated as **13**) and $\Delta_3=\{7\}$ (illustrated as **14**) are not subdivided.

Example 3. Let us examine the subduction of the skeleton (**8**). Figure 3 illustrates a classification of the positions of **8**. The six positions have been classified into three orbits. The orbits $\Delta_1=\{1, 2, 3\}$, $\Delta_2=\{4, 5\}$, and $\Delta_3=\{6\}$ are subject to $\mathbf{D}_{2h}(/\mathbf{C}_{2v})$, $\mathbf{D}_{3h}(/\mathbf{C}_{3v})$, and $\mathbf{D}_{3h}(/\mathbf{D}_{3h})$. We first examine subductions into $\mathbf{C}_s=\{I, \sigma_{v(1)}\}$, where $\sigma_{v(1)}$ is a reflection with respect to a mirror plane intersecting node 1. The subductions of the CRs are found in Table 12. Thus,

$$\mathbf{D}_{3h}(/\mathbf{C}_{2v})\downarrow\mathbf{C}_s=\mathbf{C}_s(\mathbf{C}_1)+\mathbf{C}_s(/\mathbf{C}_s), \tag{23}$$

$$\mathbf{D}_{3h}(/\mathbf{C}_{3v})\downarrow\mathbf{C}_s=2\mathbf{C}_s(/\mathbf{C}_s), \tag{24}$$

and

$$\mathbf{C}_{3h}(/\mathbf{C}_{3h})\downarrow\mathbf{C}_s=\mathbf{C}_s(/\mathbf{C}_s). \tag{25}$$

The actions of the CRs appearing in the right-hand sides are illustrated in Fig. 3.

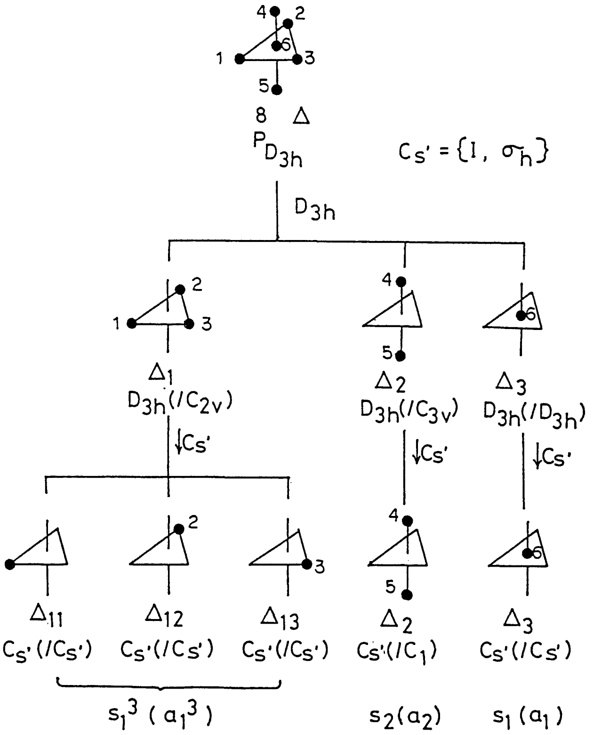


Fig. 4. Orbits and suborbits of the trigonal-bipyramid-plus-center skeleton (**8**) during the subduction into the $\mathbf{C}_s'$ group. Each set of positions with a heavy dot constitutes an orbit (or suborbit) that is subject to the coset representation cited.

Figure 4 depicts another manipulation of the skeleton (**8**). Each of the CRs is subduced into $\mathbf{C}_s'=\{I, \sigma_h\}$, where σ_h is a mirror plane containing positions 1, 2, and 3. Table 12 indicates

$$\mathbf{D}_{3h}(\mathbf{C}_{2v})\downarrow\mathbf{C}_s'=3\mathbf{C}_s'(/\mathbf{C}_s), \tag{26}$$

$$\mathbf{D}_{3h}(/\mathbf{C}_{3v})\downarrow\mathbf{C}_s'=\mathbf{C}_s'(/\mathbf{C}_1), \tag{27}$$

and

$$\mathbf{C}_{3h}(/\mathbf{C}_{3h})\downarrow\mathbf{C}_s'=\mathbf{C}_s'(/\mathbf{C}_s). \tag{28}$$

V. The SCR Notation for Case II

We now arrive at notations for Case II. Our idea is that, in order to realize a $\mathbf{G}_j$-subsymmetry, each of the suborbits (Eq. 19) is filled up with the same kind of atoms $A^{(ijk)}$. Note that the suborbit is subject to the corresponding coset representation (CR) in terms of Eq. 16. Since the length of the suborbit is $r=|\mathbf{G}_j|/|\mathbf{G}_k|$, the mode of filling-up is represented by

$$\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j[\cdots, /\mathbf{H}_k(A_r^{(ijk)}), \cdots], \tag{29}$$

which are hyphened in ascending order of $i=1, 2, \cdots, s$. This SCR notation indicates that r of atoms $A^{(ijk)}$ fill up the suborbit on which $\mathbf{G}_j(/\mathbf{H}_k)$ acts. Thereby, the SCR notation affords a full piece of information about the $\mathbf{G}_j$-molecule.

The symmetry of compound **11** is represented by

$$\mathbf{C}_{2v}(/\mathbf{C}_1)\downarrow\mathbf{C}_2[2/\mathbf{C}_1(\mathrm{H}_2, \mathrm{F}_2)]-\mathbf{C}_{2v}(/\mathbf{C}_2)\downarrow\mathbf{C}_2[/\mathbf{C}_1(\mathrm{C}_2)]-\mathbf{C}_{2v}(/\mathbf{C}_{2v})\downarrow\mathbf{C}_2[/\mathbf{C}_2(\mathrm{O})]. \tag{30}$$

This notation is based on the subdivision shown in Fig. 2, which is also represented by Eqs. 20—22 (Example 2). Thus, the first part indicates the respective packing of orbits **12a** and **12b** with H_2 and F_2. The 2nd part of Eq. 30 shows that C_2 occupy the orbit (**13**). The 3rd one shows the substitution of the orbit (**14**) with one oxygen.

The SCR notation for **11** (Eq. 30) can be abbreviated to

$$\mathbf{C}_2[2/\mathbf{C}_1(\mathrm{H}_2, \mathrm{F}_2); /\mathbf{C}_1(\mathrm{C}_2); /\mathbf{C}_2(\mathrm{O})] \tag{31}$$

by collecting the terms in the brackets and punctuating with semicolons. Although this short notation loses the information on the parent skeleton (**10**), it is still informative enough to indicate the symmetry of molecule **11**.

A notation for compound **3** is obtained by using the subdivisions shown by Eqs. 26—28 (Example 3), i.e.,

$$\mathbf{D}_{3h}(/\mathbf{C}_{2v})\downarrow\mathbf{C}_s'[3/\mathbf{C}_s(\mathrm{X,\ Y,\ Z})]-\mathbf{D}_{3h}(/\mathbf{C}_{3v})\downarrow\mathbf{C}_s'[/\mathbf{C}_1(\mathrm{X}_2)]-\mathbf{D}_{3h}(/\mathbf{D}_{3h})\downarrow\mathbf{C}_s'[/\mathbf{C}_s(\mathrm{P})]. \quad (32)$$

This SCR notation indicates the mode of filling-up of the suborbits illustrated in Fig. 4. Thus, the first brackets of Eq. 32 indicate that atoms X, Y, and Z occupy the suborbits, Δ_{11}, Δ_{12}, and Δ_{13}, respectively, where all of the suborbits are subject to $\mathbf{C}_s'(/\mathbf{C}_s')$. The second brackets correspond to the fact that Δ_2 of Fig. 4 is operated by $\mathbf{C}_s'(/\mathbf{C}_1)$ and filled with X_2. The third one specifies the substitution of phosphorus.

Notations for compounds **4** and **5** can be obtained by using Eqs. 23—25. That is,

$$\mathbf{D}_{3h}(/\mathbf{C}_{2v})\downarrow\mathbf{C}_s[/\mathbf{C}_1(\mathrm{X}_2),\ /\mathbf{C}_s(\mathrm{Z})]-\mathbf{D}_{3h}(/\mathbf{C}_{3v})\downarrow\mathbf{C}_s[2/\mathbf{C}_s(\mathrm{X,Y})]-\mathbf{D}_{3h}(/\mathbf{D}_{3h})\downarrow\mathbf{C}_s[/\mathbf{C}_s(\mathrm{P})]\ \text{for } \mathbf{4} \quad (33)$$

and

$$\mathbf{D}_{3h}(/\mathbf{C}_{2v})\downarrow\mathbf{C}_s[/\mathbf{C}_1(\mathrm{X}_2),/\mathbf{C}_s(\mathrm{Y})]-\mathbf{D}_{3h}(/\mathbf{C}_{3v})\downarrow\mathbf{C}_s[2/\mathbf{C}_s(\mathrm{X,Z})]-\mathbf{D}_{3h}(/\mathbf{D}_{3h})\downarrow\mathbf{C}_s[/\mathbf{C}_s(\mathrm{P})]\ \text{for } \mathbf{5}. \quad (34)$$

Figure 3 depicts the construction of these SCR notations. Note that a set of equivalent atoms occupies a suborbit. These notations (Eqs. 32—34) faithfully reflect the fact that molecule **4** can be converted into **5** by exchanging Y and Z.

The SCR notations (Eqs. 32—34) are converted to abbreviated forms by selecting the subgroups in question and by collecting the terms in the brackets:

$$\mathbf{C}_s'[3/\mathbf{C}_s(\mathrm{X,\ Y,\ Z,});\ /\mathbf{C}_1(\mathrm{X}_2);\ /\mathbf{C}_s(\mathrm{P})]\ \text{for } \mathbf{3}, \quad (35)$$

$$\mathbf{C}_s[/\mathbf{C}_1(\mathrm{X}_2),\ /\mathbf{C}_s(\mathrm{Z});\ 2/\mathbf{C}_s(\mathrm{X,Y});\ /\mathbf{C}_s(\mathrm{P})]\ \text{for } \mathbf{4}, \quad (36)$$

and

$$\mathbf{C}_s[/\mathbf{C}_s(\mathrm{X}_2),\ /\mathbf{C}_s(\mathrm{Y});\ 2/\mathbf{C}_s(\mathrm{X,\ Z});\ /\mathbf{C}_s(\mathrm{P})]\ \text{for } \mathbf{5}. \quad (37)$$

These abbreviated notations are still capable of distinguishing the three molecules (**3**, **4**, and **5**). This fact reveals an advantage of the present notation over the framework group as well as over the modified Schönflies notation.

It should be noted that the notations for Case I molecules are special cases of those for Case II. For example, the notation of compound **9** (Table 8) is represented by

$$\mathbf{C}_{2v}(/\mathbf{C}_1)\downarrow\mathbf{C}_{2v}[/\mathbf{C}_1(\mathrm{H}_4)]-\mathbf{C}_{2v}(/\mathbf{C}_s')\downarrow\mathbf{C}_{2v}[/\mathbf{C}_s'(\mathrm{C}_2)]-\mathbf{C}_{2v}(/\mathbf{C}_{2v})\downarrow\mathbf{C}_{2v}[/\mathbf{C}_{2v}(\mathrm{O})] \quad (38)$$

in a full manner described in this section. This notation can be abbreviated to

$$\mathbf{C}_{2v}[/\mathbf{C}_1(\mathrm{H}_4);\ /\mathbf{C}_s'(\mathrm{C}_2);\ /\mathbf{C}_{2v}(\mathrm{O})] \quad (39)$$

by collecting the terms in the brackets of Eq. 38. The abbreviated form (Eq. 39) is identical to that listed in Table 8.

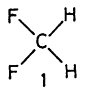
Table 13 lists several molecules having $\mathbf{C}_{2v}$ symmetry that are derived from skeletons of higher symmetry.

An abbreviated SCR notation (or its slightly simplified counterpart in some cases) can be directly obtained without considering a parent skeleton. Let us examine compound **2**, which is here considered to directly take $\mathbf{C}_{2v}$ symmetry and not to be a derivative of a $\mathbf{T}_d$ skeleton. This process corresponds to a consideration of a $\mathbf{C}_{2v}$-set $\{1, 2, \cdots, 5\}$ and a permutation group ($\mathbf{P}_{\mathbf{C}_{2v}}$): (1)(2)(3)(4)(5) for I (an identity operation), (1 2)(3 4)(5) for C_2, (1)(2)(3 4)(5) for $\sigma_{v(1)}$, and (1 2)(3)(4)(5) for $\sigma_{v(2)}$. This case affords FPV =(5 1 3 3 1), which in turn yields MV=(0 0 1 1 1) by multiplying the inverse of the mark table (Table 3). This MV indicates the following reduction:

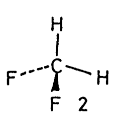
$$\mathbf{P}_{\mathbf{C}_{2v}}=\mathbf{C}_{2v}(/\mathbf{C}_s)+\mathbf{C}_{2v}(/\mathbf{C}_s')+\mathbf{C}_{2v}(/\mathbf{C}_{2v}). \quad (40)$$

Table 13. $\mathbf{C}_{2v}$ Subsymmetries Based on Skeletons of Higher Symmetry

Molecule	SCR notation	Abbreviated SCR notation
1	$\mathbf{D}_{4h}(/\mathbf{C}_{2v}'')\downarrow\mathbf{C}_{2v}'''[2/\mathbf{C}_s(\mathrm{H}_2,\ \mathrm{F}_2)]$- $\mathbf{D}_{4h}(/\mathbf{D}_{4h})\downarrow\mathbf{C}_{2v}'''[/\mathbf{C}_{2v}(\mathrm{C})]$	$\mathbf{C}_{2v}'''[2/\mathbf{C}_s(\mathrm{H}_2,\ \mathrm{F}_2);\ /\mathbf{C}_{2v}(\mathrm{C})]$
2	$\mathbf{T}_d(/\mathbf{C}_{3v})\downarrow\mathbf{C}_{2v}[\mathbf{C}_s(\mathrm{H}_2),\ /\mathbf{C}_s'(\mathrm{F}_2)]$- $\mathbf{T}_d(/\mathbf{T}_d)\downarrow\mathbf{C}_{2v}[/\mathbf{C}_{2v}(\mathrm{C})]$	$\mathbf{C}_{2v}[/\mathbf{C}_s(\mathrm{H}_2),\ /\mathbf{C}_s'(\mathrm{F}_2);\ /\mathbf{C}_{2v}(\mathrm{C})]$
37	$\mathbf{T}_d(/\mathbf{C}_s)\downarrow\mathbf{C}_{2v}[2/\mathbf{C}_1(2\mathrm{H}_4),\ /\mathbf{C}_s(\mathrm{A}_2),\ /\mathbf{C}_s'(\mathrm{A}_2)]$- $\mathbf{T}_d(/\mathbf{C}_{2v})\downarrow\mathbf{C}_{2v}[/\mathbf{C}_1(\mathrm{C}_4),\ 2/\mathbf{C}_{2v}(2/\mathrm{C})]$- $\mathbf{T}_d(/\mathbf{C}_{3v})\downarrow\mathbf{C}_{2v}[/\mathbf{C}_s(\mathrm{C}_2),\ /\mathbf{C}_s'(\mathrm{C}_2)]$- $\mathbf{T}_d(/\mathbf{C}_{3v})\downarrow\mathbf{C}_{2v}[/\mathbf{C}_s(\mathrm{H}_2),\ /\mathbf{C}_s'(\mathrm{B}_2)]$	$\mathbf{C}_{2v}[2/\mathbf{C}_1(2\mathrm{H}_4),\ /\mathbf{C}_s(\mathrm{A}_2),\ /\mathbf{C}_s'(\mathrm{A}_2);$ $/\mathbf{C}_1(\mathrm{C}_4),\ 2/\mathbf{C}_{2v}(2\mathrm{C});\ /\mathbf{C}_s(\mathrm{C}_2),\ /\mathbf{C}_s'(\mathrm{C}_2);$ $/\mathbf{C}_s(\mathrm{H}_2),\ /\mathbf{C}_s'(\mathrm{B}_2)]$
38	$\mathbf{D}_{3h}(/\mathbf{C}_{2v})\downarrow\mathbf{C}_{2v}[/\mathbf{C}_s'(\mathrm{X}_2),\ /\mathbf{C}_{2v}(\mathrm{Z}),]$- $\mathbf{D}_{3h}(/\mathbf{C}_{3v})\downarrow\mathbf{C}_{2v}[/\mathbf{C}_s(\mathrm{Y}_2)]$- $\mathbf{D}_{3h}(/\mathbf{D}_{3h})\downarrow\mathbf{C}_{2v}[/\mathbf{C}_{2v}(\mathrm{P})]$	$\mathbf{C}_{2v}[/\mathbf{C}_s'(\mathrm{X}_2),\ /\mathbf{C}_{2v}(\mathrm{Z});\ /\mathbf{C}_s(\mathrm{Y}_2);\ /\mathbf{C}_{2v}(\mathrm{P})]$
39	$\mathbf{D}_{3h}(/\mathbf{C}_s)\downarrow\mathbf{C}_{2v}[/\mathbf{C}_1(\mathrm{H}_4),\ /\mathbf{C}_s(\mathrm{F}_2)]$- $\mathbf{D}_{3h}(/\mathbf{C}_{2v})\downarrow\mathbf{C}_{2v}[/\mathbf{C}_s'(\mathrm{C}_2),\ /\mathbf{C}_{2v}(\mathrm{C})]$	$\mathbf{C}_{2v}[/\mathbf{C}_1(\mathrm{H}_4),\ /\mathbf{C}_s(\mathrm{F}_2);\ /\mathbf{C}_s'(\mathrm{C}_2),\ /\mathbf{C}_{2v}(\mathrm{C})]$
40	$\mathbf{D}_{2d}(/\mathbf{C}_s)\downarrow\mathbf{C}_{2v}[/\mathbf{C}_s(\mathrm{H}_2),\ /\mathbf{C}_s'(\mathrm{F}_2)]$- $\mathbf{D}_{2d}(/\mathbf{C}_{2v})\downarrow\mathbf{C}_{2v}[2/\mathbf{C}_{2v}(2\mathrm{C})]$- $\mathbf{D}_{2d}(/\mathbf{D}_{2d})\downarrow\mathbf{C}_{2v}[/\mathbf{C}_{2v}(\mathrm{C})]$	$\mathbf{C}_{2v}[/\mathbf{C}_s(\mathrm{H}_2),\ /\mathbf{C}_s'(\mathrm{F}_2);\ 2/\mathbf{C}_{2v}(2\mathrm{C});\ /\mathbf{C}_{2v}(\mathrm{C})]$



1



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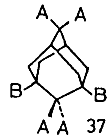

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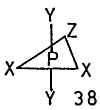
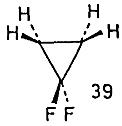


38



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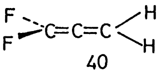


40

Hence, we obtain

$$\mathbf{C}_{2v}[/\mathbf{C}_s(\mathrm{H}_2),\ /\mathbf{C}_s'(\mathrm{F}_2),\ /\mathbf{C}_{2v}(\mathrm{C})] \qquad (41)$$

as a notation for compound **2**. This notation has a context equivalent to that shown in Table 13.

It is worthwhile comparing the present SCR notation with the previous systems. The abbreviated SCR notations are closely related to framework-group notations in some cases. Compare the following notations:

$\mathbf{C}_{2v}'''[2/\mathbf{C}_s(\mathrm{H}_2,\mathrm{F}_2);\ /\mathbf{C}_{2v}(\mathrm{C})]$ vs. $\mathbf{C}_{2v}[\mathrm{C}_2(\mathrm{C}),\ \sigma_v\ (\mathrm{F}_2,\ \mathrm{H}_2)]$ for **1**,

$\mathbf{C}_{2v}[/\mathbf{C}_s(\mathrm{H}_2),\ /\mathbf{C}_s'(\mathrm{F}_2);\ /\mathbf{C}_{2v}(\mathrm{C})]$ vs.
$\mathbf{C}_{2v}[\mathrm{C}_2(\mathrm{C}),\ \sigma_v(\mathrm{F}_2),\ \sigma_v'(\mathrm{H}_2)]$ for **2**,

and

$\mathbf{C}_{2v}[/\mathbf{C}_1(\mathrm{H}_4);\ /\mathbf{C}_s'(\mathrm{C}_2);\ /\mathbf{C}_{2v}(\mathrm{O})]$ vs.
$\mathbf{C}_{2v}[\mathrm{C}_2(\mathrm{O}),\ \sigma_v(\mathrm{C}_2),\ \mathrm{X}(\mathrm{H}_4)]$ for **9**.

Here, the former of each pair is an abbreviated SCR notation (Tables 8 and 13) and the latter is based on a framework group. The apparent resemblances can be explained by considering the meaning of an abbreviated SCR notation. Thus, a calculation of the fixed-point vector (FPV) is closely related to the procedure of obtaining subspaces in the framework-group approach. However, the present approach is more discriminative than the framework group in the manipulation of the subspace X, as well as in cases where two or more non-conjugate isomorphic subgroups are present. An example of the latter case has been described for compounds **3**, **4**, and **5**.

Table 14. Unit Subduced Cycle Indices of $\mathbf{C}_{2v}$

i	j				
	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{C}_s'$	$\downarrow\mathbf{C}_{2v}$
$\mathbf{C}_{2v}(/\mathbf{C}_1)$	s_1^4 (b_1^4)	s_2^2 (b_2^2)	s_2^2 (c_2^2)	s_2^2 (c_2^2)	s_4 (c_4)
$\mathbf{C}_{2v}(/\mathbf{C}_2)$	s_1^2 (b_1^2)	s_1^2 (b_1^2)	s_2 (c_2)	s_2 (c_2)	s_2 (c_2)
$\mathbf{C}_{2v}(/\mathbf{C}_s)$	s_1^2 (b_1^2)	s_2 (b_2)	s_1^2 (a_1^2)	s_2 (c_2)	s_2 (a_2)
$\mathbf{C}_{2v}(/\mathbf{C}_s')$	s_1^2 (b_1^2)	s_2 (b_2)	s_2 (c_2)	s_1^2 (a_1^2)	s_2 (a_2)
$\mathbf{C}_{2v}(/\mathbf{C}_{2v})$	s_1 (b_1)	s_1 (b_1)	s_1 (a_1)	s_1 (a_1)	s_1 (a_1)
$\sum_i m_i^{(j)}$	1/4	1/4	1/4	1/4	0

VI. Unit Subduced Cycle Index

In this section we introduce a novel concept called "unit subduce cycle index (USCI)." First, we assign a variable $s_{d_{jk}}$ to each suborbit $\Delta_{\beta k}^{(i\alpha)}$ (Eq. 19), since its length is represented by

$$d_{jk}=|\mathbf{G}_i|/|\mathbf{H}_k|. \qquad (42)$$

We then define a unit subduced cycle index (USCI) as follows.

Definition 1. A unit subduced cycle index (USCI) is defined as

$$Z(\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j;\ s)=\prod_{k=1}^{v}(s_{d_{jk}})^{\beta_k^{(ij)}} \qquad (43)$$

(for $i=1, 2, \cdots, s$ and $j=1, 2, \cdots, s$),

where the power $\beta_k^{(ij)}$ has appeared in Eq. 17. Tables 14—16 collected USCIs for the subduction of $\mathbf{C}_{2v}$, $\mathbf{D}_{3h}$, and $\mathbf{T}_d$ groups.

A USCI describes an allowed mode of substitution

Table 15. Unit Subduced Cycle Indices of $\mathbf{D}_{3h}$

i	j									
	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{C}_s'$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{C}_{2v}$	$\downarrow\mathbf{C}_{3v}$	$\downarrow\mathbf{C}_{3h}$	$\downarrow\mathbf{D}_3$	$\downarrow\mathbf{D}_{3h}$
$\mathbf{D}_{3h}(/\mathbf{C}_1)$	s_1^{12} (b_1^{12})	s_2^6 (b_2^6)	s_2^6 (c_2^6)	s_2^6 (c_2^6)	s_3^4 (b_3^4)	s_4^3 (c_4^3)	s_6^2 (c_6^2)	s_6^2 (c_6^2)	s_6^2 (b_6^2)	s_{12} (c_{12})
$\mathbf{D}_{3h}(/\mathbf{C}_2)$	s_1^6 (b_1^6)	$s_1^2s_2^2$ $(b_1^2b_2^2)$	s_2^3 (c_2^3)	s_2^3 (c_2^3)	s_3^2 (b_3^2)	s_2s_4 (c_2c_4)	s_6 (c_6)	s_6 (c_6)	s_3^2 (b_3^2)	s_6 (c_6)
$\mathbf{D}_{3h}(/\mathbf{C}_3)$	s_1^6 (b_1^6)	s_2^3 (b_2^3)	$s_1^2s_2^2$ $(a_1^2c_2^2)$	s_2^3 (c_2^3)	s_3^2 (b_3^2)	s_2s_4 (a_2c_4)	s_3^2 (a_3^2)	s_6 (c_6)	s_6 (b_6)	s_6 (a_6)
$\mathbf{D}_{3h}(/\mathbf{C}_s')$	s_1^6 (b_1^6)	s_2^3 (b_2^3)	s_2^3 (c_2^3)	s_1^6 (a_1^6)	s_3^2 (b_3^2)	s_2^3 (a_2^3)	s_6 (c_6)	s_3^2 (a_3^2)	s_3^2 (b_3^2)	s_6 (a_6)
$\mathbf{D}_{3h}(/\mathbf{C}_3)$	s_1^4 (b_1^4)	s_2^2 (b_2^2)	s_2^2 (c_2^2)	s_2^2 (c_2^2)	s_1^4 (b_1^4)	s_4 (c_4)	s_2^2 (c_2^2)	s_2^2 (c_2^2)	s_2^2 (b_2^2)	s_4 (c_4)
$\mathbf{D}_{3h}(/\mathbf{C}_{2v})$	s_1^3 (b_1^3)	s_1s_2 (b_1b_2)	s_1s_2 (a_1c_2)	s_1^3 (a_1^3)	s_3 (b_3)	s_1s_2 (a_1a_2)	s_3 (a_3)	s_3 (a_3)	s_3 (b_3)	s_3 (a_3)
$\mathbf{D}_{3h}(/\mathbf{C}_{3v})$	s_1^2 (b_1^2)	s_2 (b_2)	s_1^2 (a_1^2)	s_2 (c_2)	s_1^2 (b_1^2)	s_2 (a_2)	s_1^2 (a_1^2)	s_2 (c_2)	s_2 (b_2)	s_2 (a_2)
$\mathbf{D}_{3h}(/\mathbf{C}_{3h})$	s_1^2 (b_1^2)	s_2 (b_2)	s_2 (c_2)	s_1^2 (a_1^2)	s_1^2 (b_1^2)	s_2 (a_2)	s_2 (c_2)	s_1^2 (a_1^2)	s_2 (b_2)	s_2 (a_2)
$\mathbf{D}_{3h}(/\mathbf{D}_3)$	s_1^2 (b_1^2)	s_1^2 (b_1^2)	s_2 (c_2)	s_2 (c_2)	s_1^2 (b_1^2)	s_2 (c_2)	s_2 (c_2)	s_2 (c_2)	s_1^2 (b_1^2)	s_2 (c_2)
$\mathbf{D}_{3h}(/\mathbf{D}_{3h})$	s_1 (b_1)	s_1 (b_1)	s_1 (a_1)	s_1 (a_1)	s_1 (b_1)	s_1 (a_1)	s_1 (a_1)	s_1 (a_1)	s_1 (b_1)	s_1 (a_1)
$\sum_i \overline{m}_i^{(j)}$	1/12	1/4	1/4	1/12	1/6	0	0	1/6	0	0

Table 16. Unit Subduced Cycle Indices for $\mathbf{T}_d$

i	j										
	$\downarrow\mathbf{C}_1$	$\downarrow\mathbf{C}_2$	$\downarrow\mathbf{C}_s$	$\downarrow\mathbf{C}_3$	$\downarrow\mathbf{S}_4$	$\downarrow\mathbf{D}_2$	$\downarrow\mathbf{C}_{2v}$	$\downarrow\mathbf{C}_{3v}$	$\downarrow\mathbf{D}_{2d}$	$\downarrow\mathbf{T}$	$\downarrow\mathbf{T}_d$
$\mathbf{T}_d(/\mathbf{C}_1)$	s_1^{24} (b_1^{24})	s_2^{12} (b_2^{12})	s_2^{12} (c_2^{12})	s_3^8 (b_3^8)	s_4^6 (c_4^6)	s_4^6 (b_4^6)	s_4^6 (c_4^6)	s_6^4 (c_4^6)	s_8^3 (c_8^3)	s_{12}^2 (b_{12}^2)	s_{24} (c_{24})
$\mathbf{T}_d(/\mathbf{C}_2)$	s_1^{12} (b_1^{12})	$s_1^4s_2^4$ $(b_1^4b_2^4)$	s_2^6 (c_2^6)	s_3^4 (b_3^4)	$s_2^2s_4^2$ $(c_2^2c_4^2)$	s_2^6 (b_2^6)	$s_2^2s_4^2$ $(c_2^2c_4^2)$	s_6^2 (c_6^2)	s_4^3 (c_4^3)	s_6^2 (b_6^2)	s_{12} (c_{12})
$\mathbf{T}_d(/\mathbf{C}_s)$	s_1^{12} (b_1^{12})	s_2^6 (b_2^6)	$s_1^2s_2^5$ $(a_1^2c_2^5)$	s_3^4 (b_3^4)	s_4^3 (c_4^3)	s_4^3 (b_4^3)	$s_2^2s_4^2$ $(a_2^2c_4^2)$	$s_3^2s_6$ $(a_3^2c_6)$	s_4s_8 (a_4c_8)	s_{12} (b_{12})	s_{12} (a_{12})
$\mathbf{T}_d(/\mathbf{C}_3)$	s_1^8 (b_1^8)	s_2^4 (b_2^4)	s_2^4 (c_2^4)	$s_1^2s_3^2$ $(b_1^2b_3^2)$	s_4^2 (c_4^2)	s_4^2 (b_4^2)	s_4^2 (c_4^2)	s_2s_6 (c_2c_6)	s_8 (c_8)	s_4^2 (b_4^2)	s_8 (c_8)
$\mathbf{T}_d(/\mathbf{S}_4)$	s_1^6 (b_1^6)	$s_1^2s_2^2$ $(b_1^2b_2^2)$	s_2^3 (c_2^3)	s_2^3 (b_3^2)	$s_1^2s_4$ $(a_1^2c_4)$	s_2^3 (b_2^3)	s_2s_4 (c_2c_4)	s_6 (c_6)	s_2s_4 (a_2c_4)	s_6 (b_6)	s_6 (a_6)
$\mathbf{T}_d(/\mathbf{D}_2)$	s_1^6 (b_1^6)	s_1^6 (b_1^6)	s_2^3 (c_2^3)	s_3^2 (b_3^2)	s_2^3 (c_2^3)	s_1^6 (b_1^6)	s_2^3 (c_2^3)	s_6 (c_6)	s_2^3 (c_2^3)	s_3^2 (b_3^2)	s_6 (c_6)
$\mathbf{T}_d(/\mathbf{C}_{2v})$	s_1^6 (b_1^6)	$s_1^2s_2^2$ $(b_1^2b_2^2)$	$s_1^2s_2^2$ $(a_1^2c_2^2)$	s_3^2 (b_3^2)	s_2s_4 (c_2c_4)	s_2^3 (b_2^3)	$s_1^2s_4$ $(a_1^2c_4)$	s_3^2 (a_3^2)	s_2s_4 (a_2c_4)	s_6 (b_6)	s_6 (a_6)
$\mathbf{T}_d(/\mathbf{C}_{3v})$	s_1^4 (b_1^4)	s_2^2 (b_2^2)	$s_1^2s_2$ $(a_1^2c_2)$	s_1s_3 (b_1b_3)	s_4 (c_4)	s_4 (b_4)	s_2^2 (a_2^2)	s_1s_3 (a_1a_3)	s_4 (a_4)	s_4 (b_4)	s_4 (a_4)
$\mathbf{T}_d(/\mathbf{D}_{2d})$	s_1^3 (b_1^3)	s_1^3 (b_1^3)	s_1s_2 (a_1c_2)	s_3 (b_3)	s_1s_2 (a_1c_2)	s_1^3 (b_1^3)	s_1s_2 (a_1c_2)	s_3 (a_3)	s_1s_2 (a_1c_2)	s_3 (b_3)	s_3 (a_3)
$\mathbf{T}_d(/\mathbf{T})$	s_1^2 (b_1^2)	s_1^2 (b_1^2)	s_2 (c_2)	s_1^2 (b_1^2)	s_2 (a_2)	s_1^2 (b_1^2)	s_2 (c_2)	s_2 (c_2)	s_2 (c_2)	s_1^2 (b_1^2)	s_2 (c_2)
$\mathbf{T}_d(/\mathbf{T}_d)$	s_1 (b_1)	s_1 (b_1)	s_1 (a_1)	s_1 (b_1)	s_1 (a_1)	s_1 (b_1)	s_1 (a_1)	s_1 (a_1)	s_1 (a_1)	s_1 (b_1)	s_1 (a_1)
$\sum_i \overline{m}_i^{(j)}$	1/24	1/8	1/4	1/3	1/4	0	0	0	0	0	0

with achiral atoms (or ligands) during the subduction of a coset representation (CR). For example, Fig. 3 is an illustration of the fact that $\mathbf{D}_{3h}(/\mathbf{C}_{2v})\downarrow\mathbf{C}_s$ corresponds to the USCI (s_1s_2). This appears at the intersection of the $\mathbf{C}_s$ column and the $\mathbf{D}_{3h}(/\mathbf{C}_{2v})$ row of Table 15. The index (s_1s_2) means that, in order to realize a $\mathbf{C}_s$ symmetry, achiral atoms (or ligands) should occupy the corresponding positions in the manner of A_1B_2, if A and B denote such achiral atoms. This discussion applies in the other $\mathbf{D}_{3h}(/\mathbf{C}_{3v})$ and $\mathbf{D}_{3h}(/\mathbf{D}_{3h})$, as depicted in Fig. 3. As a result, a set of USCIs,

$$s_1s_2;\ s_1^2;\ s_1, \tag{44}$$

is a descriptor for characterizing the $\mathbf{C}_s$-molecule derived from the parent $\mathbf{D}_{3h}$ skeleton (**8**).

Because Eq. 5 indicates that the multiplicity of $\mathbf{G}(/\mathbf{G}_i)$ is α_i, the term

$$\prod_{k=1}^{v}(s_{d_{jk}})^{\alpha_i\beta_k^{(ij)}} \tag{45}$$

which is derived from Eq. 43, concerns $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$ and determines the mode of substitution on the corresponding orbits. Hence, a $\mathbf{G}_j$-molecule derived from a parent $\mathbf{G}$-skeleton is characterized by a set of unit subduced cycle indices (USCIs) defined by

Definition 2. A set of USCIs is defined as

$$\prod_{k=1}^{v}(s_{d_{jk}})^{\alpha_1\beta_k^{(1j)}};\ \prod_{k=1}^{v}(s_{d_{jk}})^{\alpha_2\beta_k^{(2j)}};\ \cdots;\ \prod_{k=1}^{v}(s_{d_{jk}})^{\alpha_s\beta_k^{(sj)}} \tag{46}$$

for any substitution of achiral atoms (or ligands) generating the $\mathbf{G}_j$-molecule.

We now consider a case that allows chiral ligands as well as achiral ligands. In order to manipulate this case, we shall extend the concept of "a set of USCIs." Coset representations, $\mathbf{G}_j(/\mathbf{H}_k)$, are classified into three cases: (a) both $\mathbf{G}_j$ and $\mathbf{H}_k$ contain improper symmetry operation (an achiral part), (b) both $\mathbf{G}_i$ and $\mathbf{H}_k$ contain only proper symmetry operations (a neutral part), and (c) $\mathbf{G}_j$ is improper and $\mathbf{H}_k$ is proper (a chiral part). We then define a unit subduced cycle index with chirallity fittingnes (USCI-CF).

Definition 3. A USCI-CF is defined as

$$Z(\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j;\ a,\ b,\ c) = \prod_{k=1}^{v}(\$_{d_{jk}})^{\beta_k^{(ij)}} \tag{47}$$

wherein \$ denotes a for an achiral part, b for a neutral part, and c for a chiral part.

Tables 14—16 also collects USCI-CFs for $\mathbf{C}_{2v}$, $\mathbf{D}_{3h}$, and $\mathbf{T}_d$ groups.

In a similar way as described in Def. 2, we now end up with

Definition 4. A set of USCI-CFs is defined as

$$\prod_{k=1}^{v}(\$_{d_{jk}})^{\alpha_1\beta_k^{(1j)}};\ \prod_{k=1}^{v}(\$_{d_{jk}})^{\alpha_2\beta_k^{(2j)}};\ \cdots;\ \prod_{k=1}^{v}(\$_{d_{jk}})^{\alpha_s\beta_k^{(sj)}} \tag{48}$$

for any substitution of achiral atoms (or ligands) generating the $\mathbf{G}_j$-molecule.

Let us again examine the $\mathbf{C}_s$-molecule of Fig. 3. The $\mathbf{C}_s$-molecule is characterized by a set of USCI-CFs,

$$a_1c_2;\ a_1^2;\ a_1 \tag{49}$$

The index (a_1c_2) for $\mathbf{D}_{3h}(/\mathbf{C}_{2v})\downarrow\mathbf{C}_s$ part shows that only one achiral ligand can occupies and two achiral (or chiral) ligands can attach in the manner of AB_2 or

AQQ′, where Q denotes a chiral ligand and Q′ is the antipode of Q. This restriction comes from the condition that realizes $\mathbf{C}_s$ symmetry. It should be noted that the positions of an achiral part can only take achiral ligands.

The discussions in the last paragraph can be applied to a general case characterized by Eq. 48. Hence, we arrive at

Theorem 2. Any orbit of an achiral part (characterized by variable a) can take only achiral ligands. An orbit of a neutral part (characterized by variable b) can take achiral or chiral ligands. An orbit of a chiral part (characterized by variable c) can take achiral ligands or is capable of carrying chiral ones in the manner QQ′QQ′⋯.

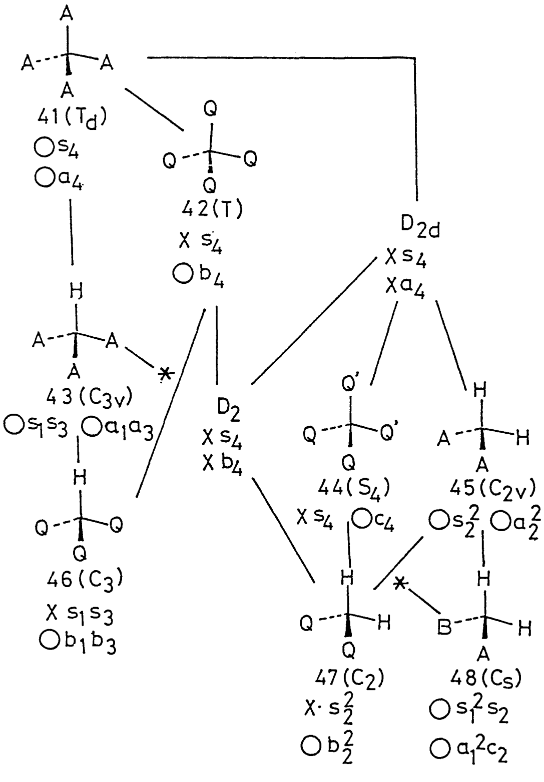


Fig. 5. Allowed molecules on the tetrahedron skeleton (**7**). The symbol (○) on each USCI (or USCI-CF) indicates that it predicts the existence of a molecule of the corresponding subsymmetry. The symbol (X) indicates a forbidden subsymmetry. The centeral position of **7** is not considered.

VII. A Selection Rule for Judging the Existence of Subsymmetries

When a skeleton of **G**-symmetry is substituted by an appropriate number of atoms (or ligands) to create a subsymmetry of **G**, several subsymmetries cannot be realized. For example, a $\mathbf{T}_d$ skeleton (**7**) cannot affords **T**, $\mathbf{D}_{2d}$, $\mathbf{D}_2$, $\mathbf{S}_4$, $\mathbf{C}_3$, and $\mathbf{C}_2$ molecules by considering only achiral (structureless) ligands or atoms (Fig. 5).[5] On the other hand, if we permit the substitution of chiral ligands as well as achiral ones, only $\mathbf{D}_{2d}$ and $\mathbf{D}_2$ remain impossible to exist. What factor controls these selections?

The USCI and USCI-CF are effective for detecting such factors. Let a given skeleton have a point group **G** in the manner of Eq. 5. We then construct a lattice of conjugate subgroups of $\mathbf{G}_j$ in which all group-subgroup relations are determined. If a (sub)group contains another subgroup, we call the former a supergroup of the latter. Let us first discuss the case of permitting only achiral atoms. Consider a coset representation (CR): $\mathbf{G}(/\mathbf{G}_i)$. The subgroups $\mathbf{G}_j$ and $\mathbf{G}_k$ of **G** are selected as being $\mathbf{G}_j \leqslant \mathbf{G}_k \leqslant \mathbf{G}$. If the USCI of $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_k$ is equal to that of $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$, the molecule having $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_k$ symmetry is identical to that having $\mathbf{G}(/\mathbf{G}_i)\downarrow\mathbf{G}_j$ symmetry. As a result, the $\mathbf{G}_j$ symmetry cannot exist.

As for a general molecule, we should consider a set of USCIs for achiral substituents and a set of USCI-CFs for achiral and chiral substituents. Hence, we arrive at the following selection rule:

Theorem 3. Let a parent skeleton of **G** symmetry be reduced into transitive CRs in accord with Eq. 5. Suppose that the subduction of CRs by $\mathbf{G}_j$ results in a set of USCIs (Eq. 46) or USCI-CFs (Eq. 48). A molecule of $\mathbf{G}_j$ symmetry on the skeleton exists, only if no supergroups of $\mathbf{G}_j$ have the same set of USCIs (or USCI-CFs) as that of $\mathbf{G}_j$.

Let us verify this theorem by using the $\mathbf{T}_d$ skeleton (**7**) shown in Fig. 5, where we consider only $\mathbf{T}_d(/\mathbf{C}_{3v})$ for simplicity of discussion. The set of USCIs for subgroup **T** is s_4, which is the same as that of $\mathbf{T}_d$. On the other hand, the set of USCI-CFs for **T** (b_4) is different from that of $\mathbf{T}_d$ (a_4); therefore, a **T**-molecule is possible only when chiral ligands are permitted. If we start from the skeleton (**7**), no $\mathbf{D}_{2d}$ molecule can

Table 17. Molecules based on the Skeleton (**7**)

Molecule	SCR notation	Abbreviated SCR notation
41	$\mathbf{T}_d[/\mathbf{C}_{3v}(A_3); /\mathbf{T}_d(C)]$[a]	
43	$\mathbf{T}_d(/\mathbf{C}_{3v})\downarrow\mathbf{C}_{3v}[/\mathbf{C}_s(A_3), /\mathbf{C}_{3v}(H)]$- $\mathbf{T}_d(/\mathbf{T}_d)\downarrow\mathbf{C}_{3v}[/\mathbf{C}_{3v}(C)]$	$\mathbf{C}_{3v}[/\mathbf{C}_s(A_3), /\mathbf{C}_{3v}(H); /\mathbf{C}_{3v}(C)]$
45	$\mathbf{T}_d(/\mathbf{C}_{3v})\downarrow\mathbf{C}_{2v}[/\mathbf{C}_s(H_2), /\mathbf{C}_s'(A_2)]$- $\mathbf{T}_d(/\mathbf{T}_d)\downarrow\mathbf{C}_{2v}[/\mathbf{C}_{2v}(C)]$	$\mathbf{C}_{2v}[/\mathbf{C}_s(H_2), /\mathbf{C}_s'(A_2); /\mathbf{C}_{2v}(/C)]$
48	$\mathbf{T}_d(/\mathbf{C}_{3v})\downarrow\mathbf{C}_s[/\mathbf{C}_1(H_2), 2/\mathbf{C}_s(A, B)]$- $\mathbf{T}_d(/\mathbf{T}_d)\downarrow\mathbf{C}_s[/\mathbf{C}_s(C)]$	$\mathbf{C}_s[/\mathbf{C}_1(H_2), /\mathbf{C}_s(A, B); /\mathbf{C}_s(/C)]$

a) This is a Case-I notation. The other data are Case-II notations.

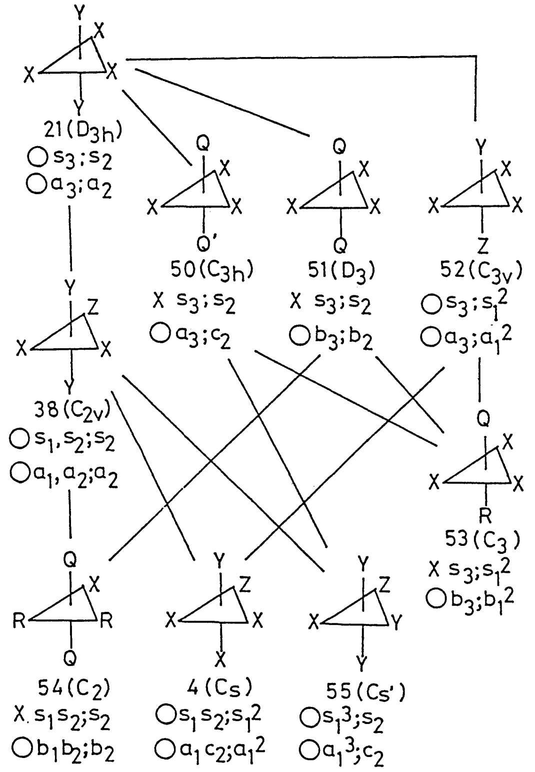
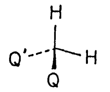


Fig. 6. Allowed molecules on the trigonal-bipyramid skeleton (**8**). The symbol (○) on each subsymmetry indicates that a molecule of the subsymmetry exists. The symbol (X) denotes a forbidden subsymmetry. The center of **8** is not considered.

possibly exist, because both s_4 and a_4 are the same as the respective counterparts of $\mathbf{T}_d$. A $\mathbf{C}_{2v}$ molecule exists, since s_1s_3 and a_1a_3 are different from s_4 and a_4 for $\mathbf{T}_d$. The symbol a_1a_3 indicates that four ligands should be achiral in order to realize $\mathbf{C}_{3v}$-symmetry, even when chiral ligands are allowed.

No $\mathbf{C}_2$ molecules with achiral ligands exist, because the symbol s_2^2 is equal to that of a supergroup ($\mathbf{C}_{2v}$). On the other hand, a $\mathbf{C}_2$ molecule with chiral ligands is allowed, because it is different from all supergroups in the set of USCI-CFs. Since both $s_1^2s_2$ and $a_1^2c_2$ are different from the counterparts of all supergroups, $\mathbf{C}_s$ molecules with achiral ligands (**43**) and with chiral ligands (**44**) are allowed. Note that the c_2 part of $a_1^2c_2$ can take Q and Q′ to afford an alternative $\mathbf{C}_s$ compound **49**.

The SCR notations for several derivatives in this series are found in Table 17.



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Theorem 3 is also verified in the case of skeleton **8** ($\mathbf{D}_{3h}$), as shown in Fig. 6. Allowed molecules are those having $\mathbf{D}_{3h}$, $\mathbf{C}_{3v}$, $\mathbf{C}_{2v}$, $\mathbf{C}_s$, $\mathbf{C}_{s'}$, and $\mathbf{C}_1$ symmetries, if only achiral ligands are permitted. Molecules with $\mathbf{C}_{3h}$, $\mathbf{D}_3$, $\mathbf{C}_3$, and $\mathbf{C}_2$ symmetries are forbidden.[14] On the other hand, if we permit chiral substituents as well, all subsymmetries of this lattice are realized.

VIII. Conclusion

Several concepts are presented for the chracterization of molecular symmetry, where a parent skeleton of a given symmetry is considered to afford a molecule having a subsymmetry in terms of appropriate substitution. The representative concepts are (1) subduction of coset representations for classification of positions of the skeleton, (2) the SCR notation for describing molecular symmetry,[15] (3) the abbreviated SCR notation,[15] (4) a set of unit subduced cycle indices, and (5) a selection rule for judging the existence of a molecule having a subsymmetry.

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10) This correspondence can be proved by clarifying the relationship between coset representations and a regular representation. The proof will be reported in detail elsewhere, since this relationship provides us with a broad prospect to stereochemisty.

11) For the proof of Theorem 1, see Ref. 7.

12) It should be noted that the term "mark" of the text is used in a slightly different sense from Ref. 13. The mark of $\mathbf{G}_j$ in $\mathbf{G}(/\mathbf{G}_i)$ in the present usage corresponds to the mark of $\mathbf{G}_j$ in $\mathbf{G}_i$ defined in Ref 13.

13) a) W. Hässelbarth, *Theor. Chim. Acta,* **67**, 339 (1985). b) C. A. Mead, *J. Am. Chem. Soc.,* **109**, 2130 (1987).

14) Brocas called this type of forbidden subsymmetry *a phantom subgroup*. See Ref. 3.

15) (Note added in proof) The present SCR notation explicitly contains the multiplicity of each CR before a slash. This multiplicity, however, may be abbreviated for simplicity.