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Regular Representations and Coset Representations Combined with a Mirror-Permutation. Concordant Construction of the Mark Table and the USCI-CF Table of the Point Group $\boldsymbol{T}_d$

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Abstract

A combined-permutation representation (CPR) of degree 26 (= 24 + 2) for a regular representation (RR) of degree 24 is derived algebraically from a multiplication table of the point group $\boldsymbol{T}_d$, where reflections are explicitly considered in the form of a mirror-permutation of degree 2. Thereby, the standard mark table and the standard USCI-CF table (unit-subduced-cycle-index-with-chirality-fittingness table) are concordantly generated by using the GAP functions `MarkTableforUSCI` and `constructUSCITable`, which have been developed by Fujita for the purpose of systematizing the concordant construction. A CPR for each coset representation (CR) $(\boldsymbol{G}_i \backslash)\boldsymbol{T}_d$ is obtained algebraically by means of the GAP function `CosetRepCF` developed by Fujita (Appendix A). On the other hand, CPRs for CRs are obtained geometrically as permutation groups by considering appropriate skeletons, where the point group $\boldsymbol{T}_d$ acts on an orbit of $|\boldsymbol{T}_d|/|\boldsymbol{G}_i|$ positions to be equivalent in a given skeleton so as to generate the CPR of degree $|\boldsymbol{T}_d|/|\boldsymbol{G}_i|$. An RR as a CPR is obtained by considering a regular body (RB), the $|\boldsymbol{T}_d|$ positions of which are considered to be governed by RR $(\boldsymbol{C}_1\backslash)\boldsymbol{T}_d$. These geometrically derived CPRs as groups are compared with the corresponding CPRs obtained algebraically.

1 Introduction

Regular bodies (RBs) as geometric entities for characterizing point groups [1] have been discussed in connection with *regular representations* (RRs) as algebraic entities in Section 6.4 of Ref. [2], where multiplication tables of the point groups were used as essential clues. By staring from RBs and RRs, orbits of given skeletons have been shown to be governed by coset representations (CRs), where the former geometric entities due to point groups are correlated to the latter algebraic entities due to permutation representations (PRs) [3, 4]. So long as we obey the conventional way of the group theory, however, PRs as they are have not taken chirality/achirality into explicit consideration. This means that CRs as PRs as they are have been incapable of treating 3D structures with chirality/achirality. To treat 3D structures, the author (Fujita) has proposed the concepts of *sphericity* and of *chirality fittingness* (CF), which control an orbit governed by a CR [5]. Thus, each orbit is categorized into a homospheric orbit, an enantiospheric orbit, or a hemispheric orbit by examining the global and local symmetries of the corresponding CR. The sphericity of such an orbit determines the capability of accommodating chiral or achiral ligands, where the mode of accommodation is referred to in terms of CF. Thereby, *unit subduced cycle indices with chirality fittingness* (USCI-CFs) are introduced to enumerate 3D structures in symmetry-itemized fashion under the name *the USCI approach* by Fujita [3].

To treat chirality/achirality more systematically by computer, the author (Fujita) has proposed *combined permutation representations* (CPRs), where respective PRs are combined with a mirror-permutation which differentiates between a rotation and a reflection [6–8]. The CPRs are found to be useful to generate mark tables of permutation groups [9] under the GAP (Groups, Algorithms, Programming) system, which has been available freely [10]. The remaining task is to examine the above-mentioned RBs and RRs from the viewpoint of CPRs under the GAP system. This paper deals mainly with the point group $\boldsymbol{T}_d$, where we start from the multiplication table of $\boldsymbol{T}_d$ as an essential clue.

2 Backgrounds

The practices of Fujita's USCI approach [3] has been originally based on computer-manipulation under the FORTRAN77 programming language. For example, the point group $\boldsymbol{T}_d$ having 24 symmetry operations:

$$\boldsymbol{T}_d = \{ \underbrace{I}_{1}, \underbrace{C_{2(1)}}_{2}, \underbrace{C_{2(2)}}_{3}, \underbrace{C_{2(3)}}_{4}, \underbrace{C_{3(1)}}_{5}, \underbrace{C_{3(3)}}_{6}, \underbrace{C_{3(2)}}_{7}, \underbrace{C_{3(4)}}_{8}, \underbrace{C^2_{3(1)}}_{9}, \underbrace{C^2_{3(4)}}_{11}, \underbrace{C^2_{3(3)}}_{11}, \underbrace{C^2_{3(2)}}_{12},$$
$$\underbrace{\sigma_{d(1)}}_{13}, \underbrace{S_{4(3)}}_{14}, \underbrace{S^3_{4(3)}}_{15}, \underbrace{\sigma_{d(6)}}_{16}, \underbrace{\sigma_{d(2)}}_{17}, \underbrace{\sigma_{d(4)}}_{18}, \underbrace{S_{4(1)}}_{19}, \underbrace{S^3_{4(1)}}_{20}, \underbrace{\sigma_{d(3)}}_{21}, \underbrace{S^3_{4(2)}}_{22}, \underbrace{\sigma_{d(5)}}_{23}, \underbrace{S_{4(2)}}_{24}, \} \tag{1}$$

is treated in the form of a multiplication table, which is a 24×24 matrix. The horizontal direction contains respective first operations m_j ($j = 1, 2, \ldots, 24$ for Eq. 1), the vertical direction contains respective second operations m_i ($i = 1, 2, \ldots, 24$ for Eq. 1), and the intersection between the j-th column and the i-th row indicates the result of multiplication $m_j m_i$.

Algebraically speaking, the point group $\boldsymbol{T}_d$ is defined by the multiplication table concerning the symmetry operations collected in Eq. 1. To specify the action of such point group as $\boldsymbol{T}_d$ on substitution positions of a given skeleton, a CR is calculated by starting from the multiplication table. As an extreme case of a CR, a skeleton having 24 equivalent positions is called an RB, which is governed by an RR based on the multiplication table itself.

Because the sequence of symmetry operations can be changed freely, there are 24! multiplication tables different but equivalent to each other under the point group $\boldsymbol{T}_d$. In the present article, the multiplication table corresponding to Eq. 1 is adopted as a standard by considering a coset decomposition of $\boldsymbol{T}_d$ by $\boldsymbol{D}_2$ $(= \{\underbrace{I}_{1}, \underbrace{C_{2(1)}}_{2}, \underbrace{C_{2(2)}}_{3}, \underbrace{C_{2(3)}}_{4}\})$:

$$\boldsymbol{T}_d = \boldsymbol{D}_2 + \boldsymbol{D}_2 C_{3(1)} + \boldsymbol{D}_2 C^2_{3(1)} + \boldsymbol{D}_2 \sigma_{d(1)} + \boldsymbol{D}_2 \sigma_{d(2)} + \boldsymbol{D}_2 \sigma_{d(3)} \tag{2}$$

This selection is tentative but does not lose generality.

An orbit of equivalent positions in a given skeleton is governed by a CR $(\boldsymbol{G}_i \backslash) \boldsymbol{T}_d$, where the subgroup $\boldsymbol{G}_i$ is selected from a non-redundant set of subgroups $\mathrm{SSG}_{\boldsymbol{T}_d}$:

$$\mathrm{SSG}_{\boldsymbol{T}_d} = \{ \underbrace{\boldsymbol{C}_1}_{1}, \underbrace{\boldsymbol{C}_2}_{2}, \underbrace{\boldsymbol{C}_s}_{3}, \underbrace{\boldsymbol{C}_3}_{4}, \underbrace{\boldsymbol{S}_4}_{5}, \underbrace{\boldsymbol{D}_2}_{6}, \underbrace{\boldsymbol{C}_{2v}}_{7}, \underbrace{\boldsymbol{C}_{3v}}_{8}, \underbrace{\boldsymbol{D}_{2d}}_{9}, \underbrace{\boldsymbol{T}}_{10}, \underbrace{\boldsymbol{T}_d}_{11} \} \tag{3}$$

where the alignment of subgroups are according to the orders of subgroups (cf. Example 6.4 of Ref. [3] and Eq. 1.3 (page 10) of Ref. [4]). For subgroups of the same size e.g., $\boldsymbol{S}_4$, $\boldsymbol{D}_2$, and $\boldsymbol{C}_{2v}$ (order 4), a cyclic subgroup (e.g., $\boldsymbol{S}_4$) is placed to have a younger sequence, and then, a subgroup with proper rotations only (e.g., $\boldsymbol{D}_2$) is placed to have a younger sequence.

Such coset representations (CRs) are calculated by considering coset decompositions, which are derived from the multiplication table. Note that an RR can be regarded as a CR by a trivial subgroup $\boldsymbol{C}_1$ $(= \{I\})$, i.e., $(\boldsymbol{C}_1\backslash)\boldsymbol{T}_d$. The concept of *subduction of coset representations* $(\boldsymbol{G}_i\backslash)\boldsymbol{T}_d \downarrow \boldsymbol{G}_j$ proposed by the author (cf. Theorem 9.1 of [3]) is essential to derive USCI-CFs, which are keys for conducting symmetry-itemized enumeration of 3D structures [3]. The calculation of $(\boldsymbol{G}_i\backslash)\boldsymbol{T}_d \downarrow \boldsymbol{G}_j$ is based on a mark table of $\boldsymbol{T}_d$, which collects fixed-point vectors (FPVs) in the form of row vectors concerning the subgroups of the SSG (Eq. 3). The results of $(\boldsymbol{G}_i\backslash)\boldsymbol{T}_d \downarrow \boldsymbol{G}_j$ are used to construct the corresponding USCI-CF table.

Because a mark table (cf. Table 2 of Ref. [11]) and a USCI-CF table (cf. Table 5 of the Ref. [11]) depends on the selected SSG (Eq. 3), they are called a standard mark table and a standard USCI-CF table.

Note that the concept of mark tables (tables of marks) has been originally proposed by Burnside [12] and applied to symmetry-itemized enumeration of chemical structures [13, 14]. On the other hand, the concept of USCI-CF table has been proposed by the author (Fujita) [3] and applied to symmetry-itemized enumeration of chemical structures as 3D objects [3].

3 Multiplication Tables into Regular Representations Combined with a Mirror Permutation

The multiplication table of $\boldsymbol{T}_d$ contains the multiplication result $m_j m_i$ at the intersection between j-th column and i-th row, where m_j $(j = 1, 2, \ldots 24)$ in the horizontal direction represents the first operation and m_i $(i = 1, 2, \ldots 24)$ in the vertical direction represents the second operation. If the serial numbers under respective operations in Eq. 1 are used for the sake of simplicity, the multiplication table is represented by the following `List` format (`[...]`) of the GAP system:

```
gap> m1 := PermList([ 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]);; # I
gap> m2 := PermList([ 2, 1, 4, 3, 8, 7, 6, 5,11,12, 9,10,15,16,13,14,18,17,20,19,24,23,22,21]);; #C2(1)
gap> m3 := PermList([ 3, 4, 1, 2, 6, 5, 8, 7,12,11,10, 9,14,13,16,15,20,19,18,17,23,24,21,22]);; #C2(2)
gap> m4 := PermList([ 4, 3, 2, 1, 7, 8, 5, 6,10, 9,12,11,16,15,14,13,19,20,17,18,22,21,24,23]);; #C2(3)
gap> m5 := PermList([ 5, 6, 7, 8, 9,10,11,12, 1, 2, 3, 4,21,22,23,24,13,14,15,16,17,18,19,20]);; #C3(1)
gap> m6 := PermList([ 6, 5, 8, 7,12,11,10, 9, 3, 4, 1, 2,23,24,21,22,14,13,16,15,20,19,18,17]);; #C3(3)
gap> m7 := PermList([ 7, 8, 5, 6,10, 9,12,11, 4, 3, 2, 1,22,21,24,23,16,15,14,13,19,20,17,18]);; #C3(2)
gap> m8 := PermList([ 8, 7, 6, 5,11,12, 9,10, 2, 1, 4, 3,24,23,22,21,15,16,13,14,18,17,20,19]);; #C3(4)
gap> m9 := PermList([ 9,10,11,12, 1, 2, 3, 4, 5, 6, 7, 8,17,18,19,20,21,22,23,24,13,14,15,16]);; #C3(1)^2
gap> m10 := PermList([10, 9,12,11, 4, 3, 2, 1, 7, 8, 5, 6,19,20,17,18,22,21,24,23,16,15,14,13]);; #C3(4)^2
gap> m11 := PermList([11,12, 9,10, 2, 1, 4, 3, 8, 7, 6, 5,18,17,20,19,24,23,22,21,15,16,13,14]);; #C3(3)^2
gap> m12 := PermList([12,11,10, 9, 3, 4, 1, 2, 6, 5, 8, 7,20,19,18,17,23,24,21,22,14,13,16,15]);; #C3(2)^2
gap> m13 := PermList([13,14,15,16,17,18,19,20,21,22,23,24, 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12]);; #sd(1)
```

```
gap> m14 := PermList([14,13,16,15,20,19,18,17,23,24,21,22, 3, 4, 1, 2, 6, 5, 8, 7,12,11,10, 9]);; #S4(3)
gap> m15 := PermList([15,16,13,14,18,17,20,19,24,23,22,21, 2, 1, 4, 3, 8, 7, 6, 5,11,12, 9,10]);; #S4(3)^3
gap> m16 := PermList([16,15,14,13,19,20,17,18,22,21,24,23, 4, 3, 2, 1, 7, 8, 5, 6,10, 9,12,11]);; #sd(6)
gap> m17 := PermList([17,18,19,20,21,22,23,24,13,14,15,16, 9,10,11,12, 1, 2, 3, 4, 5, 6, 7, 8]);; #sd(2)
gap> m18 := PermList([18,17,20,19,24,23,22,21,15,16,13,14,11,12, 9,10, 2, 1, 4, 3, 8, 7, 6, 5]);; #sd(4)
gap> m19 := PermList([19,20,17,18,22,21,24,23,16,15,14,13,10, 9,12,11, 4, 3, 2, 1, 7, 8, 5, 6]);; #S4(1)
gap> m20 := PermList([20,19,18,17,23,24,21,22,14,13,16,15,12,11,10, 9, 3, 4, 1, 2, 6, 5, 8, 7]);; #S4(1)^3
gap> m21 := PermList([21,22,23,24,13,14,15,16,17,18,19,20, 5, 6, 7, 8, 9,10,11,12, 1, 2, 3, 4]);; #sd(3)
gap> m22 := PermList([22,21,24,23,16,15,14,13,19,20,17,18, 7, 8, 5, 6,10, 9,12,11, 4, 3, 2, 1]);; #S4(2)^3
gap> m23 := PermList([23,24,21,22,14,13,16,15,20,19,18,17, 6, 5, 8, 7,12,11,10, 9, 3, 4, 1, 2]);; #sd(5)
gap> m24 := PermList([24,23,22,21,15,16,13,14,18,17,20,19, 8, 7, 6, 5,11,12, 9,10, 2, 1, 4, 3]);; #S4(2)
```

For example, if we obey the GAP system, we obtain the following multiplication results:

$$\underbrace{C_{3(1)}}_{5}\underbrace{\sigma_{d(1)}}_{13} = \underbrace{\sigma_{d(2)}}_{17} \tag{4}$$

$$\underbrace{\sigma_{d(1)}}_{13}\underbrace{C_{3(1)}}_{5} = \underbrace{\sigma_{d(3)}}_{21} \tag{5}$$

where $\underbrace{C_{3(1)}}_{5}$ (the first operation in the horizontal direction) multiplied by $\underbrace{\sigma_{d(1)}}_{13}$ (the second operation in the vertical direction) generates $\underbrace{\sigma_{d(2)}}_{17}$ (Eq. 4), while $\underbrace{\sigma_{d(1)}}_{13}$ (the first operation) multiplied by $\underbrace{C_{3(1)}}_{5}$ (the second operation) generates $\underbrace{\sigma_{d(3)}}_{21}$ (Eq. 5).

The first row of the multiplication table can be regarded as the coset decomposition by $\boldsymbol{C}_1$ $(= \{I\})$, where each column corresponds to a trivial coset $\boldsymbol{C}_1 m_j$ $(= \{m_j\})$. As a result, the i-th row (`List`) is a collection of $\boldsymbol{C}_1 m_j m_i$ $(= m_j m_i)$ for $j = 1, 2, \ldots, 24$, i.e.,

$$[\boldsymbol{C}_1 m_1 m_i, \boldsymbol{C}_1 m_2 m_i, \ldots, \boldsymbol{C}_1 m_{24} m_i] = [m_1 m_i, m_2 m_i, \ldots, m_{24} m_i], \tag{6}$$

which can be regarded as the m_i-value of a regular representation $(\boldsymbol{C}_1\backslash)\boldsymbol{T}_d$. Note that the GAP function `PermList` converts each `List` format (`[...]`) into the corresponding permutation (`m1` to `m24`). According to the resulting regular representation, Eqs. 4 and 5 are confirmed by using the GAP system:

```
gap> Display(m5 * m13 = m17);
true
gap> Display(m13 * m5 = m21);
true
```

The regular representation shown above ($(\boldsymbol{C}_1\backslash)\boldsymbol{T}_d = \{\mathtt{m1}, \mathtt{m2}, \cdots, \mathtt{m24}\}$) does not taken chirality/achirality into explicit consideration. The combined-permutation representation (CPR) [6–8] is defined by adding a 2-cycle `(25,26)` as a mirror-permutation representation to each reflection (`m13` to `m24`) contained in the RR $(\boldsymbol{C}_1\backslash)\boldsymbol{T}_d$. Thus, a set of generators `gen_Td_multable_CF` is produced to give the corresponding CPR `RR_Td_CF`, which is isomorphic to the point group $\boldsymbol{T}_d$ of order 24. Note that a pair of 1-cycles `(25)(26)` is attached to each rotation (`m1` to `m12`), but it is omitted according to the convention of the GAP system. The resulting CPR `RR_Td_CF` as a permutation group of order 24 is represented by a simplified set of four generators as follows:

```
gap> gen_Td_multable_CF :=
> [m1,m2,m3,m4,m5,m6,m7,m8,m9,m10,m11,m12,
> m13*(25,26),m14*(25,26),m15*(25,26),m16*(25,26),m17*(25,26),
> m18*(25,26),m19*(25,26),m20*(25,26),m21*(25,26),m22*(25,26),m23*(25,26),m24*(25,26)];;
gap> RR_Td_CF := AsGroup(gen_Td_multable_CF);
<permutation group of size 24 with 4 generators>
gap> Display(RR_Td_CF);
Group( [ ( 1, 2)( 3, 4)( 5, 8)( 6, 7)( 9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
  ( 1, 3)( 2, 4)( 5, 6)( 7, 8)( 9,12)(10,11)(13,14)(15,16)(17,20)(18,19)(21,23)(22,24),
  ( 1, 5, 9)( 2, 6,10)( 3, 7,11)( 4, 8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20),
  ( 1,13)( 2,14)( 3,15)( 4,16)( 5,17)( 6,18)( 7,19)( 8,20)( 9,21)(10,22)(11,23)(12,24)(25,26) ] )
gap> Display(Size(RR_Td_CF));
24
```

A set of generators `gen_T_multable_CF` is also obtained by collecting 12 permutations (`m1`, `m2`, $\cdots$, `m12`), so as to generate the corresponding CPR `RR_T_CF` as a permutation group of order 12, which is isomorphic to the point group $\boldsymbol{T}$ of order 12 as follows:

```
gap> gen_T_multable_CF :=
> [m1,m2,m3,m4,m5,m6,m7,m8,m9,m10,m11,m12];;
gap> RR_T_CF := AsGroup(gen_T_multable_CF);
Group([ (1,2)(3,4)(5,8)(6,7)(9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
(1,3)(2,4)(5,6)(7,8)(9,12)(10,11)(13,14)(15,16)(17,20)(18,19)(21,23)(22,24),
(1,5,9)(2,6,10)(3,7,11)(4,8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20) ])
gap> Display(Size(RR_T_CF));
12
```

As found above, the CPR `RR_Td_CF`, which has been obtained as a regular representation of degree 26 (= 24 + 2) by starting from a multiplication table of the point group $\boldsymbol{T}_d$, is alternatively shown to be a permutation group of order (size) 24 with 4 generators. In fact, the CPR `RR_Td_CF` is constructed from the set of 4 generators, i.e., `m2` (for $C_{2(1)}$), `m3` (for $C_{2(2)}$), `m5` (for $C_{3(1)}$), and `m13*(25,26)` (for $\sigma_{d(1)}$), which is represented by the following set of permutations in the GAP function `Group`:

```
gap> #Alternative expression of regular representation
gap> RR_Td_CF :=
> Group( [ ( 1, 2)( 3, 4)( 5, 8)( 6, 7)( 9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
> ( 1, 3)( 2, 4)( 5, 6)( 7, 8)( 9,12)(10,11)(13,14)(15,16)(17,20)(18,19)(21,23)(22,24),
> ( 1, 5, 9)( 2, 6,10)( 3, 7,11)( 4, 8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20),
> ( 1,13)( 2,14)( 3,15)( 4,16)( 5,17)( 6,18)( 7,19)( 8,20)( 9,21)(10,22)(11,23)(12,24)(25,26) ] );;
gap> Display(Size(RR_Td_CF));
24
```

The CPR `RR_Td_CF`, which has been constructed from the set of 4 generators, may be adopted in place of the CPR derived from the multiplication table for the sake of convenience in the following discussions.

A mark table (`tom_RR_Td_CF`) of the CPR `RR_Td_CF` as a permutation group of degree

26 (= 24 + 2), which is isomorphic to the point group $\boldsymbol{T}_d$, is obtained by using the GAP function `TableOfMarks`:

```
gap> tom_RR_Td_CF := TableOfMarks(RR_Td_CF);;
gap> Display(tom_RR_Td_CF);
 1: 24
 2: 12 4
 3: 12 . 2
 4: 8 . . 2
 5: 6 6 . . 6
 6: 6 2 2 . . 2
 7: 6 2 . . . . 2
 8: 4 . 2 1 . . . 1
 9: 3 3 1 . 3 1 1 . 1
10: 2 2 . 2 2 . . . . 2
11: 1 1 1 1 1 1 1 1 1 1 1
```

The resulting mark table (`tom_RR_Td_CF`) called *a primary mark table* is different in the sequence of subgroups from the mark table of $\boldsymbol{T}_d$ reported previously [11], which is based on $\mathrm{SSG}_{\boldsymbol{T}_d}$ (Eq. 3) and called *a standard mark table.* For example, the subgroup `r_tom_7` corresponding to the 7th row of `tom_RR_Td_CF` is calculated as follows:

```
gap> r_tom_7 := RepresentativeTom(tom_RR_Td_CF,7);
Group([ (1,2)(3,4)(5,8)(6,7)(9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
(1,19,2,20)(3,17,4,18)(5,22,8,23)(6,21,7,24)(9,16,11,14)(10,15,12,13)(25,26) ])
```

This group corresponds to the subgroup $\boldsymbol{S}_4$, which appears in the 5th row of the standard mark table based on $\mathrm{SSG}_{\boldsymbol{T}_d}$ (Eq. 3). Let us refer to this correspondence by the symbol $\overbrace{\underbrace{\boldsymbol{S}_4}_{5}}^{7}$. The above procedure using the function `RepresentativeTom` is repeated to cover all of the subgroups of a non-redundant set subgroups. Thereby, the following correspondence is obtained:

$$\mathrm{SSR}^{(RR)}_{\boldsymbol{T}_d} = \{\overbrace{\underbrace{\boldsymbol{C}_1}_{1}}^{1}, \overbrace{\underbrace{\boldsymbol{C}_2}_{2}}^{2}, \overbrace{\underbrace{\boldsymbol{C}_s}_{3}}^{3}, \overbrace{\underbrace{\boldsymbol{C}_3}_{4}}^{4}, \overbrace{\underbrace{\boldsymbol{D}_2}_{6}}^{5}, \overbrace{\underbrace{\boldsymbol{C}_{2v}}_{7}}^{6}, \overbrace{\underbrace{\boldsymbol{S}_4}_{5}}^{7}, \overbrace{\underbrace{\boldsymbol{C}_{3v}}_{8}}^{8}, \overbrace{\underbrace{\boldsymbol{D}_{2d}}_{9}}^{9}, \overbrace{\underbrace{\boldsymbol{T}}_{10}}^{10}, \overbrace{\underbrace{\boldsymbol{T}_d}_{11}}^{11}\} \tag{7}$$

where the upper numbers are taken from the leftmost column of the primary mark table `tom_RR_Td_CF`, while the lower numbers are taken from $\mathrm{SSG}_{\boldsymbol{T}_d}$ (Eq. 3) for giving the standard mark table.

4 Concordant Construction of a Standard Mark Table and a Standard USCI-CF Table

Now that the correspondence shown by $\mathrm{SSR}^{(RR)}_{\boldsymbol{T}_d}$ (Eq. 7) is obtained, the concordant construction of a standard mark table and a standard USCI-CF table should be tried systematically.

In order to convert the primary mark table `tom_RR_Td_CF` into the standard mark table based on SSG$_{\boldsymbol{T}_d}$ (Eq. 3) and to assure the concordance between the two tables, the alignment of the list of subgroups derived from $\mathrm{SSR}^{(RR)}_{\boldsymbol{T}_d}$ (the upper sequence numbers in Eq. 7) is changed into a list of sets of generators `gen[1]`–`gen[11]` derived from SSG$_{\boldsymbol{T}_d}$ (Eq. 3, i.e., the lower sequence numbers in Eq. 7).

GAP functions `MarkTableforUSCI` and `constructUSCITable` have been developed by the author (Fujita) for the purpose of systematizing the concordant construction of a standard mark table and a standard USCI-CF table [9]. They are stored in the file named `USCICF.gapfunc` (Appendix A of Ref. [9]), which is loaded at the beginning. Then, the CPR `RR_Td_CF` for $\boldsymbol{T}_d$ and the CPR `RR_T_CF` are defined as described above. The conversion list of subgroups (`gen[1]`–`gen[11]`) due to $\mathrm{SSR}^{(RR)}_{\boldsymbol{T}_d}$ is described as follows. For example, the set of generators for $\boldsymbol{S}_4$ (`r_tom_7`) appears as `gen[5]` in this conversion list of subgroups.

```
gap> Read("c:/fujita00/fujita2018/multitable-Td/gap/USCICF.gapfunc");
(# definitions of CPR RR_Td_CF and CPR RR_T_CF are omitted.)
gap> #Subgroups of Td given
gap> gen := [];;
gap> gen[1] := [ ];; #C1-- 1
gap> gen[2] := [ (1,2)(3,4)(5,8)(6,7)(9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23) ];; #C2 -- 2
gap> gen[3] := [ (1,13)(2,14)(3,15)(4,16)(5,17)(6,18)(7,19)(8,20)(9,21)(10,22)(11,23)(12,24)(25,26) ];; #
    ↪ Cs -- 3
gap> gen[4] := [ (1,5,9)(2,6,10)(3,7,11)(4,8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20) ];; #C3 -- 4
gap> gen[6] := [ (1,2)(3,4)(5,8)(6,7)(9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
> (1,3)(2,4)(5,6)(7,8)(9,12)(10,11)(13,14)(15,16)(17,20)(18,19)(21,23)(22,24) ];; #D2 -- 5
gap> gen[7] := [ (1,2)(3,4)(5,8)(6,7)( 9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
> (1,17)(2,18)(3,19)(4,20)(5,21)(6,22)(7,23)(8,24)(9,13)(10,14)(11,15)(12,16)(25,26) ];; #C2v -- 6
gap> gen[5] := [ (1,2)(3,4)(5,8)(6,7)(9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
> (1,19,2,20)(3,17,4,18)(5,22,8,23)(6,21,7,24)(9,16,11,14)(10,15,12,13)(25,26) ];; #S4 -- 7
gap> gen[8] := [ (1,5,9)(2,6,10)(3,7,11)(4,8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20),
> (1,13)(2,14)(3,15)(4,16)(5,17)(6,18)(7,19)(8,20)(9,21)(10,22)(11,23)(12,24)(25,26) ];; #C3v -- 8
gap> gen[9] := [ (1,2)(3,4)(5,8)(6,7)(9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
> (1,3)(2,4)(5,6)(7,8)(9,12)(10,11)(13,14)(15,16)(17,20)(18,19)(21,23)(22,24),
> (1,13)(2,14)(3,15)(4,16)(5,17)(6,18)(7,19)(8,20)(9,21)(10,22)(11,23)(12,24)(25,26) ];; #D2d -- 9
gap> gen[10] := [ (1,2)(3,4)(5,8)(6,7)(9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
> (1,3)(2,4)(5,6)(7,8)(9,12)(10,11)(13,14)(15,16)(17,20)(18,19)(21,23)(22,24),
> (1,5,9)(2,6,10)(3,7,11)(4,8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20) ];; #T 10
gap> gen[11] := [ (1,2)(3,4)(5,8)(6,7)(9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
> (1,3)(2,4)(5,6)(7,8)(9,12)(10,11)(13,14)(15,16)(17,20)(18,19)(21,23)(22,24),
> (1,5,9)(2,6,10)(3,7,11)(4,8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20),
> (1,13)(2,14)(3,15)(4,16)(5,17)(6,18)(7,19)(8,20)(9,21)(10,22)(11,23)(12,24)(25,26) ];; #Td 11
gap>
```

The function `MarkTableforUSCI` stored in the file `USCICF.gapfunc` (Appendix A of Ref. [9]) is loaded to generate the standard mark table named `MarkTableTd_RR`.

```
gap> #mark table sorted for USCI table
gap> MarkTableTd_RR := MarkTableforUSCI(RR_Td_CF,RR_T_CF,11,gen,24,26);;
gap> Display(MarkTableTd_RR);
 1: 24
 2: 12 4
 3: 12 . 2
 4: 8 . . 2
 5: 6 2 . . 2
 6: 6 6 . . . 6
```

```
 7: 6 2 2 . . . 2
 8: 4 . 2 1 . . . 1
 9: 3 3 1 . 1 3 1 . 1
10: 2 2 . 2 . 2 . . . 2
11: 1 1 1 1 1 1 1 1 1 1 1

gap>
```

The standard mark table `MarkTableTd_RR`, which is calculated by applying the function `MarkTableforUSCI` to the above-mentioned CPR of degree 26 (= 24 + 2), is identical with Table 2 of Ref. [11], which was, in turn, calculated by using a FORTRAN77 program. The standard mark table `MarkTableTd_RR` is also identical with Source Code 4 (`MarkTableTd`) of Ref. [9], which was calculated by applying `MarkTableforUSCI` to the CPR of degree 6 (= 4 + 2) in the GAP system.

The concordant generation of the standard USCI-CF table named `USCITableTd_RR` is achieved by using the function `constructUSCITable`, which is also stored in the file `USCICF.gapfunc` (Appendix A of Ref. [9]).

```
gap> Display("##USCI-CF table (USCITableTd_RR) :");
##USCI-CF table (USCITableTd_RR) :
gap> USCITableTd_RR := constructUSCITable(RR_Td_CF,RR_T_CF,11,gen,24,26);;
gap> Display(USCITableTd_RR);
[ [ b_1^24, b_2^12, c_2^12, b_3^8, c_4^6, b_4^6, c_4^6, c_6^4, c_8^3, b_12^2, c_24 ],
  [ b_1^12, b_1^4*b_2^4, c_2^6, b_3^4, c_2^2*c_4^2, b_2^6, c_2^2*c_4^2, c_6^2, c_4^3, b_6^2, c_12 ],
  [ b_1^12, b_2^6, c_2^5*a_1^2, b_3^4, c_4^3, b_4^3, c_4^2*a_2^2, c_6*a_3^2, c_8*a_4, b_12, a_12 ],
  [ b_1^8, b_2^4, c_2^4, b_1^2*b_3^2, c_4^2, b_4^2, c_4^2, c_2*c_6, c_8, b_4^2, c_8 ],
  [ b_1^6, b_1^2*b_2^2, c_2^3, b_3^2, c_4*a_1^2, b_2^3, c_2*c_4, c_6, c_4*a_2, b_6, a_6 ],
  [ b_1^6, b_1^6, c_2^3, b_3^2, c_2^3, b_1^6, c_2^3, c_6, c_2^3, b_3^2, c_6 ],
  [ b_1^6, b_1^2*b_2^2, c_2^2*a_1^2, b_3^2, c_2*c_4, b_2^3, c_4*a_1^2, a_3^2, c_4*a_2, b_6, a_6 ],
  [ b_1^4, b_2^2, c_2*a_1^2, b_1*b_3, c_4, b_4,a_2^2, a_1*a_3, a_4, b_4, a_4 ],
  [ b_1^3, b_1^3, c_2*a_1, b_3, c_2*a_1, b_1^3, c_2*a_1, a_3, c_2*a_1, b_3, a_3 ],
  [ b_1^2, b_1^2, c_2,b_1^2, c_2, b_1^2, c_2, c_2, c_2, b_1^2, c_2 ],
  [ b_1, b_1, a_1, b_1, a_1, b_1, a_1, a_1, a_1, b_1, a_1 ] ]
gap>
```

The standard USCI-CF table `USCITableTd_RR`, which is derived from the CPR of degree 26 (= 24 + 2), is identical with Table 5 of Ref. [11], which was calculated by using a FORTRAN77 program. The standard USCI-CF table `USCITableTd_RR` is also identical with Source Code 5 (`USCITableTd`) of Ref. [9], which was calculated by applying `constructUSCITable` to the CPR of degree 6 (= 4 + 2) in the GAP system.

5 Coset Representations

Each subgroup $\boldsymbol{G}_i$ for the standard mark table `MarkTableTd_RR` corresponds to a coset representation $(\boldsymbol{G}_i\backslash)\boldsymbol{T}_d$. If the CPR of degree 26 (= 24 + 2) `RR_Td_CF` for $\boldsymbol{T}_d$ is considered, the corresponding set of generators is represented by `gen[i]` described above. The GAP function `CosetRepCF` is developed to calculate such a coset representation (CR) in the form of CPR.

Although the file `USCICF.gapfunc` attached as Appendix A in the previous report [9] contains the function `CosetRepCF`, this function suffers from an error. Hence, the revised version of `CosetRepCF` is contained in Appendix A (`CosetRepresentation.gapfunc`) of the present article, which should be loaded after the file `USCICF.gapfunc`.

5.1 The CR $(\boldsymbol{C}_{3v}\backslash)\boldsymbol{T}_d$

Let us first calculate the CR $(\boldsymbol{C}_{3v}\backslash)\boldsymbol{T}_d$. After loading `RR_Td_CF` of $\boldsymbol{T}_d$ and `RR_T_CF` of $\boldsymbol{T}$, the CPR `C3v` for the subgroup $\boldsymbol{C}_{3v}$ derived from `gen[8]` is used in the function `CosetRepCF` in order to calculate the corresponding CR $(\boldsymbol{C}_{3v}\backslash)\boldsymbol{T}_d$ in the form of CPR `CRTd_C3v` of degree 6 (= 4 + 2). Note that the degree of the CR $(\boldsymbol{C}_{3v}\backslash)\boldsymbol{T}_d$ is calculated to be $|\boldsymbol{T}_d|/|\boldsymbol{C}_{3v}| = 24/6 = 4$. The resulting CR `CRTd_C3v` is converted into a group `Td_C3vTd` based on a set of 3 generators.

```
gap> Read("c:/fujita00/fujita2018/multitable-Td/gap/USCICF.gapfunc"); #Loading of USCICF.gapfunc
gap> Read("c:/fujita00/fujita2018/multitable-Td/gap/CosetRepresentation.gapfunc");
gap> #CosetRepresentation.gapfunc should be loaded after USCICF.gapfunc
gap>
gap> RR_Td_CF :=
> Group( [ ( 1, 2)( 3, 4)( 5, 8)( 6, 7)( 9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
> ( 1, 3)( 2, 4)( 5, 6)( 7, 8)( 9,12)(10,11)(13,14)(15,16)(17,20)(18,19)(21,23)(22,24),
> ( 1, 5, 9)( 2, 6,10)( 3, 7,11)( 4, 8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20),
> ( 1,13)( 2,14)( 3,15)( 4,16)( 5,17)( 6,18)( 7,19)( 8,20)( 9,21)(10,22)(11,23)(12,24)(25,26) ] );;
gap> RR_T_CF :=
> Group( [ ( 1, 2)( 3, 4)( 5, 8)( 6, 7)( 9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
> ( 1, 3)( 2, 4)( 5, 6)( 7, 8)( 9,12)(10,11)(13,14)(15,16)(17,20)(18,19)(21,23)(22,24),
> ( 1, 5, 9)( 2, 6,10)( 3, 7,11)( 4, 8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20)] );;
gap> ###Coset Representation C3v-Td###
gap> C3v := Group([ (1,5,9)(2,6,10)(3,7,11)(4,8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20),
> (1,13)(2,14)(3,15)(4,16)(5,17)(6,18)(7,19)(8,20)(9,21)(10,22)(11,23)(12,24)(25,26) ]);; #C3v -- gen[8]
gap> ##CR: C3v-Td"
gap> CRTd_C3v := CosetRepCF(RR_Td_CF,C3v,RR_T_CF,24,26);;
gap> Display(CRTd_C3v);
[ (), (1,2)(3,4), (1,3)(2,4), (1,4)(2,3), (2,3,4), (1,3,2), (1,4,3), (1,2,4), (2,4,3), (1,4,2), (1,2,3),
  (1,3,4), (2,3)(5,6), (1,3,4,2)(5,6), (1,2,4,3)(5,6), (1,4)(5,6), (3,4)(5,6), (1,2)(5,6), (1,4,2,3)(5,6),
  (1,3,2,4)(5,6), (2,4)(5,6), (1,4,3,2)(5,6), (1,3)(5,6), (1,2,3,4)(5,6) ]
gap> ##CR: a set of generators for C3v-Td
gap> Td_C3vTd := AsGroup(CRTd_C3v);;
gap> Display(Td_C3vTd);
Group( [ (3,4)(5,6), (2,3)(5,6), (1,2)(5,6) ] )
gap> Display(Size(Td_C3vTd));
24
```

5.2 The CR $(\boldsymbol{C}_{2v}\backslash)\boldsymbol{T}_d$

Let us next calculate the CR $(\boldsymbol{C}_{2v}\backslash)\boldsymbol{T}_d$. After loading `RR_Td_CF` of $\boldsymbol{T}_d$ and `RR_T_CF` of $\boldsymbol{T}$ (omitted), the CPR `C2v` for the subgroup $\boldsymbol{C}_{2v}$ derived from `gen[7]` is used in the function `CosetRepCF` in order to calculate the corresponding CR $(\boldsymbol{C}_{2v}\backslash)\boldsymbol{T}_d$ in the form of CPR `CRTd_C2v` of degree 8 (= 6 + 2). Note that the degree of the CR $(\boldsymbol{C}_{2v}\backslash)\boldsymbol{T}_d$ is calculated to be $|\boldsymbol{T}_d|/|\boldsymbol{C}_{2v}| = 24/4 = 6$. The resulting CR `CRTd_C2v` is converted into a group `Td_C2vTd` based on a set of 4 generators.

```
gap> ###Coset Representation C2v-Td###
gap> C2v := Group([ (1,2)(3,4)(5,8)(6,7)( 9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
> (1,17)(2,18)(3,19)(4,20)(5,21)(6,22)(7,23)(8,24)(9,13)(10,14)(11,15)(12,16)(25,26) ]);; #C2v -- gen[7]
gap> ##CR: C2v-Td"
gap> CRTd_C2v := CosetRepCF(RR_Td_CF,C2v,RR_T_CF,24,26);;
gap> Display(CRTd_C2v);
[ (), (3,4)(5,6), (1,2)(5,6), (1,2)(3,4), (1,3,5)(2,4,6), (1,3,6)(2,4,5), (1,4,6)(2,3,5), (1,4,5)(2,3,6),
  (1,5,3)(2,6,4), (1,5,4)(2,6,3), (1,6,3)(2,5,4), (1,6,4)(2,5,3), (1,3)(2,4)(7,8), (1,3,2,4)(5,6)(7,8),
  (1,4,2,3)(5,6)(7,8), (1,4)(2,3)(7,8), (3,5)(4,6)(7,8), (3,6)(4,5)(7,8), (1,2)(3,5,4,6)(7,8), (1,2)
      ↪ (3,6,4,5)(7,8),
  (1,5)(2,6)(7,8), (1,5,2,6)(3,4)(7,8), (1,6)(2,5)(7,8), (1,6,2,5)(3,4)(7,8) ]
gap> ##CR: a set of generators for C2v-Td##"
gap> Td_C2vTd := AsGroup(CRTd_C2v);;
gap> Display(Td_C2vTd);
Group( [ (3,4)(5,6), (3,5)(4,6)(7,8), (1,2)(5,6), (1,3)(2,4)(7,8) ] )
gap> Display(Size(Td_C2vTd));
24
```

5.3 The CR $(\boldsymbol{C}_s\backslash)\boldsymbol{T}_d$

The CR $(\boldsymbol{C}_s\backslash)\boldsymbol{T}_d$ is calculated in a similar way. After loading `RR_Td_CF` of $\boldsymbol{T}_d$ and `RR_T_CF` of $\boldsymbol{T}$ (omitted), the CPR `Cs` for the subgroup $\boldsymbol{C}_s$ derived from `gen[3]` is used in the function `CosetRepCF` in order to calculate the corresponding CR $(\boldsymbol{C}_s\backslash)\boldsymbol{T}_d$ in the form of CPR `CRTd_Cs` of degree 14 (= 12 + 2). Note that the degree of the CR $(\boldsymbol{C}_s\backslash)\boldsymbol{T}_d$ is calculated to be $|\boldsymbol{T}_d|/|\boldsymbol{C}_s| = 24/2 = 12$. The resulting CR `CRTd_Cs` is converted into a group `Td_CsTd` based on a set of 3 generators.

```
gap> ###Coset Representation Cs-Td###
gap> Cs := Group([ (1,13)(2,14)(3,15)(4,16)(5,17)(6,18)(7,19)(8,20)(9,21)(10,22)(11,23)(12,24)(25,26) ]);;
    ↪ # Cs -- gen[3]
gap> ##CR: Cs-Td
gap> CRTd_Cs := CosetRepCF(RR_Td_CF,Cs,RR_T_CF,24,26);;
gap> Display(CRTd_Cs);
[ (), ( 1, 2)( 3, 4)( 5, 7)( 6, 8)( 9,12)(10,11), ( 1, 3)( 2, 4)( 5, 8)( 6, 7)( 9,10)(11,12),
  ( 1, 4)( 2, 3)( 5, 6)( 7, 8)( 9,11)(10,12), ( 1, 9, 5)( 2,10, 6)( 3,11, 7)( 4,12, 8),
  ( 1,10, 7)( 2, 9, 8)( 3,12, 5)( 4,11, 6), ( 1,11, 8)( 2,12, 7)( 3, 9, 6)( 4,10, 5),
  ( 1,12, 6)( 2,11, 5)( 3,10, 8)( 4, 9, 7), ( 1, 5, 9)( 2, 6,10)( 3, 7,11)( 4, 8,12),
  ( 1, 6,12)( 2, 5,11)( 3, 8,10)( 4, 7, 9), ( 1, 7,10)( 2, 8, 9)( 3, 5,12)( 4, 6,11),
  ( 1, 8,11)( 2, 7,12)( 3, 6, 9)( 4, 5,10), ( 2, 3)( 5, 9)( 6,11)( 7,10)( 8,12)(13,14),
  ( 1, 3, 4, 2)( 5,10, 6,12)( 7, 9, 8,11)(13,14), ( 1, 2, 4, 3)( 5,12, 6,10)( 7,11, 8, 9)(13,14),
  ( 1, 4)( 5,11)( 6, 9)( 7,12)( 8,10)(13,14), ( 1, 5)( 2, 7)( 3, 6)( 4, 8)(10,11)(13,14),
  ( 1, 7)( 2, 5)( 3, 8)( 4, 6)( 9,12)(13,14), ( 1, 6, 2, 8)( 3, 5, 4, 7)( 9,11,12,10)(13,14),
  ( 1, 8, 2, 6)( 3, 7, 4, 5)( 9,10,12,11)(13,14), ( 1, 9)( 2,11)( 3,10)( 4,12)( 6, 7)(13,14),
  ( 1,11, 3,12)( 2, 9, 4,10)( 5, 6, 8, 7)(13,14), ( 1,10)( 2,12)( 3, 9)( 4,11)( 5, 8)(13,14),
  ( 1,12, 3,11)( 2,10, 4, 9)( 5, 7, 8, 6)(13,14) ]
gap> ##CR: a set of generators for Cs-Td
gap> Td_CsTd := AsGroup(CRTd_Cs);;
gap> Display(Td_CsTd);
Group( [ ( 2, 3)( 5, 9)( 6,11)( 7,10)( 8,12)(13,14), ( 1, 2)( 3, 4)( 5, 7)( 6, 8)( 9,12)(10,11),
  ( 1, 5, 9)( 2, 6,10)( 3, 7,11)( 4, 8,12) ] )
gap> Display(Size(Td_CsTd));
24
```

5.4 The CR $(\boldsymbol{D}_2\backslash)\boldsymbol{T}_d$

The above-mentioned CPRs, i.e., `CRTd_C3v` (for $(\boldsymbol{C}_{3v}\backslash)\boldsymbol{T}_d$), `CRTd_C2v` (for $(\boldsymbol{C}_{2v}\backslash)\boldsymbol{T}_d$), and `CRTd_s` (for $(\boldsymbol{C}_s\backslash)\boldsymbol{T}_d$), can be regarded as permutation groups of order 24, i.e., `Td_C3vTd` (degree 6 (= 4 +2)), `Td_C2vTd` (degree 8 (= 6 +2)), and `Td_CsTd` (degree 14 (= 12 + 2)), which are isomorphic to the point group $\boldsymbol{T}_d$ of order 24. Although these permutation groups differ in their degrees, they are capable of constructing the standard mark table and the standard USCI-CF table for the point group $\boldsymbol{T}_d$.

On the other hand, there are several CPRs (for CRs) which exhibit degenerate characters. For example, the CR $(\boldsymbol{D}_2\backslash)\boldsymbol{T}_d$ corresponding to the coset decomposition shown in Eq. 2 is represented by the CPR `CRTd_D2` of degree 8 (= 6 + 2), where 24 permutations degenerate into 6 permutations so as to give a permutation group `Td_D2Td` of order 6 as follows:

```
gap> ###Coset Representation D2-Td###
gap> D2 :=
> Group([ (1,2)(3,4)(5,8)(6,7)(9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
> (1,3)(2,4)(5,6)(7,8)(9,12)(10,11)(13,14)(15,16)(17,20)(18,19)(21,23)(22,24) ]);; #D2 -- gen[6] 5
gap> ##CR: D2-Td
gap> CRTd_D2 := CosetRepCF(RR_Td_CF,D2,RR_T_CF,24,26);;
gap> Display(CRTd_D2);
[ (), (), (), (), (1,2,3)(4,6,5), (1,2,3)(4,6,5), (1,2,3)(4,6,5), (1,2,3)(4,6,5),
  (1,3,2)(4,5,6), (1,3,2)(4,5,6), (1,3,2)(4,5,6), (1,3,2)(4,5,6),
  (1,4)(2,5)(3,6)(7,8), (1,4)(2,5)(3,6)(7,8), (1,4)(2,5)(3,6)(7,8), (1,4)(2,5)(3,6)(7,8),
  (1,5)(2,6)(3,4)(7,8), (1,5)(2,6)(3,4)(7,8), (1,5)(2,6)(3,4)(7,8), (1,5)(2,6)(3,4)(7,8),
  (1,6)(2,4)(3,5)(7,8), (1,6)(2,4)(3,5)(7,8), (1,6)(2,4)(3,5)(7,8), (1,6)(2,4)(3,5)(7,8) ]
gap> ##CR: a set of generators for D2-Td
gap> Td_D2Td := AsGroup(CRTd_D2);;
gap> Display(Td_D2Td);
Group( [ (1,2,3)(4,6,5), (1,4)(2,5)(3,6)(7,8) ] )
gap> Display(Size(Td_D2Td));
6
```

6 Geometric Meaning of the Standard Mark Table

6.1 Orbits in $\boldsymbol{T}_d$-Skeletons

As described in the preceding section, each row of the standard mark table `MarkTableTd_RR` corresponds to a coset representation $(\boldsymbol{G}_i\backslash)\boldsymbol{T}_d$, where the symbol $\boldsymbol{G}_i$ represents the i-th subgroup (up to conjugacy)

selected from $\mathrm{SSG}_{\boldsymbol{T}_d}$ (Eq. 3). Geometrically speaking, the coset representation $(\mathbf{G_i}\backslash)\boldsymbol{T}_\mathbf{d}$ controls an orbit of equivalent positions in a given skeleton of the point group $\boldsymbol{T}_d$, where each equivalent position is fixed to exhibit the local symmetry $\boldsymbol{G}_i$ (up to conjugacy) under the action of the point group $\boldsymbol{T}_d$. Each row of the standard mark table `MarkTableTd_RR` indicates the corresponding fixed-point vector (FPV), where the value at the j-th column represents the number of fixed points (positions) under the subduction into a subgroup $\boldsymbol{G}_j$, which is represented by the symbol $(\boldsymbol{G}_i\backslash)\boldsymbol{T}_d \downarrow \boldsymbol{G}_j$.

For example, the numbered skeletons **1**–**3** shown in Figure 1 indicate orbits of equivalent positions, which appear in an adamantane skeleton. The orbit of four tertiary positions in **1** is governed by the coset representation $(\boldsymbol{C}_{3v}\backslash)\boldsymbol{T}_d$, which corresponds to the 8th row of the standard mark table `MarkTableTd_RR`. The orbit of six secondary vertices in **2** is governed by the coset representation $(\boldsymbol{C}_{2v}\backslash)\boldsymbol{T}_d$, which corresponds to the 7th row of the standard mark table `MarkTableTd_RR`. The orbit of twelve secondary positions in **3** is governed by the coset representation $(\boldsymbol{C}_{s}\backslash)\boldsymbol{T}_d$, which corresponds to the 3rd row of the standard mark table `MarkTableTd_RR`.

On the other hand, a regular body of the point group $\boldsymbol{T}_d$ is shown as an adamantane derivative **4** (or **5**), where each cyclopropane ring linked in spiro fashion provides four substitution positions. Hence, there appear an orbit of 24 positions governed by the coset representation $(\boldsymbol{C}_1\backslash)\boldsymbol{T}_d$, which corresponds to the first row of the standard mark table `MarkTableTd_RR`.

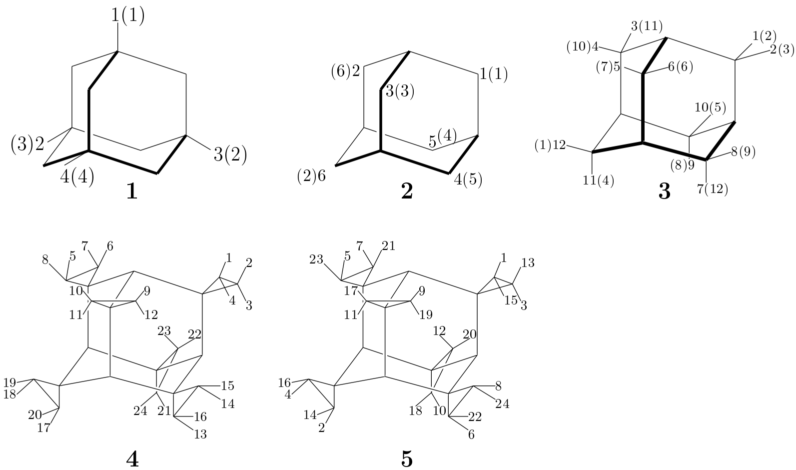

Figure 1. Orbits of equivalent positions (**1**–**3**) in an adamantane skeleton of the point group $\boldsymbol{T}_d$ as well as two modes of numbering (**4** and **5**) for a regular body of the point group $\boldsymbol{T}_d$ derived from an adamantane skeleton.

These coset representations $(\boldsymbol{G}_i\backslash)\boldsymbol{T}_d$ ($\boldsymbol{G}_i \in \mathrm{SSG}_{\boldsymbol{T}_d}$ (Eq. 3)) are permutation representations, which do not taken chirality/achirality into explicit consideration. They are converted into combined-permutation representations (CPRs) [6–8] by adding a 2-cycle.

6.2 The Four Tertiary Positions in an Adamantane Skeleton

The four tertiary positions in an adamantane skeleton **1** can be considered to construct a hypothetical tetrahedral skeleton when they are linked directly. After they are numbered sequentially from 1 to 4, they are moved under the action of the point group $\boldsymbol{T}_d$, so as to give a permutation representation of degree 4, which is regarded as a CR $(\boldsymbol{C}_{3v}\backslash)\boldsymbol{T}_d$. The skeleton **1** has a two-fold rotation axis running through the two secondary carbons to give a rotation (1,3)(2,4), a three-fold rotation axis running through the position 1 to give a rotation (2,3,4), and a mirror plane containing positions 1 and 4 to give a reflection (2,3)(5,6), where the permutation (5,6) represents a mirror-permutation. Thereby, a set of generators `gen_Td_tetra` constructs a combined permutation representation (CPR) of degree 6 (= 4 + 2) by using the GAP function `Group`. The resulting CPR `Td_tetra` is regarded as a permutation group of order 24.

```
gap> #Tetrahedral skeleton in an adamantane skeleton
gap> gen_Td_tetra := [(1,3)(2,4), (2,3,4), (2,3)(5,6)];;
gap> Td_tetra := Group(gen_Td_tetra);;
gap> Display(Td_tetra);
Group( [ (1,3)(2,4), (2,3,4), (2,3)(5,6) ] )
gap> Display(Size(Td_tetra));
24
```

The isomorphism between the CPR `Td_tetra` of degree 6 (= 4 + 2) and the CPR `Td_C3vTd` of degree 6 (= 4 + 2) described above is confirmed by using the GAP function `IsomorphismGroups`. Note that the CPR `Td_tetra` has been obtained geometrically on the basis of an adamantane skeleton **1**, while the CPR `Td_C3vTd` has been obtained algebraically on the basis of the multiplication table of $\boldsymbol{T}_d$.

```
gap> Td_tetra := Group( [ (1,3)(2,4), (2,3,4), (2,3)(5,6) ] );;
gap> Td_C3vTd := Group( [ (3,4)(5,6), (2,3)(5,6), (1,2)(5,6) ] );;
gap> #Isomorphism
gap> IsomorphismGroups(Td_tetra,Td_C3vTd);
[ (1,3)(2,4), (2,3,4), (2,3)(5,6) ] -> [ (1,2)(3,4), (1,2,4), (2,4)(5,6) ]
```

It follows that the set of generators for `Td_C3vTd` can be obtained by starting the renumbered skeleton, which is obtained by the exchange of the numbers 2 and 3 in the adamantane skeleton **1** as shown in pairs of parentheses.

On the other hand, the isomorphism between the CPR `Td_tetra` of degree 6 (= 4 + 2) and the CPR `RR_Td_CF` of degree 26 (= 24 + 2) described above is confirmed by using the GAP function `IsomorphismGroups`.

```
gap> #Isomorphism
gap> IsomorphismGroups(Td_tetra,RR_Td_CF);
[ (1,3)(2,4), (2,3,4), (2,3)(5,6) ] ->
```

```
[ (1,4)(2,3)(5,7)(6,8)(9,10)(11,12)(13,16)(14,15)(17,19)(18,20)(21,22)(23,24),
  (1,10,8)(2,9,7)(3,12,6)(4,11,5)(13,19,24)(14,20,23)(15,17,22)(16,18,21),
  (1,21)(2,22)(3,23)(4,24)(5,13)(6,14)(7,15)(8,16)(9,17)(10,18)(11,19)(12,20)(25,26) ]
gap>
```

It follows that the CPR `RR_Td_CF` is also generated from a set of three generators, which corresponds to `m4` (for $C_{2(3)}$), `m10` (for $C^2_{3(4)}$), and `m21*(25,26)` (for $\sigma_{d(3)}$) appearing in the multiplication table shown above.

6.3 The Six Secondary Vertices in an Adamantane Skeleton

The six secondary vertices in an adamantane skeleton **2** can be regarded to construct a hypothetical octahedral skeleton incorporated in an adamantane skeleton. They are controlled by the CR $(\boldsymbol{C}_{2v}\backslash)\boldsymbol{T}_d$. They are numbered sequentially from 1 to 6 to give a set of generators `gen_Td_octa`, which constructs a combined permutation representation (CPR) of degree 8 (= 6 + 2) by using the GAP function `Group`. The resulting CPR `Td_octa` is regarded as a permutation group of order 24.

```
gap> #Octahedral skeleton in an adamantane skeleton
gap> gen_Td_octa := [(2,4)(3,5), (1,2,3)(4,5,6), (1,2)(4,6)(7,8)];;
gap> Td_octa := Group(gen_Td_octa);;
gap> Display(Td_octa);
Group( [ (2,4)(3,5), (1,2,3)(4,5,6), (1,2)(4,6)(7,8) ] )
gap> Display(Size(Td_octa));
24
gap>
```

The isomorphism between the CPR `Td_octa` of degree 8 (= 6 + 2) and the CPR `Td_C2vTd` of degree 8 (= 6 + 2) described above is confirmed by using the GAP function `IsomorphismGroups`. Note that the CPR `Td_octa` has been obtained geometrically on the basis of an adamantane skeleton **2**, while the CPR `Td_C2vTd` has been obtained algebraically on the basis of the multiplication table of $\boldsymbol{T}_d$.

```
gap> Td_octa := Group( [ (2,4)(3,5), (1,2,3)(4,5,6), (1,2)(4,6)(7,8) ] );;
gap> Td_C2vTd := Group( [ (3,4)(5,6), (3,5)(4,6)(7,8), (1,2)(5,6), (1,3)(2,4)(7,8) ] );;
gap> #Isomorphism
gap> IsomorphismGroups(Td_octa,Td_C2vTd);
[ (2,4)(3,5), (1,2,3)(4,5,6), (1,2)(4,6)(7,8) ] -> [ (1,2)(3,4), (1,6,3)(2,5,4), (3,6)(4,5)(7,8) ]
```

It follows that the set of generators for `Td_C2vTd` can be obtained by starting from the renumbered skeleton, which is obtained by the permutation (2,6)(4,5) of 6 positions in the adamantane skeleton **2** as shown in pairs of parentheses.

On the other hand, the isomorphism between the CPR `Td_octa` of degree 8 (= 6 + 2) and the CPR `RR_Td_CF` of degree 26 (= 24 + 2) described above is confirmed by using the GAP function `IsomorphismGroups`.

```
gap> #Isomorphism
gap> IsomorphismGroups(Td_octa,RR_Td_CF);
[ (2,4)(3,5), (1,2,3)(4,5,6), (1,2)(4,6)(7,8) ] ->
[ (1,3)(2,4)(5,6)(7,8)(9,12)(10,11)(13,14)(15,16)(17,20)(18,19)(21,23)(22,24),
  (1,6,11)(2,5,12)(3,8,9)(4,7,10)(13,23,18)(14,24,17)(15,21,20)(16,22,19),
  (1,18)(2,17)(3,20)(4,19)(5,24)(6,23)(7,22)(8,21)(9,15)(10,16)(11,13)(12,14)(25,26) ]
```

It follows that the CPR RR_Td_CF is also generated from a set of three generators, which corresponds to m3 (for $C_{2(2)}$), m6 (for $C_{3(3)}$), and m18*(25,26) (for $\sigma_{d(4)}$) appearing in the multiplication table shown above.

6.4 The 12 Positions in an Adamantane Skeleton

The 12 positions in an adamantane skeleton **3** are controlled by the CR $(\boldsymbol{C}_s\backslash)\boldsymbol{T}_d$. They are numbered sequentially from 1 to 12 to give a set of generators gen_Td_12, which constructs a combined permutation representation (CPR) of degree 14 (= 12 + 2) by using the GAP function Group. The resulting CPR Td_12 is regarded as a permutation group of order 24.

```
gap> #Adamantane with 12 positions
gap> gen_Td_12 := [(1,2)(3,8)(4,7)(5,9)(6,10)(11,12),
> (1,4,6)(2,3,5)(7,9,11)(8,10,12), (1,3)(2,4)(5,6)(7,11)(8,12)(13,14)];;
gap> Td_12 := Group(gen_Td_12);;
gap> Display(Td_12);
Group( [ ( 1, 2)( 3, 8)( 4, 7)( 5, 9)( 6,10)(11,12), ( 1, 4, 6)( 2, 3, 5)( 7, 9,11)( 8,10,12),
  ( 1, 3)( 2, 4)( 5, 6)( 7,11)( 8,12)(13,14) ] )
gap> Display(Size(Td_12));
24
```

The isomorphism between the CPR Td_12 of degree 14 (= 12 + 2) and the CPR Td_CsTd of degree 14 (= 12 + 2) described above is confirmed by using the GAP function IsomorphismGroups. Note that the CPR Td_12 has been obtained geometrically on the basis of an adamantane skeleton **3**, while the CPR Td_CsTd has been obtained algebraically on the basis of the multiplication table of $\boldsymbol{T}_d$.

```
gap> Td_12 := Group( [ ( 1, 2)( 3, 8)( 4, 7)( 5, 9)( 6,10)(11,12),
> ( 1, 4, 6)( 2, 3, 5)( 7, 9,11)( 8,10,12),
> ( 1, 3)( 2, 4)( 5, 6)( 7,11)( 8,12)(13,14) ] );;
gap> Td_CsTd := Group( [ ( 2, 3)( 5, 9)( 6,11)( 7,10)( 8,12)(13,14),
> ( 1, 2)( 3, 4)( 5, 7)( 6, 8)( 9,12)(10,11),
> ( 1, 5, 9)( 2, 6,10)( 3, 7,11)( 4, 8,12) ] );;
gap> #Isomorphism
gap> IsomorphismGroups(Td_12,Td_CsTd);
[ (1,2)(3,8)(4,7)(5,9)(6,10)(11,12), (1,4,6)(2,3,5)(7,9,11)(8,10,12),
  (1,3)(2,4)(5,6)(7,11)(8,12)(13,14) ] ->
[ (1,2)(3,4)(5,7)(6,8)(9,12)(10,11), (1,9,5)(2,10,6)(3,11,7)(4,12,8),
  (2,3)(5,9)(6,11)(7,10)(8,12)(13,14) ]
```

It follows that the set of generators for Td_CsTd can be obtained by starting from the renumbered skeleton, which is obtained by the permutation (1,2,3,11,4,10,5,7,12)(8,9) of 12 positions in the adamantane skeleton **3** as shown in pairs of parentheses.

The isomorphism between the CPR `Td_12` of degree 14 (= 12 + 2) and the CPR `RR_Td_CF` of degree 26 (= 24 + 2) described above is confirmed by using the GAP function `IsomorphismGroups`.

```
gap> #Isomorphism
gap> IsomorphismGroups(Td_12,RR_Td_CF);
[ (1,2)(3,8)(4,7)(5,9)(6,10)(11,12), (1,4,6)(2,3,5)(7,9,11)(8,10,12),
  (1,3)(2,4)(5,6)(7,11)(8,12)(13,14) ] ->
[ (1,2)(3,4)(5,8)(6,7)(9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
  (1,7,12)(2,8,11)(3,5,10)(4,6,9)(13,22,20)(14,21,19)(15,24,18)(16,23,17),
  (1,16)(2,15)(3,14)(4,13)(5,19)(6,20)(7,17)(8,18)(9,22)(10,21)(11,24)(12,23)(25,26) ]
gap>
```

It follows that the CPR `RR_Td_CF` is also generated from a set of three generators, which corresponds to `m2` (for $C_{2(1)}$), `m7` (for $C_{3(2)}$), and `m16*(25,26)` (for $\sigma_{d(6)}$) appearing in the multiplication table shown above.

6.5 The 24 Positions in a Regular Body

The 24 positions in a regular body **4** are controlled by the CR $(\boldsymbol{C}_1\backslash)\boldsymbol{T}_d$, which is referred to under the name *regular representation* (RR). They are numbered sequentially from 1 to 24 to give a set of generators `gen_Td_RB`, which constructs a combined permutation representation (CPR) of degree 26 (= 24 + 2) by using the GAP function `Group`. The resulting CPR `Td_RB` is regarded as a permutation group of order 24.

```
gap> gen_Td_RB :=
> [(1,3)(2,4)(5,16)(6,15)(7,14)(8,13)(9,22)(10,21)(11,24)(12,23)(17,19)(18,20),
> (1,5,9)(2,6,10)(3,7,11)(4,8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20),
> (1,6)(2,5)(3,8)(4,7)(9,10)(11,12)(13,20)(14,19)(15,18)(16,17)(21,24)(22,23)(25,26)];;
gap> Td_RB := Group(gen_Td_RB);;
gap> Display(Td_RB);
Group( [ ( 1, 3)( 2, 4)( 5,16)( 6,15)( 7,14)( 8,13)( 9,22)(10,21)(11,24)(12,23)(17,19)(18,20),
  ( 1, 5, 9)( 2, 6,10)( 3, 7,11)( 4, 8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20),
  ( 1, 6)( 2, 5)( 3, 8)( 4, 7)( 9,10)(11,12)(13,20)(14,19)(15,18)(16,17)(21,24)(22,23)(25,26) ] )
gap> Display(Size(Td_RB));
24
```

The isomorphism between the CPR `Td_RB` of degree 26 (= 24 + 2) and the CPR `RR_Td_CF` of degree 26 (= 24 + 2) described above is confirmed by using the GAP function `IsomorphismGroups`.

```
gap> #Isomorphism
gap> IsomorphismGroups(Td_RB,RR_Td_CF);
[ (1,3)(2,4)(5,16)(6,15)(7,14)(8,13)(9,22)(10,21)(11,24)(12,23)(17,19)(18,20),
  (1,5,9)(2,6,10)(3,7,11)(4,8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20),
  (1,6)(2,5)(3,8)(4,7)(9,10)(11,12)(13,20)(14,19)(15,18)(16,17)(21,24)(22,23)(25,26) ] ->
[ (1,2)(3,4)(5,8)(6,7)(9,11)(10,12)(13,15)(14,16)(17,18)(19,20)(21,24)(22,23),
  (1,5,9)(2,6,10)(3,7,11)(4,8,12)(13,21,17)(14,22,18)(15,23,19)(16,24,20),
  (1,13)(2,14)(3,15)(4,16)(5,17)(6,18)(7,19)(8,20)(9,21)(10,22)(11,23)(12,24)(25,26) ]
```

It follows that the CPR `RR_Td_CF` is also generated from a set of three generators, which corresponds to `m2` (for $C_{2(1)}$), `m5` (for $C_{3(1)}$), and `m13*(25,26)` (for $\sigma_{d(1)}$) appearing in the multiplication table shown above.

Geometrical speaking, the set of three generators [m2,m5,m13*(25,26)] corresponds to another mode of numbering for the regular body **5**.

7 Conclusion

A regular representation (RR) of the point group $\boldsymbol{T}_d$ is derived algebraically from a multiplication table of $\boldsymbol{T}_d$, where reflections are explicitly considered by means of a mirror-permutation to give a combined-permutation representation (CPR) of degree 26 (= 24 + 2). Thereby, the standard mark table and the standard USCI-CF table (unit-subduced-cycle-index-with-chirality-fittingness table) are concordantly generated by using the GAP functions `MarkTableforUSCI` and `constructUSCITable`, which have been developed by Fujita for the purpose of systematizing the concordant construction [9]. A coset representation (CR) $(\boldsymbol{G}_i\backslash)\boldsymbol{T}_d$, which corresponds to a respective subgroup $\boldsymbol{G}_i$ appearing in the i-th row of the standard mark table, is obtained algebraically as a CPR by means of the GAP function `CosetRepCF` developed by Fujita (Appendix A). On the other hand, CPRs for an RR and CRs are obtained geometrically as permutation groups by considering appropriate skeletons. They are compared with the corresponding ones obtained algebraically.

8 Appendix A. CosetRepresentation.gapfunc

The function `CosetRepCF` provides us with a utility for calculating a coset representation (CR) as a combined permutation representation (CPR). This function is contained in the following file:

File Name: CosetRepresentation.gapfunc

```
#CosetRepresentation.gapfunc should be loaded
#after USCICF.gapfunc

####################################################
## Function for Calculating a Coset Representation #
## globalgr(/localgrp) #
####################################################
fixedpoint := 1; #Global fixed point (default)
isstabilizer := 1; #Global stabilizer or not
CosetRepCF := function(globalgrp,localgrp,maxchgrp,degree,degreefull)
#CosetRepCF := function(Glgrp,Locgrp,MxChgrp,DegCGr,DegGr)
local i, j, k,
#Glgrp, Locgrp, MxChgrp, DegCGr, DegGr,
l_elm_Glgrp, l_elm_MxChgrp,
cd_Gl_MxC,cd_Gl_Loc, l_rep, calcdegree,
perm_cd, s_perm_cd, l_perm, ll_perm, cosetrep;
```

```
Glgrp := globalgrp;
Locgrp := localgrp;
MxChgrp := maxchgrp;
DegCGr := degree; DegGr := degreefull;
l_elm_Glgrp := Elements(Glgrp); l_elm_MxChgrp := Elements(MxChgrp);
####################################################
#Display("#Coset Decomposition Global/MaxChiral"); # #for debug
####################################################
cd_Gl_MxC := CosetDecomposition(Glgrp, MxChgrp);
#Display(IsList(cd_Gl_MxC)); Display(cd_Gl_MxC); #for debug
###############################################
#Display("#Coset Decomposition Global/Local");# #for debug
###############################################
calcdegree := Size(Glgrp)/Size(Locgrp);
#Display(calcdegree); Display(calcdegree = DegCGr); #for debug
if calcdegree = DegCGr then
if isstabilizer = 1 then #harmonization
l_rep := []; cd_Gl_Loc := [];
for j in [1..DegCGr] do
#Print("####### j = ", j, "#########\n"); #for debug
l_rep[j] := RepresentativeAction(Glgrp, fixedpoint, j);
cd_Gl_Loc[j] := Elements(RightCoset(Locgrp, l_rep[j]));
od;
#Display(IsList(l_rep)); Display(l_rep); #for debug
#Display(IsList(cd_Gl_Loc)); Display(cd_Gl_Loc); #for debug
else #no harmonization
cd_Gl_Loc := CosetDecomposition(Glgrp, Locgrp);
#Display(IsList(cd_Gl_Loc)); Display(cd_Gl_Loc); #for debug
fi;
else #no harmonization
cd_Gl_Loc := CosetDecomposition(Glgrp, Locgrp);
#Display(IsList(cd_Gl_Loc)); Display(cd_Gl_Loc); #for debug
fi;
##################################################
#Display("#Coset Representation Global(/Local)");# #for debug
##################################################
s_perm_cd := [1..DegGr]; cosetrep := [];
for k in [1..Size(l_elm_Glgrp)] do
#Print("#### k:=", k, "#### \n"); #for debug
l_perm := cd_Gl_Loc*l_elm_Glgrp[k];
ll_perm := cd_Gl_MxC*l_elm_Glgrp[k];
#Display("###A###"); Display(l_elm_Glgrp[k]); #for debug
#Display("###B###"); Display(l_perm); #for debug
#Display("###BB###"); Display(cd_Gl_Loc); #for debug
#Display("###C###"); Display(ll_perm); #for debug
#Display("###CC###"); Display(cd_Gl_MxC); #for debug
perm_cd := [];
for j in [1..Size(cd_Gl_Loc)] do
for i in [1..Size(cd_Gl_Loc)] do
if IsEqualSet(cd_Gl_Loc[i],l_perm[j]) then
#Display(cd_Gl_Loc[i]); #for debug
#Display(l_perm[j]); #for debug
#perm_cd[j] := i; break; fi;
perm_cd[j] := i; fi;
od; od;
if DegCGr <> DegGr then
#Display("#### DegCGr <> DegGr####"); # for debug
for j in [1..Size(cd_Gl_MxC)] do
for i in [1..Size(cd_Gl_MxC)] do
if IsEqualSet(cd_Gl_MxC[i],ll_perm[j]) then

#perm_cd[DegCGr+j] := DegCGr+i; break; fi; #error
perm_cd[Size(cd_Gl_Loc)+j] := Size(cd_Gl_Loc)+i; break; fi;
od; od;
fi;
#Display(perm_cd); #for debug
#cosetrep[k] := PermListList(s_perm_cd, perm_cd); #error
cosetrep[k] := PermList(perm_cd);
#Display(cosetrep[k]); #for debug
od;
return cosetrep;
end; #end of CosetRepCF
```

References

[1] S. Fujita, Application of coset representations to the construction of symmetry adapted functions, *Theor. Chim. Acta* **78** (1990) 45–63.

[2] S. Fujita, *Diagrammatical Approach to Molecular Symmetry and Enumeration of Stereoisomers*, Univ. Kragujevac, Kragujevac, 2007.

[3] S. Fujita, *Symmetry and Combinatorial Enumeration in Chemistry*, Springer, Berlin, 1991.

[4] S. Fujita, *Combinatorial Enumeration of Graphs, Three–Dimensional Structures, and Chemical Compounds*, Univ. Kragujevac, Kragujevac, 2013.

[5] S. Fujita, Chirality fittingness of an orbit governed by a coset representation. Integration of point-group and permutation-group theories to treat local chirality and prochirality, *J. Am. Chem. Soc.* **112** (1990) 3390–3397.

[6] S. Fujita, Computer-oriented representations of point groups and cycle indices with chirality fittingness (CI-CFs) calculated by the GAP system. Enumeration of three-dimensional structures of ligancy 4 by Fujita's proligand method, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 379–400.

[7] S. Fujita, Computer-oriented representations of $\boldsymbol{O}_h$-skeletons for supporting combinatorial enumeration by Fujita's proligand method. GAP calculation of cycle indices with chirality fittingness (CI-CFs), *MATCH Commun. Math. Comput. Chem.* **77** (2017) 409–442.

[8] S. Fujita, Hierarchical enumeration based on skeletons of ligancy 6 by using combined-permutation representations. Part 1. Cyclopropane derivatives, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 103–142.

[9] S. Fujita, Concordant generation of mark tables and USCI-CF (unit subduced cycle indices with chirality fittingness) tables on the basis of combined-permutation representations, *MATCH Commun. Math. Comput. Chem.*, in press.

[10] https://www.gap-system.org/.

[11] S. Fujita, Systematic enumeration of high symmetry molecules by means of unit subduced cycle indices with and without chirality fittingness, *Bull. Chem. Soc. Jpn.* **63** (1990) 203–215.

[12] W. Burnside, *Theory of Groups of Finite Order*, Cambridge Univ. Press, Cambridge, 1911.

[13] C. A. Mead, Table of marks and double cosets in isomer counting, *J. Am. Chem. Soc.* **109** (1987) 2130–2137.

[14] C. A. Mead, Symmetry and combinatorial enumeration in chemistry, *J. Am. Chem. Soc.* **114** (1992) 4018–4019.