Journal of Mathematical Chemistry Vol. 33, Nos. 3–4, May 2003 (© 2003)

Graphical models of characters of groups

Shinsaku Fujita [a] and Sherif El-Basil [b]

[a] *Department of Chemistry and Materials Technology, Kyoto Institute of Technology, Matsugasaki, Sakyo-ku, 606-8585 Japan*
[b] *Faculty of Pharmacy, Kasr El-Aini Street, Cairo, Egypt 11562*

A graphical method of generating one- and (some) two-dimensional characters (Γ) has been developed on the basis of a reduced homomer set, which has been derived from a new concept of negative graphs. Thus, a homomer set $\mathcal{H}[\boldsymbol{G}(/\boldsymbol{G}_i)] = \{\mathrm{h}_1, \ldots, \mathrm{h}_{d-1}, \mathrm{h}_d\}$ ($d = |\boldsymbol{G}|/|\boldsymbol{G}_i|$) has been generated from a regular body of $\boldsymbol{G}$ so that it has been governed by the coset representation $\boldsymbol{G}(/\boldsymbol{G}_i)$. The homomer set has been reduced into a reduced homomer set $\mathcal{H}'[\Gamma] = \{\mathrm{h}_1, \ldots, \mathrm{h}_{d-1}\}$, where we have placed $\mathrm{h}_d \equiv -(\mathrm{h}_1 + \cdots + \mathrm{h}_{d-1})$ in terms of negative graphs. The action of the symmetry operations of $\boldsymbol{G}$ on the reduced homomer set $\mathcal{H}'[\Gamma]$ has graphically generated a one- or (some) two-dimensional character (Γ). The versatility of the graphical method has been tested by using $\boldsymbol{C}_{3v}$, $\boldsymbol{D}_{2h}$, $\boldsymbol{C}_{2h}$, $\boldsymbol{C}_{2v}$, $\boldsymbol{D}_{3h}$, and $\boldsymbol{C}_{3h}$ as examples. The graphical method has been compared with an alternative algebraic generation using marks (or markaracters), i.e., $\Gamma = \boldsymbol{G}(/\boldsymbol{G}_i) - \boldsymbol{G}(/\boldsymbol{G})$.

1. Introduction

There are two disciplines of chemical group theory. The first discipline is based on permutation groups and permutation representations. Because of its discrete nature, it has found its applications in chemical combinatorics [1–5], especially in isomer enumerations, as summarized in excellent reviews [6–8] and books [9–11]. The second discipline is based on point groups and linear representations and has been applied to other chemical fields that treat problems of continuous nature, e.g., quantum chemistry [12], molecular spectroscopy [13], and related fields [14]. Many textbooks detail the concepts [15–21].

The two disciplines, however, have common features at the traditional stage described in the preceding paragraph[1], as we have recently discussed in [22]: namely, both of them are based on conjugacy classes in discussing invariants of a group. The first discipline, e.g., Pólya's theorem, emphasizes cycle indices, each term of which is ascribed to a conjugacy class, as discussed for clarifying the nature of chemical combinatorics [23]. As known widely, the second discipline uses linear representations, irreducible representations and characters for point groups, which stem from conjugacy classes.

[1] Methods based on conjugacy classes are here called "the traditional stage". On the other hand, methods characterized by conjugate subgroups are referred to as "the present stage".

0259-9791/03/0500-0255/0 © 2003 Plenum Publishing Corporation

The common features have been more clearly demonstrated now that the Pólya's theorem has been shown to stem from permutation representations, dominant representations and dominant markaracters (mark-character) [24,25]. Thus, characters for the second discipline have been shown to correspond to markaracters of the first discipline [26–29]. Because such markaracters have been defined as marks for cyclic subgroups [30], various group-theoretical tools developed for the present stage of the first discipline [31] have become applicable to the problems that has been usually ascribed to the second discipline[2].

As a continuation of our study on the graphical method of generating marks for the first discipline, this work is devoted to present a graphical (almost nonmathematical) method for generating characters for the second discipline, where one-dimensional characters of chemically important groups are graphically evaluated as **Q**-conjugacy characters. Then, the two methods are compared with each other by considering the relationship between markaracters (marks for cyclic subgroups) for the first discipline and **Q**-conjugacy characters for the second discipline. The concepts of "negative graphs" and "reduced homomer sets" are proposed as key concepts to comprehend the relationship between the two desciplines graphically. The approaches can be applied to cases which contain imaginary units.

2. Algebraic approach of characters from marks

2.1. *Marks and markaracters*

Marks have been earlier proposed by Burnside [33] but have remained less familiar to mathematicians and chemists compared to characters, probably because the calculation of the mark table of a given group requires the full information of the subgroup lattice. Thus, the current trends (in mathematics as well as in chemistry) have selected approaches which do not necessitate first knowing such a full subgroup lattice. This explains why characters and linear representations have been more widely used than marks and coset representations. However, chemists interested in stereochemistry should examine the symmetries of derivatives based on a molecular skeleton belonging to a given group. It follows that they have to know the corresponding full subgroup lattice in order to discuss the group–subgroup relationships of the derivatives. This situation has caused the revival of interest in marks, as summarized in several books [31,34].

Fujita has demonstrated that a row of marks can be regarded as a sum of irreducible characters, which are capable of constructing symmetry adapted functions [35]. Fujita has called such sums *markaracters* (mark-characters) by taking account of the columns (and sometimes the rows) corresponding to cyclic subgroups only and has further developed an algebraic procedure to discuss marks and characters on a common basis [24].

[2] In an alternative approach, marks have been referred to as *supercharacters* and markaracters have been characterized as transitive permutation characters [32, pp. 134, 135].

Table 1
Mark table of $\boldsymbol{C}_{3v}$.

	$\boldsymbol{C}_1$	$\boldsymbol{C}_s$	$\boldsymbol{C}_3$	$\boldsymbol{C}_{3v}$
$\boldsymbol{C}_{3v}(/\boldsymbol{C}_1)$	6	0	0	0
$\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)$	3	1	0	0
$\uparrow$ $\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)$	2	0	2	0
$\boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v})$	1	1	1	1

Table 2
Markaracter table of $\boldsymbol{C}_{3v}$.

	$\boldsymbol{C}_1$ I	$\boldsymbol{C}_s$ $3\sigma_v$	$\boldsymbol{C}_3$ $2C_3$	(**Q**-conjugacy) character
$\boldsymbol{C}_{3v}(/\boldsymbol{C}_1)$	6	0	0	$A_1 + A_2 + 2E$
$\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)$	3	1	0	$A_1 + E$
$\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)$	2	0	2	$A_1 + A_2$
$\boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v})$	1	1	1	A_1

Table 3
(**Q**-conjugacy) character table of $\boldsymbol{C}_{3v}$.

	I $\boldsymbol{C}_1$	$3\sigma_v$ $\boldsymbol{C}_s$	$2C_3$ $\boldsymbol{C}_3$	Markaracter
A_1	1	1	1	$\boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v})$
A_2	1	-1	1	$\boldsymbol{C}_{3v}(/\boldsymbol{C}_3) - \boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v})$
E	2	0	-1	$\boldsymbol{C}_{3v}(/\boldsymbol{C}_s) - \boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v})$

In this subsection, the algebraic procedure is first outlined by examining simple examples in order that the present graphical procedure is compared with the algebraic one by using the same example.

Let us consider the mark table of $\boldsymbol{C}_{3v}$ shown in table 1. When we take the columns corresponding to cyclic subgroups only, we obtain a markaracter table shown in table 2. Although the mark rows for the cyclic subgroups are sufficient to describe the remaining mark rows, we leave the row of $\boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v})$ for convenience[3].

The resulting markaracter table can be resolved into a sum of irreducible characters, as found in the last column of table 2. The symbols in the column are notations of irreducible representations in the corresponding table of characters (table 3)[4].

[3] For a general approach, we should consider *modified mark tables* in place of mark tables [24], since markaracter tables are derived from such modified mark tables. Although the two types of mark tables for $\boldsymbol{C}_{3v}$ are identical with each other, they are different in general cases.

[4] Strictly speaking, such a character table should be a **Q**-conjugacy character table in order to cover the cases of cyclic groups or others that contain characters of imaginary units. Note that a **Q**-conjugacy relationship has been defined on the basis of the conjugation of two or more subgroups, while a (usual) conjugacy relationship has been defined in terms of the conjugation of two or more elements of a group. See [26,37]. For the sake of simplicity, we mainly take account of the cases that do not contain characters of imaginary

2.2. Characters via markaracters

Let us now consider how the character table (table 3) is resolved in terms of the markaracter table (table 3). This resolution can be easily carried out to give the last column of table 3 [24][5]. *It should be emphasized that rows of markaracters can be added and/or subtracted* [24], *whereas rows of marks can undergo addition only* [31][6].

The result of the $\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)$ row of table 2,

$$\boldsymbol{C}_{3v}(/\boldsymbol{C}_3) = A_1 + A_2, \tag{1}$$

and the result of the A_2 row of table 3,

$$A_2 = \boldsymbol{C}_{3v}(/\boldsymbol{C}_3) - \boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v}), \tag{2}$$

can be considered to describe the same thing from two distinct viewpoints, when the totally symmetric irreducible character $A_1 = (1, 1, 1)$ is equalized to the mark $\boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v})$[7]. In other words, we are able to discuss characters as mar*karacters* (the right-hand side of equation (1)) and marks as *mark*aracters (the right-hand side of equation (2)) on a common basis [24].

In general, a coset representation $\boldsymbol{G}(/\boldsymbol{G}_i^{\max})$ with $|\boldsymbol{G}|/|\boldsymbol{G}_i^{\max}| = 2$ gives the corresponding mark row (MR), the elements of which are 0 or 2. Hence, the row calculated by the expression $\boldsymbol{G}(/\boldsymbol{G}_i^{\max}) - \boldsymbol{G}(/\boldsymbol{G})$ (e.g., equation (2)) produces a one-dimensional irreducible character which is denoted as $\Gamma_{\pm 1}$, where the subscript (± 1) indicates the fact that 1-dimensional irreducible representations (other than the totally symmetry irreducible character) are composed of plus and minus ones only. This fact is summarized symbolically as follows:

$$\Gamma_{\pm 1} = \boldsymbol{G}(/\boldsymbol{G}_i^{\max}) - \boldsymbol{G}(/\boldsymbol{G}), \tag{3}$$

where $\boldsymbol{G}_i^{\max}$ is a maximum subgroup of $\boldsymbol{G}$ and $|\boldsymbol{G}|/|\boldsymbol{G}_i^{\max}| = 2$; namely, there is no subgroups between $\boldsymbol{G}$ and $\boldsymbol{G}_i^{\max}$[8].

Since marks of a group can be algebraically calculated by means of coset representations [31], equation (3) indicates that such one-dimensional characters ($\Gamma_{\pm 1}$) can be calculated algebraically. Hence, the procedure is described as a *purely algebraic*

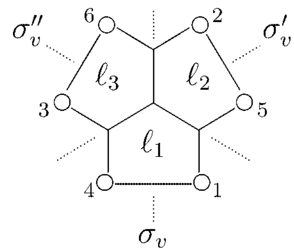
units. In other words, we mainly consider *matured* cases [28] in this paper, where **Q**-conjugacy character tables are identical with usual character tables.

[5] A given coset representation (CR) $\boldsymbol{G}(/\boldsymbol{G}_i)$ and the corresponding mark (and sometimes markaracter) are denoted by the same notation, if confusion does not occur.

[6] The expressions in the markaracter column of table 3 contain the subtractions of markaracters. If we remain within the concept of marks, such subtractions cannot be defined for the marks of non-cyclic subgroups. Thus the statement "rows of marks can undergo addition only" means that minus values are not permitted if such subtraction of rows of marks was carried out. See [24,30].

[7] Stricktly speaking, the right-hand side of equation (1) is concerned with dominant (irreducible) **Q**-conjugacy characters, but not with irreducible characters. On a similar line, equation (2) is concerned with markaracters, but not with marks. However, we sometimes use the words "character" and "mark", so long as such usage does not cause confusion.

[8] Strictly speaking, the right-hand side of equation (3) is concerned with markaracters, not with marks. The left-hand side is concerned with a **Q**-conjugacy character, not with a (usual) character.



1

Figure 1. A regular body for $\boldsymbol{C}_{3v}$-group. The three reflection planes are denoted by the symbols σ_v, σ_v', and σ_v''. The three-fold axis, which is perpendicular to the page plane and runs through the center of the regular body, is the intersection line of the three reflection planes.

approach. For further examples, characters as markaracters have been discussed algebraically to give the following equations for characterizing $\boldsymbol{T}_d$ group [24]:

$$\boldsymbol{T}_d(/\boldsymbol{T}) - \boldsymbol{T}_d(/\boldsymbol{T}_d) = (2,2,0,2,0) - (1,1,1,1,1) = (1,1,-1,1,-1) = A_2, \quad (4)$$

$$\boldsymbol{T}_d(/\boldsymbol{D}_{2d}) - \boldsymbol{T}_d(/\boldsymbol{T}_d) = (3,3,1,0,1) - (1,1,1,1,1) = (2,2,0,-1,0) = E, \quad (5)$$

$$\boldsymbol{T}_d(/\boldsymbol{D}_{3v}) - \boldsymbol{T}_d(/\boldsymbol{T}_d) = (4,0,2,1,0) - (1,1,1,1,1) = (3,-1,1,0,-1) = T_2. \quad (6)$$

The first equation of this set is an example of the general expression (equation (3)). Fujita has clarified a more fundamental relationship between marks (or strictly speaking, markaracters) and characters (or strictly speaking, **Q**-conjugacy characters) for cyclic groups by ascribing it to the relationship between Möbius' functions and Euler's ones [30]. Moreover, such relationships as equation (2) have been further subduced into subgroups so that Fujita has obtained characteristic monomials (CMs) [36]. For example, the CM $s_1^{-1}s_2$ is obtained from equation (2), because the powers are the coefficients of the respective terms on the right-hand side and the subscripts are calculated to be $|\boldsymbol{C}_{3v}|/|\boldsymbol{C}_3| = 6/3 = 2$ and $|\boldsymbol{C}_{3v}|/|\boldsymbol{C}_{3v}| = 6/6 = 1$. Note that the power of the term s_1 of each CM is identical with the corresponding character (strictly speaking **Q**-conjugacy character). Such CMs have been applied to combinatorial enumerations which led to CM (characteristic-monomial) method as an alternative method to Pólya's theorem [22][9].

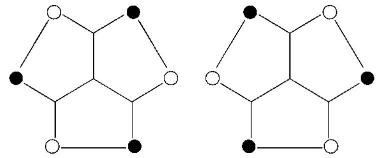
3. Semi-graphical approaches

3.1. Subtraction of markaracters

For a graphical approach for obtaining the marks of $\boldsymbol{C}_{3v}$-group, we consider a regular body ($\mathbf{1} = \mathrm{h}$) depicted in figure 1[10].

[9] Note that Fujita's CM method is based on linear representations, while Pólya's theorem is based on permutation representations.

[10] For the definition of regular bodies, see a previous paper of this series [39] and [31, chapter 7].



		2	**3**	$\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)]$	$\mathcal{H}'[A_2]$
		h_1	h_2	$\{\mathrm{h}_1, \mathrm{h}_2\}$	$\{\mathrm{h}_1\}$
			$(\equiv -\mathrm{h}_1)$	mark[a]	character
$\boldsymbol{C}_1$	I	h_1	h_2	2	1
$\boldsymbol{C}_3$	$2C_3$	h_1	h_2	2	1
$\boldsymbol{C}_s$	$3\sigma_v$	$\mathrm{h}_2(\equiv -\mathrm{h}_1)$	h_1	0	-1

[a]Strictly speaking, this column is concerned with markaracters, since each of the symmetric operations is operated on the homomer set.

Figure 2. Homomer sets for characterizing $\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)$ and A_2.

When the operations of $\boldsymbol{C}_3$ ($\subset \boldsymbol{C}_{3v}$) are applied to the set of six vertices of **1**, we obtain two sets ("color-equalities") of equivalent vertices: {1, 2, 3}, {4, 5, 6}[11]. Thereby, we take a set (orbit) of homomers of $\boldsymbol{C}_3$-symmetry (h_1 and h_2) listed in figure 2. For the sake of simplicity, we use the symbol $\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)] = \{\mathrm{h}_1, \mathrm{h}_2\}$ to designate the homomer set for characterizing $\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)$. Although such a set as $\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)]$ is called a *homomer set* in this paper, it should be noted that the resulting graphs (**2** and **3**) are enantiomeric to each other according to the chiral local symmetry $\boldsymbol{C}_3$. Thus, a homomer set contains enantiomers along with homomers, if it is concerned with a chiral graph.

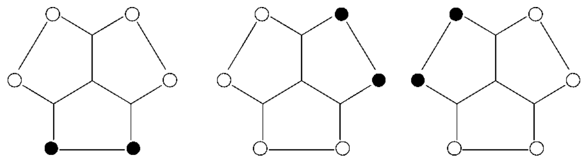
Let us consider the action of $\boldsymbol{C}_3$ on $\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)]$ (figure 2). Obviously, the symmetry operations I, C_3, and C_3^2 fix both h_1 and h_2 so that the corresponding mark is determined to be equal to 2. On the other hand, the operations σ_v, σ_v', and σ_v'' cause the interchange between h_1 and h_2. It follows that the corresponding mark is equal to 0. The resulting values are collected in the mark column of figure 2. As a result, we have graphically obtained the $\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)$-row of the mark table (table 2). Because $\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)$-row of the mark table has been obtained by the graphical procedure, we can, in turn, calculate the one-dimensional character A_2 algebraically by virtue of equation (2). In general, one-dimensional character ($\Gamma_{\pm 1}$) can be obtained by using equation (3).

This procedure for obtaining one-dimensional characters ($\Gamma_{\pm 1}$) is here called a *subtraction method*, since marks of a group are graphically evaluated and the subtraction due to equation (3) is used algebraically.

3.2. Semi-graphical method of generating characters

The subtraction due to equation (3) can be replaced by a semi-graphical operation, even though the graphical meaning of equation (3) is not clarified. Let us consider a

[11] According to the USCI approach [31], this division is ascribed to the subduction of the regular representation, i.e., $\boldsymbol{C}_{3v}(/\boldsymbol{C}_1) \downarrow \boldsymbol{C}_3 = 2\boldsymbol{C}_3(/\boldsymbol{C}_1)$.



	4	**5**	**6**	$\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)]$	$\mathcal{H}'[E]$
	h_1	h_2	h_3 $\equiv -(\mathrm{h}_1 + \mathrm{h}_2)$	$\{\mathrm{h}_1, \mathrm{h}_2, \mathrm{h}_3\}$ mark[a]	$\{\mathrm{h}_1, \mathrm{h}_2\}$ character
I	h_1	h_2	h_3	3	2
C_3	h_2	$\mathrm{h}_3(\equiv -(\mathrm{h}_1 + \mathrm{h}_2))$	h_1	0	-1
C_3^2	$\mathrm{h}_3(\equiv -(\mathrm{h}_1 + \mathrm{h}_2))$	h_1	h_2	0	-1
σ_v	h_1	$\mathrm{h}_3(\equiv -(\mathrm{h}_1 + \mathrm{h}_2))$	h_2	1	0
σ_v'	$\mathrm{h}_3(\equiv -(\mathrm{h}_1 + \mathrm{h}_2))$	h_2	h_1	1	0
σ_v''	h_2	h_1	h_3	1	0

[a] Strictly speaking, this column is concerned with markaracters, since each of the symmetry operations is operated on the homomer set.

Figure 3. Semi- and full-graphical approach to the mark row $\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)$ and the character E.

reduced set $\mathcal{H}'[A_2] = \{\mathrm{h}_1\}$ in place of the homomer set $\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)]$ (figure 2). Although the restriction of $\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)]$ into $\mathcal{H}'[A_2]$ has no foundation in this stage of this paper, we consider the action of $\boldsymbol{C}_{3v}$ on the one-membered set of $\mathcal{H}'[A_2]$. Obviously, the symmetry operations I, C_3, and C_3^2 fix h_1 so that the corresponding character is determined to be equal to 1. On the other hand, the operations σ_v, σ_v', and σ_v'' convert h_1 ($\in \mathcal{H}'[A_2]$) into h_2 ($\notin \mathcal{H}'[A_2]$) so that the value -1 is assigned to these operations. Since the graphical meaning of this assignment is not clarified, they are called *semi-graphical operations*. These values are collected in the character column of figure 2. As a result, we have graphically obtained the A_2-row of the character table (table 3). This method is called here a *semi-graphical method*.

The semi-graphical method can be applied to obtain two-dimensional characters. Figure 3 illustrates the derivation from a regular body (**1** as h) to give a homomer set:

$$\mathcal{H}\big[\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)\big] = \{\mathbf{4}, \mathbf{5}, \mathbf{6}\} = \{\mathrm{h}_1, \mathrm{h}_2, \mathrm{h}_3\}, \tag{7}$$

which is used to calculate marks of coset representation (CR) $\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)$. The homomers belong to $\boldsymbol{C}_s$-symmetry up to conjugacy.

We here take account of a reduced set $\mathcal{H}'[E] = \{\mathrm{h}_1, \mathrm{h}_2\}$ in place of the original homomer set $\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)] = \{\mathrm{h}_1, \mathrm{h}_2, \mathrm{h}_3\}$, although this restriction has no foundation in this stage. Let us examine the action of $\boldsymbol{C}_{3v}$ on $\mathcal{H}'[E]$. Obviously, the identity operation I fixes both h_1 and h_2 so that the corresponding character is determined to be equal to 2, as collected in the character column of figure 3. If an operation converts $\mathrm{h}_1 \in \mathcal{H}'[E]$ into $\mathrm{h}_2 \in \mathcal{H}'[E]$ or $\mathrm{h}_2 \in \mathcal{H}'[E]$ into $\mathrm{h}_1 \in \mathcal{H}'[E]$, its contribution to a character is evaluated to be 0. If an operation fixes $\mathrm{h}_1 \in \mathcal{H}'[E]$ or $\mathrm{h}_2 \in \mathcal{H}'[E]$, its contribution to a character is evaluated to be 1. If an operation converts $\mathrm{h}_1 \in \mathcal{H}'[E]$ into $\mathrm{h}_3 \notin \mathcal{H}'[E]$ or $\mathrm{h}_2 \in \mathcal{H}'[E]$ into $\mathrm{h}_3 \notin \mathcal{H}'[E]$, its contribution to a character is evaluated to be -1. These values are summed up to give the corresponding character. The resulting characters are collected in the character column of figure 3. Consequently, we have semi-graphically obtained the E-row of the character table (table 3) by classifying the operations into the conjugacy classes.

The semi-graphical method works well but has a conceptual drawback, since there is no graphical foundation which restricts an original homomer set (such as $\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)] = \{\mathrm{h}_1, \mathrm{h}_2, \mathrm{h}_3\}$) into a reduced set (such as $\mathcal{H}'[E] = \{\mathrm{h}_1, \mathrm{h}_2\}$), even though such a foundation can be derived algebraically from equation (3) as described later. The next interest is to clarify the graphical meaning of equation (3). This will result in the development of a purely graphical approach for obtaining one- and two-dimensional characters, as discussed in the next section.

4. Full graphical approach

4.1. *Concept of negative graphs*

To develop such a purely graphical approach for obtaining characters, we now propose the concept of *negative graphs*, which are generated from the uncolored graph by exchanging black and white ligands. For example, the graph $\mathbf{2}(\mathrm{h}_1)$ shown in figure 2 is converted into the corresponding negative graph $\mathbf{3}(\mathrm{h}_2)$ by exchanging black and white ligands. This fact is symbolically expressed as $\mathrm{h}_2 \equiv -\mathrm{h}_1$. This means that h_2 is represented by h_1 in terms of the concept of negative graphs. Thereby, the homomer set $\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_3)] = \{\mathrm{h}_1, \mathrm{h}_2\}$ can be reduced into $\mathcal{H}'[A_2] = \{\mathrm{h}_1\}$, which contains the homomer h_1 only. In this paper, such a set as $\mathcal{H}'[A_2]$ is now called a *reduced homomer set*.

A more complicated example of negative graphs is illustrated in figure 4, where the first row represents a homomer set corresponding to equation (7). The corresponding negative homomer set is obtained easily, as shown in the bottom row of figure 4:

$$\overline{\mathcal{H}}\big[\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)\big] = \big\{\overline{\mathbf{4}}, \overline{\mathbf{5}}, \overline{\mathbf{6}}\big\} = \{-\mathrm{h}_1, -\mathrm{h}_2, -\mathrm{h}_3\}. \tag{8}$$

When we superimpose $\mathbf{4}(\mathrm{h}_1)$ and $\mathbf{5}(\mathrm{h}_2)$, we obtain the negative graph $\overline{\mathbf{6}}(-\mathrm{h}_3)$[12]. This is symbolically expressed by $\mathrm{h}_1 + \mathrm{h}_2 \equiv -\mathrm{h}_3$[13]. In a similar way, the superposition of $\overline{\mathbf{4}}(-\mathrm{h}_1)$ and $\overline{\mathbf{5}}(-\mathrm{h}_2)$ gives $\mathbf{6}(\mathrm{h}_3)$ so that we obtain $-(\mathrm{h}_1 + \mathrm{h}_2) \equiv \mathrm{h}_3$[14]. This means that h_3 is represented by h_1 and h_2 in terms of the concept of negative graphs. Thereby, the homomer set $\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)] = \{\mathrm{h}_1, \mathrm{h}_2, \mathrm{h}_3\}$ (equation (7)) can be reduced into the corresponding reduced homomer set, i.e., $\mathcal{H}'[E] = \{\mathrm{h}_1, \mathrm{h}_2\}$.

[12] The superposition gives presedence to black ligands. In other words, a black ligand and a white ligand give a black ligand. Two white ligands superimposed give a white ligand. This procedure is called here "positive coloring".

[13] It should be noted that **1** and $\overline{\mathbf{1}}$ are equalized in this treatment. This means that the coloring process is considered in terms of the modulus of full coloring.

[14] The superposition gives presedence to white ligands. In other words, a white ligand and a black ligand gives a white ligand. Two black ligands superimposed give a black ligand. This procedure is called here "negative coloring".

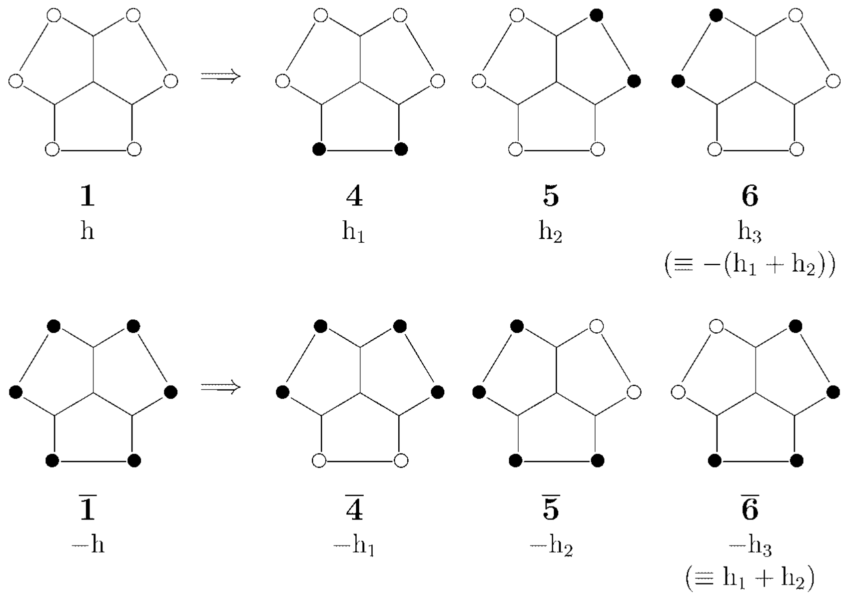


Figure 4. Homomer sets and negative graphs for characterizing $\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)$ and E.

In general, a homomer set $\mathcal{H}[\boldsymbol{G}(/\boldsymbol{G}_i)] = \{\mathrm{h}_1, \ldots, \mathrm{h}_{d-1}, \mathrm{h}_d\}$ ($d = |\boldsymbol{G}|/|\boldsymbol{G}_i|$) generated from a regular body of $\boldsymbol{G}$ is governed by the coset representation $\boldsymbol{G}(/\boldsymbol{G}_i)$. If no other subgroups are present between $\boldsymbol{G}$ and $\boldsymbol{G}_i$, the homomer set can be reduced into a reduced homomer set $\mathcal{H}'[\Gamma] = \{\mathrm{h}_1, \ldots, \mathrm{h}_{d-1}\}$, where we place $\mathrm{h}_d \equiv -(\mathrm{h}_1 + \cdots + \mathrm{h}_{d-1})$ in terms of negative graphs.

4.2. Full graphical method for generating characters

Now that we have clarified the graphical meaning of a reduced homomer set in terms of negative graphs, we are ready to develop full graphical method for obtaining characters.

The first goal of this subsection is to obatin the one-dimensional character A_2 by a full graphical approach. Thus we take account of the reduced homomer set $\mathcal{H}'[A_2] = \{\mathrm{h}_1\}$ and consider the action of $\boldsymbol{C}_{3v}$ on $\mathcal{H}'[A_2]$. This treatment is allowed in terms of the expression, $\mathrm{h}_2 \equiv -\mathrm{h}_1$. Obviously, the symmetry operations I, C_3, and C_3^2 fix h_1 so that the corresponding character is determined to be equal to 1. On the other hand, the operations σ_v, σ_v', and σ_v'' convert h_1 into h_2, which is equal to $-\mathrm{h}_1$. Thereby, the conversion from h_1 to h_2 can be regarded as the conversion from h_1 into $-\mathrm{h}_1$. Since h_1 is fixed, the corresponding character is equal to -1. These values are collected in the character column of figure 2. As a result, we have graphically obtained the A_2-row of the character table (table 3).

The second goal of this subsection is to obtain the two-dimensional character E for the $\boldsymbol{C}_{3v}$-group by a full graphical approach (figure 3). Thus we take account of the reduced homomer set $\mathcal{H}'[E] = \{\mathrm{h}_1, \mathrm{h}_2\}$ in place of the original homomer set

$\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)] = \{\mathrm{h}_1, \mathrm{h}_2, \mathrm{h}_3\}$. Let us examine the action of $\boldsymbol{C}_{3v}$ on $\mathcal{H}'[E]$, where we take the relationship $\mathrm{h}_3 \equiv -(\mathrm{h}_1 + \mathrm{h}_2)$ into consideration. Obviously, the identity operation I fixes both h_1 and h_2 so that the corresponding character is determined to be equal to 2, as collected in the character column of figure 3. The operation C_3 converts h_1 into h_2 (no homomers is fixed yielding a character of 0) and h_2 into h_3 ($\equiv -(\mathrm{h}_1 + \mathrm{h}_2)$, fixing $-\mathrm{h}_2$ to contribute to a character by -1)[15] so that we can graphically obtain $0 + (-1) = -1$ as a character. It should be emphasized that the contribution of h_3 is hidden or shut up within the reduced homomer set $\mathcal{H}'[E] = \{\mathrm{h}_1, \mathrm{h}_2\}$ by virtue of the relationship $\mathrm{h}_3 \equiv -(\mathrm{h}_1 + \mathrm{h}_2)$ derived from the concept of negative graphs. The operation C_3^2 converts h_1 into h_3 ($\equiv -(\mathrm{h}_1 + \mathrm{h}_2)$, fixing $-\mathrm{h}_1$) and h_1 into h_2 (fixing no homomers); thereby we obtain $(-1) + 0 = -1$ as a character. The operation σ_v fixes the homomer h_1 but converts h_2 into h_3 ($\equiv -(\mathrm{h}_1 + \mathrm{h}_2)$, fixing $-\mathrm{h}_2$) so that we obtain $1 + (-1) = 0$ as a character. Similarly, the character for the operation σ_v' is graphically obtained to be equal to 0. The operation σ_v'' that exchanges h_1 and h_2 to each other (fixing no homomers) is determined to have the character 0. These values are collected in the character column of figure 3. Consequently, we have graphically obtained the E-row of the character table (table 3) by classifying the operations into the conjugacy classes.

Figure 3 also involves the mark column of $\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)$ which is graphically obtained by considering the action of $\boldsymbol{C}_{3v}$ on the homomer set $\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)]$. The comparison of the behavior of $\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)]$ with that of the reduced homomer set $\mathcal{H}'[E]$ provides us with the graphical meaning of characters, which is concealed in the following equation collected in table 3:

$$E = \boldsymbol{C}_{3v}(/\boldsymbol{C}_s) - \boldsymbol{C}_{3v}(/\boldsymbol{C}_{3v}) = (3, 1, 0) - (1, 1, 1) = (2, 0, -1), \tag{9}$$

or in the following equation collected in table 2:

$$\boldsymbol{C}_{3v}(/\boldsymbol{C}_s) = A_1 + E = (1, 1, 1) + (2, -1, 0) = (3, 0, 1). \tag{10}$$

5. Applications of the graphical approach

5.1. *Graphical generation of characters of $\boldsymbol{D}_{2h}$ and its subgroups*

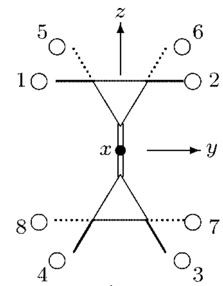
By thinking out appropriate regular bodies, the generation of characters for $\boldsymbol{D}_{2h}$ and its subgroups can be graphically discussed on a common basis.

5.1.1. *One-dimensional characters of $\boldsymbol{D}_{2h}$*

The mark table of $\boldsymbol{D}_{2h}$ that was obtained algebraically has been reported as a USCI (unit-subduced-cycle-index) table by one of the authors [38]. To clarify the usefulness of the present approach, the character of the $\boldsymbol{D}_{2h}$-group will be obtained graphically in this subsection.

To work with an actual example for organic chemistry, we select an ethylene derivative (**7**) shown in figure 5 as a regular body of the $\boldsymbol{D}_{2h}$-group, where two cyclopropane

[15] This assignment results in the same contribution as defined in the semi-graphical method.



7

Figure 5. A regular body for $\boldsymbol{D}_{2h}$-group. The three two-fold axes are chosen as the Cartesian coordinates, i.e., $\mathrm{C}_{2(x)}$, $\mathrm{C}_{2(y)}$, $\mathrm{C}_{2(z)}$. The three reflection planes are the xy-plane ($\sigma_{(xy)}$), the xz-plane ($\sigma_{(xz)}$), and the yz-plane ($\sigma_{(yz)}$).

rings are linked with a double bond. It is convenient that the three two-fold axes are used as the Cartesian coordinate axes. Thus, the z-axis is chosen as the two-fold axis ($\mathrm{C}_{2(z)}$) which passes through the two carbon atoms of the central double bond. The y-axis ($\mathrm{C}_{2(y)}$) is selected so that the two cyclopropane rings lie in the yz-plane. The x-axis ($\mathrm{C}_{2(x)}$) runs through the center of the double bond and is perpendicular to the page plane (yz-plane). The three reflection planes are the xy-plane ($\sigma_{(xy)}$), the xz-plane ($\sigma_{(xz)}$), and the yz-plane ($\sigma_{(yz)}$). The remaining element of the $\boldsymbol{D}_{2h}$-group is the inversion center (i). In summary, we obtain eight symmetry operations of $\boldsymbol{D}_{2h}$ as follows:

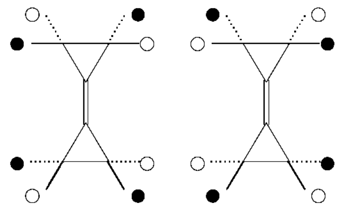
$$\boldsymbol{D}_{2h} = \{I, C_{2(x)}, C_{2(y)}, C_{2(z)}, i, \sigma_{(xy)}, \sigma_{(xz)}, \sigma_{(yz)}\}. \tag{11}$$

There are 16 subgroups, which are enumerated as follows:

$$\begin{array}{lll}
\boldsymbol{C}_1 = \{I\}; & & \\
\boldsymbol{C}_2 = \{I, C_{2(x)}\}, & \boldsymbol{C}'_2 = \{I, C_{2(y)}\}, & \boldsymbol{C}''_2 = \{I, C_{2(z)}\}; \\
\boldsymbol{C}_s = \{I, \sigma_{(xy)}\}, & \boldsymbol{C}'_s = \{I, \sigma_{(xz)}\}, & \boldsymbol{C}''_s = \{I, \sigma_{(yz)}\}; \\
\boldsymbol{C}_i = \{I, i\}; & & \\
\boldsymbol{C}_{2v} = \{I, C_{2(x)}, \sigma_{(xy)}, \sigma_{(xz)}\}, & \boldsymbol{C}'_{2v} = \{I, C_{2(z)}, \sigma_{(xz)}, \sigma_{(yz)}\}, & \boldsymbol{C}''_{2v} = \{I, C_{2(y)}, \sigma_{(xy)}, \sigma_{(yz)}\}; \\
\boldsymbol{C}_{2h} = \{I, C_{2(x)}, i, \sigma_{(yz)}\}, & \boldsymbol{C}'_{2h} = \{I, C_{2(y)}, i, \sigma_{(xz)}\}, & \boldsymbol{C}''_{2h} = \{I, C_{2(z)}, i, \sigma_{(xy)}\}; \\
\boldsymbol{D}_2 = \{I, C_{2(x)}, C_{2(y)}, C_{2(x)}\} & \multicolumn{2}{l}{\boldsymbol{D}_{2h} = \{I, C_{2(x)}, C_{2(y)}, C_{2(z)}, i, \sigma_{(xy)}, \sigma_{(xz)}, \sigma_{(yz)}\}.}
\end{array}$$

One-dimensional character A_u. Among these subgroups, those of order 4 are concerned with one-dimensional characters of $\boldsymbol{D}_{2h}$. For example, we first consider the homomer set $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{D}_2)] = \{\mathbf{8}, \mathbf{9}\} = \{\mathrm{h}_1, \mathrm{h}_2\}$ and the corresponding reduced homomer set $\mathcal{H}'[A_u]$, as illustrated in figure 6. Note that $\mathbf{9}(\mathrm{h}_2)$ is the negative graph of and $\mathbf{8}(\mathrm{h}_1)$, i.e., $\mathrm{h}_2 \equiv -\mathrm{h}_1$. The graphs of the set $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{D}_2)]$ are enantiomeric to each other, though the set is called a “homomer” set. The sets $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{D}_2)]$ and $\mathcal{H}'[A_u]$ respectively give marks of $\boldsymbol{D}_{2h}(/\boldsymbol{D}_2)$ and a one-dimensional character A_u.

Let us consider the action of $\boldsymbol{D}_{2h}$ on $\mathcal{H}'[A_u]$. Obviously, the symmetry operations I, $C_{2(x)}$, $C_{2(y)}$ and $C_{2(z)}$ fix h_1 so that the corresponding character is determined to be equal to 1. On the other hand, the operations i, $\sigma_{(xy)}$, $\sigma_{(xz)}$, and $\sigma_{(yz)}$ convert h_1 into h_2,



	8	**9**	$\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{D}_2)]$	$\mathcal{H}'[A_u]$
	h_1	h_2	$\{h_1, h_2\}$	$\{h_1\}$
		$(\equiv -h_1)$	mark[a]	character
I	h_1	h_2	2	1
$C_{2(x)}$	h_1	h_2	2	1
$C_{2(y)}$	h_1	h_2	2	1
$C_{2(z)}$	h_1	h_2	2	1
i	$h_2(\equiv -h_1)$	h_1	0	-1
$\sigma_{(xy)}$	$h_2(\equiv -h_1)$	h_1	0	-1
$\sigma_{(xz)}$	$h_2(\equiv -h_1)$	h_1	0	-1
$\sigma_{(yz)}$	$h_2(\equiv -h_1)$	h_1	0	-1

[a] Strictly speaking, this column is concerned with markaracters, since each of the symmetry operations is operated on the homomer set.

Figure 6. Homomer sets for characterizing $\boldsymbol{D}_{2h}(/\boldsymbol{D}_2)$ and A_u.

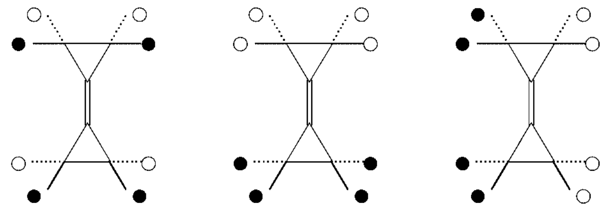
which is not a member of $\mathcal{H}'[A_u]$. However, because the latter is replaced by $-h_1$ and the h_1 is fixed, the contribution of h_2 ($\equiv -h_1$) is evaluated to be -1. This is recognized as a character. These values are collected in the character column of figure 6. This relationship is represented by the following symbolic expression:

$$A_u = \boldsymbol{D}_{2h}(/\boldsymbol{D}_2) - \boldsymbol{D}_{2h}(/\boldsymbol{D}_{2h}). \tag{12}$$

Ungerade one-dimensional characters B_{3u}, B_{2u}, and B_{1u}. Three ungerade one-dimensional characters of the $\boldsymbol{D}_{2h}$-group (B_{3u}, B_{2u}, and B_{1u}) can be discussed by considering CRs $\boldsymbol{D}_{2h}(/\boldsymbol{G}_i)$, where the subgroups $\boldsymbol{G}_i$ are of $\boldsymbol{C}_{2v}$-type. The graphical approach for these cases are shown in figure 7, where one homomer (**10**, **11**, or **12**) is selected as h_1 and the other homomer h_2 is omitted from each of the homomer sets. In other words, figure 7 contains the respective reduced homomer sets, whose homomer is h_1. Note that each h_2 is the negative graph of the corresponding h_1, i.e., $h_2 \equiv -h_1$. The action of $\boldsymbol{D}_{2h}$ on each of the reduced homomer sets fixes h_1 or generates h_2, where the latter h_2 is replaced by $-h_1$. By this procedure, the three ungerade one-dimensional characters B_{3u}, B_{2u}, and B_{1u} are generated graphically, as summarized in figure 7. The relationships between $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{C}_{2v})]$ and $\mathcal{H}'[B_{3u}]$, between $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{C}'_{2v})]$ and $\mathcal{H}'[B_{2u}]$, and between $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{C}''_{2v})]$ and $\mathcal{H}'[B_{1u}]$ are represented by the following symbolic expressions:

$$B_{3u} = \boldsymbol{D}_{2h}(/\boldsymbol{C}_{2v}) - \boldsymbol{D}_{2h}(/\boldsymbol{D}_{2h}), \tag{13}$$

$$B_{2u} = \boldsymbol{D}_{2h}\bigl(/\boldsymbol{C}'_{2v}\bigr) - \boldsymbol{D}_{2h}(/\boldsymbol{D}_{2h}), \tag{14}$$



	h$_1$ **10** of $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{C}_{2v})]$ $\mathcal{H}'[B_{3u}]$		h$_1$ **11** of $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{C}'_{2v})]$ $\mathcal{H}'[B_{2u}]$		h$_1$ **12** of $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{C}''_{2v})]$ $\mathcal{H}'[B_{1u}]$	
I	h$_1$	1	h$_1$	1	h$_1$	1
$C_{2(x)}$	h$_1$	1	$-$h$_1$	-1	$-$h$_1$	-1
$C_{2(y)}$	$-$h$_1$	-1	h$_1$	1	$-$h$_1$	-1
$C_{2(z)}$	$-$h$_1$	-1	$-$h$_1$	-1	h$_1$	1
i	$-$h$_1$	-1	$-$h$_1$	-1	$-$h$_1$	-1
σ_{xy}	h$_1$	1	h$_1$	1	$-$h$_1$	-1
σ_{xz}	h$_1$	1	$-$h$_1$	-1	h$_1$	1
σ_{yz}	$-$h$_1$	-1	h$_1$	1	h$_1$	1

Figure 7. Reduced homomer sets for characterizing one-dimensional characters, B_{3u}, B_{2u}, and B_{1u}.

$$B_{1u} = \boldsymbol{D}_{2h}\left(/\boldsymbol{C}''_{2v}\right) - \boldsymbol{D}_{2h}(/\boldsymbol{D}_{2h}). \tag{15}$$

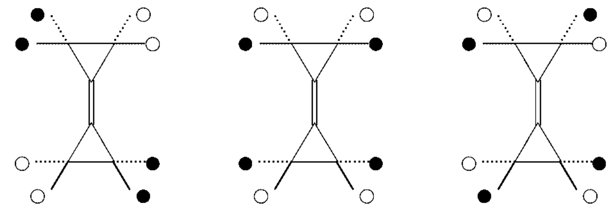
A common feature of the ungerade characters (B_{3u}, B_{2u}, and B_{1u}) collected in figure 7 is the fact that each character for the inversion i is equal to -1. Graphically speaking, the homomers **10**, **11** and **12** are not fixed on the action of i. Hence, the common feature is ascribed to the nature of the graphs whose symmetries satisfy $i \notin \boldsymbol{C}_{2v}, \boldsymbol{C}'_{2v}, \boldsymbol{C}''_{2v}$.

Gerade one-dimensional characters B_{3g}, B_{2g}, and B_{1g}. Similarly, the graphical approach for the three subgroups of $\boldsymbol{C}_{2h}$-type clarifies common features between the three gerade one-dimensional characters of the $\boldsymbol{D}_{2h}$-group (B_{3g}, B_{2g}, and B_{1g}), as shown in figure 8. Again, figure 8 depicts one homomer (**13**, **14**, or **15**) selected as h$_1$. The other homomer h$_2$ is omitted to depict the corresponding reduced homomer set, where each omitted h$_2$ is the negative graph of the corresponding h$_1$, i.e., h$_2 \equiv -$h$_1$. The action of $\boldsymbol{D}_{2h}$ on each of the reduced homomer sets fixes h$_1$ or generates h$_2$, where the latter h$_2$ is replaced by $-$h$_1$. Thereby, the three gerade one-dimensional characters B_{3g}, B_{2g}, and B_{1g} are generated graphically, as summarized in figure 8. The relationships between $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{C}_{2h})]$ and $\mathcal{H}'[B_{3g}]$, between $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{C}'_{2h})]$ and $\mathcal{H}'[B_{2g}]$, and between $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{C}''_{2h})]$ and $\mathcal{H}'[B_{1g}]$ are represented by the following symbolic expressions:

$$B_{3g} = \boldsymbol{D}_{2h}(/\boldsymbol{C}_{2h}) - \boldsymbol{D}_{2h}(/\boldsymbol{D}_{2h}), \tag{16}$$

$$B_{2g} = \boldsymbol{D}_{2h}\left(/\boldsymbol{C}'_{2h}\right) - \boldsymbol{D}_{2h}(/\boldsymbol{D}_{2h}), \tag{17}$$

$$B_{1g} = \boldsymbol{D}_{2h}\left(/\boldsymbol{C}''_{2h}\right) - \boldsymbol{D}_{2h}(/\boldsymbol{D}_{2h}). \tag{18}$$



	h_1	**13**	h_1	**14**	h_1	**15**
	of $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{C}_{2h})]$		of $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{C}'_{2h})]$		of $\mathcal{H}[\boldsymbol{D}_{2h}(/\boldsymbol{C}''_{2h})]$	
	$\mathcal{H}'[B_{3g}]$		$\mathcal{H}'[B_{2g}]$		$\mathcal{H}'[B_{1g}]$	
I	h_1	1	h_1	1	h_1	1
$C_{2(x)}$	h_1	1	$-h_1$	-1	$-h_1$	-1
$C_{2(y)}$	$-h_1$	-1	h_1	1	$-h_1$	-1
$C_{2(z)}$	$-h_1$	-1	$-h_1$	-1	h_1	1
i	h_1	1	h_1	1	h_1	1
σ_{xy}	$-h_1$	-1	$-h_1$	-1	h_1	1
σ_{xz}	$-h_1$	-1	h_1	1	$-h_1$	-1
σ_{yz}	h_1	1	$-h_1$	-1	$-h_1$	-1

Figure 8. Reduced homomer sets for characterizing one-dimensional characters of $\boldsymbol{D}_{2h}$-group, B_{3g}, B_{2g}, and B_{1g}.

A common feature of the gerade characters (B_{3g}, B_{2g}, and B_{1g}) collected in figure 8 is the fact that each character for the inversion i is equal to 1. Graphically speaking, the homomers **13**, **14** and **15** are fixed on the action of i. Hence, the common feature is ascribed to the nature of the graphs whose symmetries satisfy $i \in \boldsymbol{C}_{2h}, \boldsymbol{C}'_{2h}, \boldsymbol{C}''_{2h}$.

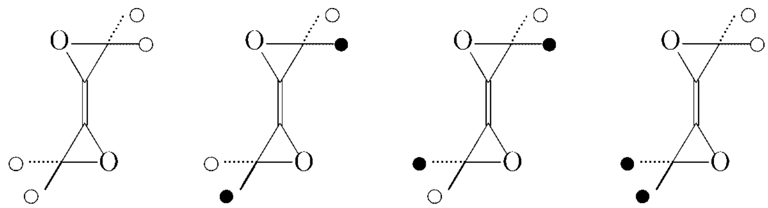
5.1.2. One-dimensional characters of $\boldsymbol{C}_{2h}$

The graphical generation of homomers discussed in this paper can be regarded as a method of generating a regular body of its subgroup from another point of view. For example, the two cyclopropane rings of the regular body of $\boldsymbol{D}_{2h}$ (**7** shown in figure 5) are replaced by two oxirane rings so that the original $C_{2(y)}$- and $C_{2(z)}$-axes of **7** are canceled. This process generates a regular body of $\boldsymbol{C}_{2h}$ (**16**) shown in figure 9. Note that the $\boldsymbol{C}_{2h}$-group listed in the subgroups of $\boldsymbol{D}_{2h}$ is selected as a mother group $\boldsymbol{C}_{2h}$ for this discussion.

$$\boldsymbol{C}_{2h} = \{I, C_2, i, \sigma_h\} \quad \sim \quad \boldsymbol{C}_{2h} = \{I, C_{2(x)}, i, \sigma_{(yz)}\}. \tag{19}$$

Obviously, this regular body is related to the homomer **13** from the symmetrical point of view, where the former is generated by the replacement of each substituted methylene ($C(\bullet)_2$) with an oxygen atom.

Figure 9 also shows the graphical approach for obtaining one-dimensional characters of $\boldsymbol{C}_{2h}$-group, where the respective reduced homomer sets (**17**–**19**), which contains h_1 only, are depicted. The action of $\boldsymbol{C}_{2h}$ on each of the reduced homomer sets fixes h_1 or generates h_2, where the latter h_2 is replaced by $-h_1$. Thereby, the characters of the $\boldsymbol{C}_{2h}$-



16	h_1 **17** of $\mathcal{H}[\boldsymbol{C}_{2h}(/\boldsymbol{C}_2)]$ $\mathcal{H}'[A_u]$		h_1 **18** of $\mathcal{H}[\boldsymbol{C}_{2h}(/\boldsymbol{C}_i)]$ $\mathcal{H}'[B_g]$		h_1 **19** of $\mathcal{H}[\boldsymbol{C}_{2h}(/\boldsymbol{C}_s)]$ $\mathcal{H}'[B_u]$	
I	h_1	1	h_1	1	h_1	1
C_2	h_1	1	$-\mathrm{h}_1$	-1	$-\mathrm{h}_1$	-1
i	$-\mathrm{h}_1$	-1	h_1	1	$-\mathrm{h}_1$	-1
σ_h	$-\mathrm{h}_1$	-1	$-\mathrm{h}_1$	-1	h_1	1

Figure 9. Reduced homomer sets for characterizing one-dimensional characters of $\boldsymbol{C}_{2h}$-group, A_u, B_g, and B_u.

group are obtained and listed in the respective columns of figure 9. The relationships between $\mathcal{H}[\boldsymbol{C}_{2h}(/\boldsymbol{C}_2)]$ and $\mathcal{H}'[A_u]$, between $\mathcal{H}[\boldsymbol{C}_{2h}(/\boldsymbol{C}_i)]$ and $\mathcal{H}'[B_g]$, and between $\mathcal{H}[\boldsymbol{C}_{2h}(/\boldsymbol{C}_s)]$ and $\mathcal{H}'[B_u]$ are represented by the following symbolic expressions:

$$A_u = \boldsymbol{C}_{2h}(/\boldsymbol{C}_2) - \boldsymbol{C}_{2h}(/\boldsymbol{C}_{2h}), \tag{20}$$

$$B_g = \boldsymbol{C}_{2h}(/\boldsymbol{C}_i) - \boldsymbol{C}_{2h}(/\boldsymbol{C}_{2h}), \tag{21}$$

$$B_u = \boldsymbol{C}_{2h}(/\boldsymbol{C}_s) - \boldsymbol{C}_{2h}(/\boldsymbol{C}_{2h}). \tag{22}$$

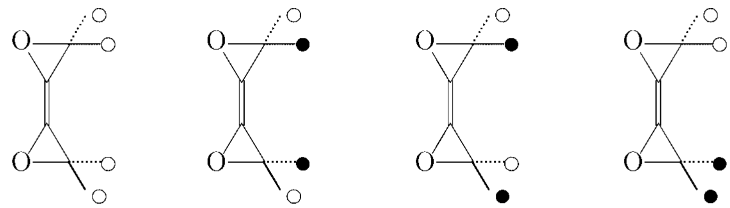
5.1.3. One-dimensional characters of $\boldsymbol{C}_{2v}$

When the two cyclopropane rings of **7** (figure 5) are replaced by two oxirane rings in an alternative way, we can generate a regular body of $\boldsymbol{C}_{2v}$ (**20**) shown in figure 10. During this process, the original $\mathrm{C}_{2(x)}$- and $\mathrm{C}_{2(z)}$-axes of **7** are canceled. Note that the $\boldsymbol{C}''_{2v}$-group listed in the subgroups of $\boldsymbol{D}_{2h}$ is selected as a mother group $\boldsymbol{C}_{2v}$ for this discussion.

$$\boldsymbol{C}_{2v} = \left\{I, C_2, \sigma_v, \sigma'_v\right\} \quad \sim \quad \boldsymbol{C}''_{2v} = \{I, C_{2(y)}, \sigma_{(xy)}, \sigma_{(yz)}\}. \tag{23}$$

Obviously, this regular body is related to the homomer **12**, where each substituted methylene (C(●)$_2$) in the latter homomer is replaced by an oxygen atom to generate the regular body (**20**).

One-dimensional characters of $\boldsymbol{C}_{2v}$-group can be obtained by the graphical approach, as shown in figure 10, where the respective reduced homomer sets (**21**–**23**) are depicted. When the action of $\boldsymbol{C}_{2v}$ on each of the reduced homomer sets fixes h_1, its contribution to the corresponding character is equal to 1. On the other hand, the action converts h_1 into h_2, where the latter h_2 is replaced by $-\mathrm{h}_1$ and its contribution is evaluated to be -1. Thereby, the characters of the $\boldsymbol{C}_{2v}$-group are obtained and listed in the respective columns of figure 10. The relationships between $\mathcal{H}[\boldsymbol{C}_{2v}(/\boldsymbol{C}_2)]$ and $\mathcal{H}'[A_2]$, between



20	h_1	**21**	h_1	**22**	h_1	**23**
	of $\mathcal{H}[\boldsymbol{C}_{2v}(/\boldsymbol{C}_2)]$		of $\mathcal{H}[\boldsymbol{C}_{2v}(/\boldsymbol{C}_s)]$		of $\mathcal{H}[\boldsymbol{C}_{2v}(/\boldsymbol{C}'_s)]$	
	$\mathcal{H}'[A_2]$		$\mathcal{H}'[B_1]$		$\mathcal{H}'[B_2]$	
I	h_1	1	h_1	1	h_1	1
C_2	h_1	1	$-\mathrm{h}_1$	-1	$-\mathrm{h}_1$	-1
σ_v	$-\mathrm{h}_1$	-1	$-\mathrm{h}_1$	-1	h_1	1
σ'_v	$-\mathrm{h}_1$	-1	h_1	1	$-\mathrm{h}_1$	-1

Figure 10. Reduced homomer sets for characterizing one-dimensional characters of $\boldsymbol{C}_{2v}$-group, A_1, B_1, and B_2.

$\mathcal{H}[\boldsymbol{C}_{2v}(/\boldsymbol{C}_s)]$ and $\mathcal{H}'[B_1]$, and between $\mathcal{H}[\boldsymbol{C}_{2v}(/\boldsymbol{C}'_s)]$ and $\mathcal{H}'[B_2]$ are represented by the following symbolic expressions:

$$A_2 = \boldsymbol{C}_{2v}(/\boldsymbol{C}_2) - \boldsymbol{C}_{2v}(/\boldsymbol{C}_{2v}), \tag{24}$$

$$B_1 = \boldsymbol{C}_{2v}(/\boldsymbol{C}_s) - \boldsymbol{C}_{2v}(/\boldsymbol{C}_{2v}), \tag{25}$$

$$B_2 = \boldsymbol{C}_{2v}\left(/\boldsymbol{C}'_s\right) - \boldsymbol{C}_{2v}(/\boldsymbol{C}_{2v}). \tag{26}$$

5.2. *Graphical generation of characters of $\boldsymbol{D}_{3h}$ and its subgroups*

This subsection deals with two-dimensional characters (or **Q**-conjugacy characters), which are generated by the graphical approach to the $\boldsymbol{D}_{3h}$- and $\boldsymbol{C}_{3h}$-groups. By thinking out appropriate regular bodies, their group–subgroup relationship is demonstrated graphically.

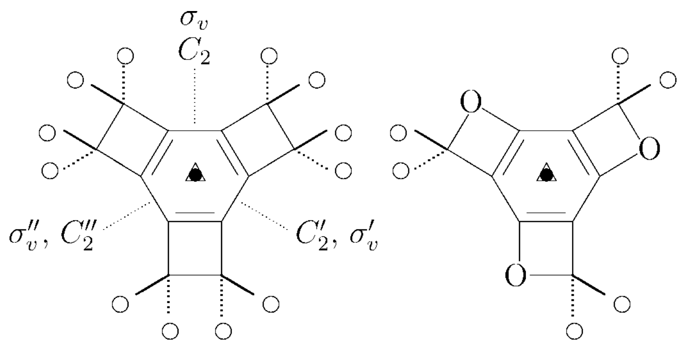
5.2.1. Two-dimensional character of $\boldsymbol{D}_{3h}$

Let us consider **24** (figure 11) as a regular body for $\boldsymbol{D}_{3h}$, where twelve open circles (white) represent substitution sites[16]. We obtain twelve symmetry operations of $\boldsymbol{D}_{3h}$ as follows:

$$\boldsymbol{D}_{3h} = \left\{I, C_3, C_3^2, C_2, C'_2, C''_2, \sigma_h, S_3, S_3^2, \sigma_v, \sigma'_v, \sigma''_v\right\}. \tag{27}$$

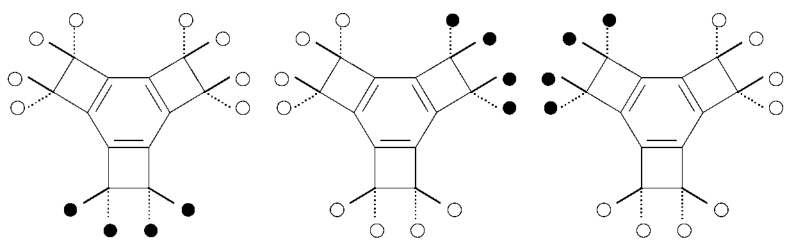
To describe the CR $\boldsymbol{D}_{3h}(/\boldsymbol{C}_{2v})$, we consider the homomer set shown in figure 12, where the four sites on either one of the cyclobutane rings are replaced by solid circles (black) to give **26**(h_1), **27**(h_2), or **28**(h_3). These homomers respectively belong to $\boldsymbol{C}_{2v} = \{I, C_2, \sigma_h, \sigma_v\}$, $\boldsymbol{C}''_{2v} = \{I, C''_2, \sigma_h, \sigma''_v\}$, and $\boldsymbol{C}'_{2v} = \{I, C'_2, \sigma_h, \sigma'_v\}$, which are conjugate to each other within the $\boldsymbol{D}_{3h}$-group.

[16] For the mark table and related data of $\boldsymbol{D}_{3h}$, see [31, appendices A–E].



24 ($\boldsymbol{D}_{3h}$) **25** ($\boldsymbol{C}_{3h}$)

Figure 11. Regular bodies for $\boldsymbol{D}_{3h}$ and $\boldsymbol{C}_{3h}$. Three two-fold axes and three mirror planes are depicted. The symbol ▲ represents a three-fold rotoreflection axis.



	26	**27**	**28**	$\mathcal{H}'[E']$
	h_1	h_2	h_3 $\equiv -(\mathrm{h}_1 + \mathrm{h}_2)$	$\{\mathrm{h}_1, \mathrm{h}_2\}$ character
I	h_1	h_2	h_3	2
$2C_3$	h_2	$\mathrm{h}_3(\equiv -(\mathrm{h}_1 + \mathrm{h}_2))$	h_1	-1
$3C_2$	h_1	$\mathrm{h}_3(\equiv -(\mathrm{h}_1 + \mathrm{h}_2))$	h_2	0
σ_h	h_1	h_2	h_3	2
$2S_3$	h_2	$\mathrm{h}_3(\equiv -(\mathrm{h}_1 + \mathrm{h}_2))$	h_1	-1
$3\sigma_v$	h_1	$\mathrm{h}_3(\equiv -(\mathrm{h}_1 + \mathrm{h}_2))$	h_2	0

Figure 12. Homomer set $\mathcal{H}[\boldsymbol{D}_{3h}(/\boldsymbol{C}_{2v})]$ for $\boldsymbol{D}_{3h}(/\boldsymbol{C}_{2v})$ and the reduced homomer set $\mathcal{H}'[E']$ for the character E'. The marks of $\mathcal{H}[\boldsymbol{D}_{3h}(/\boldsymbol{C}_{2v})]$ are omitted.

By a similar procedure for obtaining the two-dimensional character of the $\boldsymbol{C}_{3v}$-group (figure 3), we can write $\mathrm{h}_3 \equiv -(\mathrm{h}_1 + \mathrm{h}_2)$ for the homomer set $\mathcal{H}[\boldsymbol{C}_{3v}(/\boldsymbol{C}_s)] = \{\mathrm{h}_1, \mathrm{h}_2, \mathrm{h}_3\}$. Hence, we are able to use the corresponding reduced homomer set $\mathcal{H}'[E'] = \{\mathrm{h}_1, \mathrm{h}_2\}$, as shown in figure 12. Then we consider the action of the operations on $\mathcal{H}'[E']$. Obviously, the identity operation I and the reflection σ_h fix both h_1 and h_2 so that the corresponding character is determined to be equal to 2, as collected in the character column of figure 12. The operation C_3 converts h_1 into h_2 (fixing no homomers to contribute to a character by 0) and h_2 into h_3 ($\equiv -(\mathrm{h}_1 + \mathrm{h}_2)$, fixing $-\mathrm{h}_2$ to contribute to a character by -1) so that we can graphically obtain $0 + (-1) = -1$ as a character. The

Table 4
($\mathbf{Q}$-conjugacy) character table of $\boldsymbol{C}_{3h}$[a].

	I $\boldsymbol{C}_1$	σ_h $\boldsymbol{C}_s$	$2C_3$ $\boldsymbol{C}_3$	$2S_3$ $\boldsymbol{C}_{3h}$	Markaracter[b]
A'	1	1	1	1	$\boldsymbol{C}_{3h}(/\boldsymbol{C}_{3h})$
A''	1	-1	1	-1	$\boldsymbol{C}_{3h}(/\boldsymbol{C}_3) - \boldsymbol{C}_{3h}(/\boldsymbol{C}_{3h})$
E'	2	2	-1	-1	$\boldsymbol{C}_{3h}(/\boldsymbol{C}_s) - \boldsymbol{C}_{3h}(/\boldsymbol{C}_{3h})$
E''	2	-2	-1	1	$\boldsymbol{C}_{3h}(/\boldsymbol{C}_1) - \boldsymbol{C}_{3h}(/\boldsymbol{C}_s) - \boldsymbol{C}_{3h}(/\boldsymbol{C}_3) + \boldsymbol{C}_{3h}(/\boldsymbol{C}_{3h})$

[a] Strictly speaking, this table is a $\mathbf{Q}$-conjugacy character table. Thus, the symmetry operations are classified in terms of $\mathbf{Q}$-conjugacy. See [37]. In terms of the usual conjugacy, each operation belongs to a one-membered conjugacy class because the $\boldsymbol{C}_{3h}$-group is a cyclic group.

[b] This is equivalent to equations (34)–(37) described in [26], where the original $\boldsymbol{C}_6$-group is replaced by $\boldsymbol{C}_{3h}$ because of isomorphism.

same character can be obtained by the action of C_3^2 because of conjugacy. Although the exact behaviors are different, S_3 and S_3^2 give characters of the same value. It should be emphasized that the contribution of h_3 is implicitly taken into consideration by virtue of the relationship $\mathrm{h}_3 \equiv -(\mathrm{h}_1 + \mathrm{h}_2)$. The operation C_2 fixes the homomer h_1 but converts h_2 into h_3 ($\equiv -(\mathrm{h}_1 + \mathrm{h}_2)$, fixing $-\mathrm{h}_2$) so that we obtain $1 + (-1) = 0$ as a character. The action of the other two-fold rotations gives characters of the same value. Although the exact behaviors are different, the three dihedral mirrors give characters of the value 0. The results are summarized in the character column of figure 12. The relationships between $\mathcal{H}[\boldsymbol{D}_{3h}(/\boldsymbol{C}_{2v})]$ and $\mathcal{H}'[E']$ is represented by the following symbolic expression:

$$E' = \boldsymbol{D}_{3h}(/\boldsymbol{C}_{2v}) - \boldsymbol{D}_{2h}(/\boldsymbol{D}_{2h}). \tag{28}$$

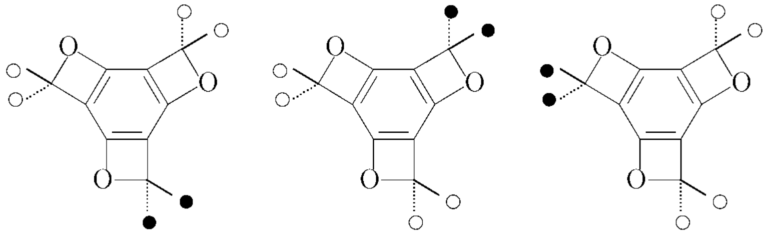
5.2.2. Two-dimensional character of $\boldsymbol{C}_{3h}$

Since the point group $\boldsymbol{C}_{3h}$ is cyclic, it has characters of imaginary units. Hence, we should use $\mathbf{Q}$-conjugacy characters to conceal such imaginary units [37]. Fujita has shown the $\mathbf{Q}$-conjugacy character table of $\boldsymbol{C}_{3h}$ [26], which is cited as table 4. The goal of this section is to obtain a two-dimensional character E' by means of the graphical approach.

A regular body of $\boldsymbol{C}_{3h}$ (**25**) can be obtained by replacing the three cyclobutane rings of **24** with three oxetane rings, as shown in figure 11. This process corresponds to the selection of six symmetry operations from $\boldsymbol{D}_{3h}$ as follows:

$$\boldsymbol{C}_{3h} = \{I, C_3, C_3^2, \sigma_h, S_3, S_3^2\}, \tag{29}$$

where the original three two-fold rotations and three vertical reflections are deleted from the right-hand side of equation (27). Then, we consider the homomer set shown in figure 13 to describe the CR $\boldsymbol{C}_{3h}(/\boldsymbol{C}_s)$. Note that the two sites on either one of the oxetane rings are replaced by solid circles (black) to give **29**(h_1), **30**(h_2), or **31**(h_3). These homomers belong to $\boldsymbol{C}_s = \{I, \sigma_h\}$. Since we have selected such a regular body (**25**) as related closely to **24**, their graphical behaviors can be easily compared.



	29	**30**	**31**	$\mathcal{H}'[E']$
	h_1	h_2	h_3 $\equiv -(\mathrm{h}_1 + \mathrm{h}_2)$	$\{\mathrm{h}_1, \mathrm{h}_2\}$ character[a]
I	h_1	h_2	h_3	2
C_3	h_2	$\mathrm{h}_3(\equiv -(\mathrm{h}_1 + \mathrm{h}_2))$	h_1	-1
C_3^2	$\mathrm{h}_3(\equiv -(\mathrm{h}_1 + \mathrm{h}_2))$	h_1	h_2	-1
σ_h	h_1	h_2	h_3	2
S_3	h_2	$\mathrm{h}_3(\equiv -(\mathrm{h}_1 + \mathrm{h}_2))$	h_1	-1
S_3^2	$\mathrm{h}_3(\equiv -(\mathrm{h}_1 + \mathrm{h}_2))$	h_1	h_2	-1

[a] Strictly speaking, this column is concerned with **Q**-conjugacy characters, since the E' of $\boldsymbol{C}_{3h}$ is further reduced into one-dimensional characters containing imaginary units.

Figure 13. Homomer set for $\boldsymbol{C}_{3h}(/\boldsymbol{C}_s)$ and the reduced homomer set for the character E'. The marks of $\mathcal{H}[\boldsymbol{C}_{3h}(/\boldsymbol{C}_s)]$ are omitted.

When a similar procedure for obtaining the two-dimensional character of the $\boldsymbol{C}_{3v}$-group (figure 3) is applied to this case, we can also write $\mathrm{h}_3 \equiv -(\mathrm{h}_1 + \mathrm{h}_2)$ for the homomer set $\mathcal{H}[\boldsymbol{C}_{3h}(/\boldsymbol{C}_s)] = \{\mathrm{h}_1, \mathrm{h}_2, \mathrm{h}_3\}$. Thereby, we are able to use the corresponding reduced homomer set $\mathcal{H}'[E'] = \{\mathrm{h}_1, \mathrm{h}_2\}$, as shown in figure 13. Then we consider the action of the operations on $\mathcal{H}'[E']$. The identity operation I and the reflection σ_h fix both h_1 and h_2 so that the corresponding character is determined to be equal to 2, as collected in the character column of figure 13. The operation C_3 converts h_1 into h_2 (fixing no homomers to contribute to a character by 0) and h_2 into h_3 ($\equiv -(\mathrm{h}_1 + \mathrm{h}_2)$, fixing $-\mathrm{h}_2$ to contribute to a character by -1) so that we can graphically obtain $0 + (-1) = -1$ as a character. The same character can be obtained by the action of C_3^2 because of **Q**-conjugacy (not because of conjugacy in this case). The **Q**-conjugate operations S_3 and S_3^2 give characters of the same value, although the exact behaviors are different. It should be again emphasized that the contribution of h_3 is implicitly taken into consideration by virtue of the relationship $\mathrm{h}_3 \equiv -(\mathrm{h}_1 + \mathrm{h}_2)$.

It is to be noted that the present graphical approach is not effective to more complicated cases such as the character E'' of $\boldsymbol{C}_{3h}$ (table 4). These cases will be the subject of future studies.

6. Remarks

Marks/markaracters vs. characters/$\boldsymbol{Q}$-conjugacy characters. In the graphical method of generating marks in a previous paper of this series [39], we have taken account of the action of $\boldsymbol{G}$ on a homomer set:

$$\mathcal{H}\big[\boldsymbol{G}(/\boldsymbol{G}_i)\big] = \big\{\mathrm{h}_1, \ldots, \mathrm{h}_{d-1}, \mathrm{h}_d\big\}, \tag{30}$$

where we place $d = |\boldsymbol{G}|/|\boldsymbol{G}_i|$. The action of $\boldsymbol{G}$ is regarded as a set of actions itemized with respect to conjugate subgroups so that marks as invariants are itemized with such conjugate subgroups. On the other hand, the action of $\boldsymbol{G}$ described in the present paper is conceptually changed to be concerned with respective symmetry operations of $\boldsymbol{G}$, where markaracters as invariants are summarized in terms of cyclic subgroups or equivalently in terms of **Q**-conjugacy. As for mark tables, this change of conceptual viewpoints results in the selection of columns for cyclic subgroups and the deletion of columns for non-cyclic subgroups so as to give the corresponding markaracter tables [24]. If no other subgroups are present between $\boldsymbol{G}$ and $\boldsymbol{G}_i$, the resulting markaracter can be converted to a **Q**-conjugacy character (Γ) according to the following equation:

$$\Gamma = \boldsymbol{G}(/\boldsymbol{G}_i) - \boldsymbol{G}(/\boldsymbol{G}), \tag{31}$$

where we have

$$\boldsymbol{G}(/\boldsymbol{G}) = (\underbrace{1, 1, \ldots, 1}_{d=|\boldsymbol{G}|/|\boldsymbol{G}_i|}). \tag{32}$$

It follows that markaracters and **Q**-conjugacy characters can be equalized to each other, though their origins are distinct. Note that such **Q**-conjugacy irreducible characters are orthogonal to each other but are not always normal. Compare this with the fact that irreducible characters are orthnormal in general.

The graphical approach described in this paper is based on equation (31). Hence, the resulting Γ is a **Q**-conjugacy characters but not a usual character, although they are identical with each other in matured cases [28].

Proof of the semi-graphical method. Let us consider the corresponding reduced homomer set:

$$\mathcal{H}'[\Gamma] = \{\mathrm{h}_1, \ldots, \mathrm{h}_{d-1}\}, \tag{33}$$

where we place $\mathrm{h}_d \equiv -(\mathrm{h}_1 + \cdots + \mathrm{h}_{d-1})$. When the action of a symmetry operation of $\boldsymbol{G}$ on h_i ($\in \mathcal{H}'[\Gamma]$) produces h_j ($\in \mathcal{H}'[\Gamma]$), the contribution to Γ can be evaluated to be $\chi_i = 0$ if $\mathrm{h}_i \neq \mathrm{h}_j$ and to be $\chi_i = 1$ if $\mathrm{h}_i = \mathrm{h}_j$.

1. If the action on any h_i ($\in \mathcal{H}'[\Gamma]$) does not produce h_d ($\notin \mathcal{H}'[\Gamma]$), the corresponding Γ is represented by $\sum_{i=1}^{d-1} \chi_i$, since the contribution of h_d ($\notin \mathcal{H}'[\Gamma]$) is always ommitted to result in the spontaneous subtraction by 1.
2. If the action on h_k ($\in \mathcal{H}'[\Gamma]$) produces h_d ($\notin \mathcal{H}'[\Gamma]$), the contribution of $\mathrm{h}_k \to \mathrm{h}_d$ should be evaluated to be $\chi_k = -1$ in order to satisfy equation (31). Note that h_d ($\notin \mathcal{H}'[\Gamma]$) have no contribution, because it is converted into either homomer of $\mathcal{H}'[\Gamma]$. Since the action on a homomer h_i ($\in \mathcal{H}'[\Gamma]$) of other than h_k can be evaluated as above, the corresponding Γ is represented by $\sum_{i=1(i\neq k)}^{d-1} \chi_i + \chi_k$, where we have $\chi_i = 0$ or 1 and $\chi_k = -1$.

Since this procedure requires equation (31) in the step of evaluating $\chi_k = -1$, it serves as a proof of the semi-graphical method described above.

Proof of the graphical method. In the above proof, we have not used the condition $\mathrm{h}_d \equiv -(\mathrm{h}_1 + \cdots + \mathrm{h}_{d-1})$, which is based on the concept of negative graphs. This condition provides us with a reason why we have placed $\chi_k = -1$ if the action on h_k ($\in \mathcal{H}'[\Gamma]$) has produced h_d ($\notin \mathcal{H}'[\Gamma]$).

When the action of a symmetry operation of $\boldsymbol{G}$ on h_i ($\in \mathcal{H}'[\Gamma]$), the same symmetry operation acts on $(\mathrm{h}_1 + \cdots + \mathrm{h}_{d-1})$ ($\equiv -\mathrm{h}_d$). Suppose that an operation g ($\in \boldsymbol{G}$) acts on h_d ($\notin \mathcal{H}'[\Gamma]$), i.e., $g : \mathrm{h}_d \to \mathrm{h}_k$. Then, we have $\mathrm{h}_d \in \mathcal{H}'[\Gamma]$ and $\mathrm{h}_k \notin \mathcal{H}'[\Gamma]$. It follows that we have the action of g on $(\mathrm{h}_1 + \cdots + \mathrm{h}_{d-1})$ as follows:

$$g : (\mathrm{h}_1 + \cdots + \mathrm{h}_{d-1}) \;\to\; (\mathrm{h}_1 + \cdots + \mathrm{h}_{d-1}) + \mathrm{h}_d - \mathrm{h}_k = -\mathrm{h}_k. \tag{34}$$

Hence, $-(\mathrm{h}_1 + \cdots + \mathrm{h}_{d-1})$ behaves in the same manner as h_d on the action of $\boldsymbol{G}$. This means that we can use the reduced homomer set $\mathcal{H}'[\Gamma] = \{\mathrm{h}_1, \ldots, \mathrm{h}_{d-1}\}$ in place of the original homomer set $\mathcal{H}[\boldsymbol{G}(/\boldsymbol{G}_i)] = \{\mathrm{h}_1, \ldots, \mathrm{h}_{d-1}, \mathrm{h}_d\}$. For example, the data collected in figure 3 exemplify equation (34) as follows:

	6	**4 + 5**	
	h_3	$\mathrm{h}_1 + \mathrm{h}_2$	$(= -\mathrm{h}_3)$
I	h_3	$\mathrm{h}_1 + \mathrm{h}_2$	$(= -\mathrm{h}_3)$
C_3	h_1	$\mathrm{h}_2 + \mathrm{h}_3$	$(= -\mathrm{h}_1)$
C_3^2	h_2	$\mathrm{h}_3 + \mathrm{h}_1$	$(= -\mathrm{h}_2)$
σ_v	h_2	$\mathrm{h}_1 + \mathrm{h}_3$	$(= -\mathrm{h}_2)$
σ_v'	h_1	$\mathrm{h}_3 + \mathrm{h}_2$	$(= -\mathrm{h}_1)$
σ_v''	h_3	$\mathrm{h}_2 + \mathrm{h}_1$	$(= -\mathrm{h}_3)$

(35)

If the action on h_k ($\in \mathcal{H}'[\Gamma]$) produces h_d ($\notin \mathcal{H}'[\Gamma]$), the contribution of $\mathrm{h}_k \to \mathrm{h}_d = -(\mathrm{h}_1 + \cdots + \mathrm{h}_k + \cdots + \mathrm{h}_{d-1})$ is evaluated to be $\chi_k = -1$, because h_k is fixed. This is identical with the criterion for the semi-graphical method and hence the remaining part of the proof is also valid for the graphical method.

7. Conclusion

By starting from a regular body of a group $\boldsymbol{G}$, we have generated graphs that belong to its subgroup $\boldsymbol{G}_i$ and are homomeric (or enantiomeric) to each other. The resulting homomer set denoted by $\mathcal{H}[\boldsymbol{G}(/\boldsymbol{G}_i)] = \{\mathrm{h}_1, \ldots, \mathrm{h}_{d-1}, \mathrm{h}_d\}$ has been determined to be governed by the coset representation $\boldsymbol{G}(/\boldsymbol{G}_i)$, where $d = |\boldsymbol{G}|/|\boldsymbol{G}_i|$. To develop a graphical method of generating characters of the $\boldsymbol{G}$-group, the concept of *negative graph* has been proposed. Thereby, the homomer set $\mathcal{H}[\boldsymbol{G}(/\boldsymbol{G}_i)]$ has been reduced into the reduced homomer set $\mathcal{H}'[\Gamma] = \{\mathrm{h}_1, \ldots, \mathrm{h}_{d-1}\}$, where we have placed $\mathrm{h}_d \equiv -(\mathrm{h}_1 + \cdots + \mathrm{h}_{d-1})$. The graphical generation of one- and (some) two-dimensional characters (Γ) of the $\boldsymbol{G}$-group has been studied on the basis of the reduced homomer set $\mathcal{H}'[\Gamma]$ in the cases of $d = |\boldsymbol{G}|/|\boldsymbol{G}_i| = 2$ and 3. It has been compared with an algebraic generation using marks (or markaracters), i.e., $\Gamma = \boldsymbol{G}(/\boldsymbol{G}_i) - \boldsymbol{G}(/\boldsymbol{G})$. The versatility of the graphical generation has been demonstrated by using $\boldsymbol{C}_{3v}$, $\boldsymbol{D}_{2h}$, $\boldsymbol{C}_{2h}$, $\boldsymbol{C}_{2v}$, $\boldsymbol{D}_{3h}$, and $\boldsymbol{C}_{3h}$ as examples.

References

[1] G. Pólya, Compt. Rend. 201 (1935) 1167–1169.
[2] G. Pólya, Helv. Chim. Acta 19 (1936) 22–24.
[3] G. Pólya, Z. Kristal. (A) 93 (1936) 415–443.
[4] G. Pólya, Acta Math. 68 (1937) 145–254.
[5] N.G. de Bruijn, Indag. Math. 21 (1959) 59–69.
[6] D.H. Rouvray, Chem. Soc. Rev. 3 (1974) 355–372.
[7] F. Harary, E.M. Palmer, R.W. Robinson and R.C. Read, in: *Chemical Aplications of Graph Theory*, ed. A.T. Balaban (Academic Press, London, 1976) pp. 11–24.
[8] K. Balasubramanian, Chem. Rev. 85 (1985) 599–618.
[9] A.T. Balaban (ed.), *Chemical Applications of Graph Theory* (Academic Press, London, 1976).
[10] G. Pólya, R.E. Tarjan and D.R. Woods, *Notes on Introductory Combinatorics* (Birkhäuser, Boston, MA, 1983).
[11] G. Pólya and R.C. Read, *Combinatorial Enumeration of Groups, Graphs, and Chemical Compounds* (Springer, New York, 1987).
[12] H. Eyring, J. Walter and G.E. Kimball, *Quantum Chemistry* (Wiley, New York–London, 1944).
[13] B.S. Tsukerblat, *Group Theory in Chemistry and Spectroscopy* (Academic Press, New York, 1994).
[14] I. Hargittai and H. Hargittai, *Symmetry through the Eyes of a Chemist* (VCH, Weinheim, 1986).
[15] F.A. Cotton, *Chemical Applications of Group Theory* (Wiley International, New York, 1971).
[16] H.H. Jaffé and M. Orchin, *Symmetry in Chemistry* (Wiley, Chichester, 1965).
[17] L.H. Hall, *Group Theory and Symmetry in Chemistry* (McGraw-Hill, New York, 1969).
[18] D.M. Bishop, *Group Theory and Chemistry* (Clarendon, Oxford, 1973).
[19] S.F.A. Kettle, *Symmetry and Structure* (Wiley, Chichester, 1985).
[20] M.F.C. Ladd, *Symmetry in Molecules and Crystals* (Ellis Horwood, Chichester, 1989).
[21] D.C. Harris and M.D. Bertolucci, *Symmetry and Spectroscopy* (Dover, New York, 1989).
[22] S. Fujita, J. Math. Chem. 30 (2002) 249–270.
[23] S. Fujita, J. Math. Chem. 5 (1990) 99–120.
[24] S. Fujita, Theor. Chem. Acta 91 (1995) 291–314.
[25] S. Fujita, Theor. Chem. Acta 91 (1995) 315–332.
[26] S. Fujita, Bull. Chem. Soc. Jpn. 71 (1998) 1587–1596.
[27] S. Fujita, Bull. Chem. Soc. Jpn. 71 (1998) 2071–2080.
[28] S. Fujita, Bull. Chem. Soc. Jpn. 71 (1998) 2309–2321.
[29] S. Fujita, Theor. Chem. Acc. 99 (1998) 404–410.
[30] S. Fujita, Theor. Chem. Acc. 101 (1999) 409–420.
[31] S. Fujita, *Symmetry and Combinatorial Enumeration in Chemistry* (Springer, Berlin, 1991).
[32] A. Kerber, *Applied Finite Group Actions*, 2nd ed. (Springer, Berlin, 1999).
[33] W. Burnside, *Theory of Groups of Finite Order*, 2nd ed. (Cambridge University Press, Cambridge, 1911).
[34] S. El-Basil, *Combinatorial Organic Chemistry: An Educational Approach* (Nova Science, New York, 1999).
[35] S. Fujita, Theor. Chim. Acta 78 (1990) 45–63.

[36] S. Fujita, Bull. Chem. Soc. Jpn. 72 (1999) 2403–2407.
[37] S. Fujita, Theor. Chem. Acc. 99 (1998) 224–230.
[38] S. Fujita, Tetrahedron 46 (1990) 365–382.
[39] S. Fujita and S. El-Basil, MATCH 46 (2002) 121–135.