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Standardization of Mark Tables and USCI-CF (Unit Subduced Cycle Indices with Chirality Fittingness) Tables Derived from Different $\boldsymbol{O_h}$-Skeletons

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Abstract

Permutation groups (PGs) are derived by respective sets of generators based on various $\boldsymbol{O}_h$-skeletons (octahedron, cube, cuboctahedron, truncated octahedron, truncated hexahedron, and rhombic dodecahedron). Each set of generators is selected from combined-permutation representations (CPRs) which stabilize the vertices of each $\boldsymbol{O}_h$-skeleton and contain 2-cycles due to mirror-permutations. Thus, the CPR of degree 8 (= 6 + 2) for octahedron, the CPR of degree 10 (= 8 + 2) for cube, the CPR of degree 14 (= 12 + 2) for cuboctahedron, the CPR of degree 26 (= 24 + 2) for truncated octahedron, the CPR of degree 26 (= 24 + 2) for truncated hexahedron, and the CPR of degree 16 (= 14 + 2) for rhombic dodecahedron are regarded as PGs. These PGs are found to be isomorphic to the point group $\boldsymbol{O}_h$, which is, in turn, composed of symmetry operations based on symmetry elements. Mark tables (tables of marks) of these PGs are different from each other when they are produced by the GAP system. By sorting rows and columns according to the respective non-redundant sets of subgroups (SSGs), however, these mark tables can be standardized to give a standard mark table for the point group $\boldsymbol{O}_h$. Concordant construction of a standard mark table and a USCI-CF (unit-subduced-cycle-index-with-chirality-fittingness) table for $\boldsymbol{O}_h$ is discussed by starting from each of the $\boldsymbol{O}_h$-skeletons. After a set of SCI-CFs (subduced cycle indices with chirality fittingness) and a set of PCI-CFs (partial cycle indices with chirality fittingness) are generated, symmetry-itemized enumeration based on the PCI method of Fujita's USCI approach (S. Fujita, *Symmetry and Combinatorial Enumeration in Chemistry*, Springer-Verlag, Berlin-Heidelberg, 1991) is conducted by starting from each of the $\boldsymbol{O}_h$-skeletons.

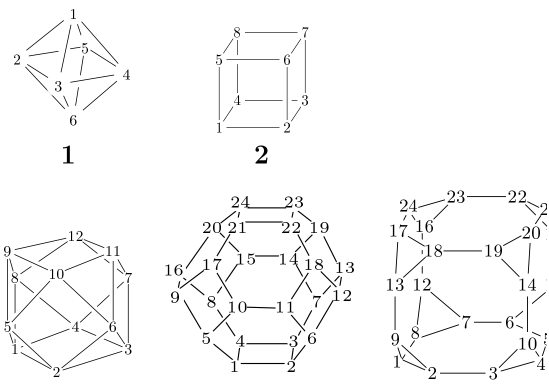
1 Introduction

The concept of *tables of marks* (mark tables) introduced by Burnside [3] was applied to isomer enumeration by Mead [4], where the concept of *double cosets* was emphasized during this application. The author (Fujita) developed the concept of *subduction of coset representations* and the concept of *unit subduced cycle indices* (USCIs) to cover symmetry-itemized enumeration of isomers [5, 6]. After the introduction of *proligands* as a new concept, chemical compounds are recognized as *promolecules* which are considered to be 3D objects derived from a rigid 3D-skeleton [7]. A set of equivalent positions of a given 3D-skeleton is regarded as an orbit (an equivalence class) governed by a coset representation, where the respective orbit is categorized into an enantiospheric orbit, a homospheric orbit, or a hemispheric orbit after formulation of the concept of *sphericity* [8]. Such an orbit is occupied by a set of equivalent proligands to give a promolecule, where the mode of occupation (referred to by the term *chirality fittingness*) is controlled by the sphericity of the orbit. Thereby, the concept of *unit subduced cycle indices with chirality fittingness* (USCI-CFs) was proposed by the author (Fujita) to enumerate isomers as 3D objects under respective point groups. As summarized in monographs [1, 9], the permutation-group theory and the point group theory have been integrated, so that the conventional enumeration of graphs under permutation groups has been extended into the enumeration of 3D objects under point groups. The integration of point-group and permutation-group theories has provided us with solid foundations to treat local chirality and prochirality [8].

Because mark tables and USCI-CF tables for point groups play important roles during the processes of symmetry-itemized enumerations due to Fujita's USCI approach [1], several examples calculated by means of the FORTRAN programming language have been reported, e.g., Appendix A (Tables A.1–A.13 for mark tables) and Appendix E (Tables E.1–E.13 for USCI-CF tables) of Ref. [1]. Recently, the advent of the GAP (Groups, Algorithms, Programming) system [10]) has brought great changes to practices concerning group theory. In particular, the GAP system provides us with useful utilities for treating mark tables, e.g., the GAP function `TableOfMarks`. However, these utilities without the concept of sphericity aim at permutation groups, so that they are originally incapable of treating enumeration of 3D objects, which requires utilities with the concept of sphericity on the basis of point groups.

The author (Fujita) has recently developed combined-permutation representations (CPRs) [11], which have been used to treat point groups [11, 12] and *RS*-stereoisomeric groups [13]. Thereby, the GAP function `MarkTableforUSCI` for calculating mark tables and the GAP function `constructUSCITable` for constructing USCI-CF tables have been developed to treat symmetry-itemized enumeration of 3D objects [14].

In the present article, we show that mark tables vary in rows and columns if the GAP function `TableOfMarks` is applied to various $\boldsymbol{O}_h$-skeletons (i.e., octahedron **1**, cube **2**, cuboctahedron **3**, truncated octahedron **4**, and truncated hexahedron **5** shown in Figure 1, as well as rhombic dodecahedron **6** shown in Figure 2). In order to pursue the symmetry-itemized enumeration under point groups, such apparently different mark tables should be sorted to give a single format, which aims at consistency with the previous result calculated by FORTRAN [1]. In the present article, we discuss the apparent difference and show a practical procedure of standardization for constructing a single format.



1 **2** **3** **4** **5**

Figure 1. $\boldsymbol{O}_h$-Skeletons: Octahedron **1** (*OC*-6), cube **2** (*CU*-8), cuboctahedron **3**, truncated octahedron **4**, and truncated hexahedron **5**.

2 Point Groups vs. Permutation Groups

The point group $\boldsymbol{O}_h$ is composed of symmetry operations based on symmetry elements, which are commonly recognized even if different $\boldsymbol{O}_h$-skeletons (e.g., octahedron, cube, cuboctahedron, truncated octahedron, truncated hexahedron, and rhombic dodecahedrons) are taken into consideration. On the other hand, a permutation group (PG) is derived from each of the $\boldsymbol{O}_h$-skeletons by using the corresponding set of generators. As a result, the mark table (table of marks) of a PG based on one set of generators is different from that of another PG based on the other set of generators, when they are produced by the GAP system.

2.1 Mark Tables and USCI-CF Tables for Point Groups

The mark table for the $\boldsymbol{O}_h$-group has been already reported for the enumeration of octahedral complexes [15]. A set of the mark table and the USCI-CF table for the $\boldsymbol{O}_h$-group has been also reported for the enumeration of cubane derivatives [16]. Although an octahedral skeleton has six substitution positions and a cubic skeleton has eight substitution positions, they are controlled by the same point group $\boldsymbol{O}_h$ through the coset representations (CRs). These CRs are commonly characterized by the mark table and the USCI-CF table, which are referred to as standard tables in the present article.

The point group $\boldsymbol{O}_h$ of order 48 has 33 subgroups up to conjugacy, which have been discussed in terms of a non-redundant set of subgroups (SSG) [15]:

$$\begin{aligned}\mathrm{SSG}_{\boldsymbol{O}_h} = \{ & \underbrace{\boldsymbol{C}_1}_{1}, \underbrace{\boldsymbol{C}_2}_{2}, \underbrace{\boldsymbol{C}'_2}_{3}, \underbrace{\boldsymbol{C}_s}_{4}, \underbrace{\boldsymbol{C}'_s}_{5}, \underbrace{\boldsymbol{C}_i}_{6}, \underbrace{\boldsymbol{C}_3}_{7}, \underbrace{\boldsymbol{C}_4}_{8}, \underbrace{\boldsymbol{S}_4}_{9}, \underbrace{\boldsymbol{D}_2}_{10}, \\ & \underbrace{\boldsymbol{D}'_2}_{11}, \underbrace{\boldsymbol{C}_{2v}}_{12}, \underbrace{\boldsymbol{C}'_{2v}}_{13}, \underbrace{\boldsymbol{C}''_{2v}}_{14}, \underbrace{\boldsymbol{C}_{2h}}_{15}, \underbrace{\boldsymbol{C}'_{2h}}_{16}, \underbrace{\boldsymbol{D}_3}_{17}, \underbrace{\boldsymbol{C}_{3v}}_{18}, \underbrace{\boldsymbol{C}_{3i}}_{19}, \underbrace{\boldsymbol{D}_4}_{20}, \\ & \underbrace{\boldsymbol{C}_{4v}}_{21}, \underbrace{\boldsymbol{C}_{4h}}_{22}, \underbrace{\boldsymbol{D}_{2d}}_{23}, \underbrace{\boldsymbol{D}'_{2d}}_{24}, \underbrace{\boldsymbol{D}_{2h}}_{25}, \underbrace{\boldsymbol{D}'_{2h}}_{26}, \underbrace{\boldsymbol{T}}_{27}, \underbrace{\boldsymbol{D}_{3d}}_{28}, \underbrace{\boldsymbol{D}_{4h}}_{29}, \underbrace{\boldsymbol{O}}_{30}, \underbrace{\boldsymbol{T}_h}_{31}, \underbrace{\boldsymbol{T}_d}_{32}, \underbrace{\boldsymbol{O}_h}_{33} \}\end{aligned} \quad (1)$$

where the subgroups are aligned and numbered sequentially in the ascending order of their orders.

The respective subgroups correspond to the coset representations $(\boldsymbol{G}_i\backslash)\boldsymbol{O}_h$ ($\boldsymbol{G}_i \in \mathrm{SSG}_{\boldsymbol{O}_h}$), the degree of which is equal to $|\boldsymbol{O}_h|/|\boldsymbol{G}_i|$. Note that the original symbol $\boldsymbol{O}_h(/\boldsymbol{G}_i)$ [1,15] is changed into the symbol $(\boldsymbol{G}_i\backslash)\boldsymbol{O}_h$ for the purpose of assuring the compatibility to the GAP system. Each row of the mark table, which is a lower triangular 33×33 matrix, corresponds to the coset representation $(\boldsymbol{G}_i\backslash)\boldsymbol{O}_h$ ($i = 1, 2, \ldots, 33$) according to the sequence of the SSG (Eq. 1). The value at the intersection between the $(\boldsymbol{G}_i\backslash)\boldsymbol{O}_h$-row and the $\boldsymbol{G}_j$-column ($i, j = 1, 2, \ldots, 33$) represents the number of fixed points during the subduction $(\boldsymbol{G}_i\backslash)\boldsymbol{O}_h \downarrow \boldsymbol{G}_j$ [1].

2.2 Utilities of Mark Tables in the GAP system

The GAP function `Group` generates a permutation group (PG) by staring from a given set of generators. The corresponding mark table is generated by means of the GAP function `TableOfMarks`.

2.2.1 Mark Table Based on the Octahedral Skeleton

The octahedral skeleton **1** possesses a four-fold axis (based on a permutation: (2 3 4 5)), a three-fold axis (based on a permutation: (1 2 3)(4 5 6)), and a mirror plane (based on a permutation (1 6)(7 8)), where the 2-cycle (7 8) represents a mirror-permutation. These permutations construct a set (`gen1`) of generators for generating a combined-permutation representation (CPR) `Oh_octa`, which can be regarded as a permutation group (PG) isomorphic to the point group $\boldsymbol{O}_h$. The CPR `Oh_octa` is used to generate a mark table named `tom_Oh_octa` by means of the GAP function `TableOfMarks` as follows:

```
gap> gen1 := [(2,3,4,5), (1,2,3)(4,5,6), (1,6)(7,8)];; #generators for Oh_octa
gap> Oh_octa := Group(gen1);; #octahedral skeleton
gap> Display(Size(Oh_octa));
48
gap> tom_Oh_octa := TableOfMarks(Oh_octa);;
gap> Display(tom_Oh_octa);
 1: 48
 2: 24 8
 3: 24 . 4
 4: 24 . . 8
 5: 24 . . . 24
 6: 24 . . . . 4
 7: 16 . . . . . 4
 8: 12 12 . . . . . 12
 9: 12 4 . 8 . . . . 4
10: 12 4 . 4 12 . . . . 4
11: 12 4 . . . 4 . . . . 4
12: 12 4 . . . . . . . . . 4
13: 12 4 . . . . . . . . . . 4
14: 12 4 4 . . . . . . . . . . 4
15: 12 . 2 4 . 2 . . . . . . . . 2
16: 12 . 2 . 12 2 . . . . . . . . . 2
17: 8 . . . 8 . 2 . . . . . . . . . 2
18: 8 . 4 . . . 2 . . . . . . . . . . 2
19: 8 . . . . 4 2 . . . . . . . . . . . 2
20: 6 6 2 . . . . 6 . . . . 2 2 . . . . . . 2
21: 6 6 . . . 2 . 6 . . 2 2 . . . . . . . . 2
22: 6 2 . 4 . 2 . . 2 . 2 . 2 . . . . . . . . 2
23: 6 2 2 4 . . . . 2 . . 2 . 2 . . . . . . . . 2
24: 6 6 . 6 6 . . 6 6 6 . . . . . . . . . . . . . 6
25: 6 2 2 2 6 2 . . . 2 2 . . 2 2 2 . . . . . . . . 2
26: 6 2 . 2 6 . . . . 2 . 2 2 . . . . . . . . . . . . 2
27: 4 . 2 . 4 2 1 . . . . . . . 2 1 1 1 . . . . . . . 1
28: 4 4 . . . . 4 4 . . . . . . . . . . . . . . . . . . . 4
29: 3 3 1 3 3 1 . 3 3 3 1 1 1 1 1 1 . . . 1 1 1 1 3 1 1 . . 1
30: 2 2 2 . . . 2 2 . . . . 2 2 . . . 2 . 2 . . . . . . . 2 . 2
31: 2 2 . 2 2 . 2 2 2 2 . . . . . . 2 . . . . . . 2 . . . 2 . . 2
32: 2 2 . . . 2 2 2 . . 2 2 . . . . . . 2 . 2 . . . . . . . 2 . . . 2
33: 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

Each sequential number at the left-most column of the mark table `tom_Oh_octa` shows the corresponding group in SSG, which can be designated by means of the GAP function `RepresentativeTom`. For example, the fifth row is found to correspond to the following group:

```
gap> RepresentativeTom(tom_Oh_octa,5);
Group([ (1,6)(2,4)(3,5)(7,8) ])
```

This group of order 2 is found to correspond to the point group $\boldsymbol{C}_i$, which is the sixth subgroup appearing in $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1). This correspondence is represented by the symbol $\overbrace{\underbrace{\boldsymbol{C}_i}_{6}}^{5}$, where the upper number 5 is concerned with the SSG for the mark table `tom_Oh_octa` (named $\mathrm{SSG}^{octa}_{\boldsymbol{O}_h}$), while the lower number 6 is concerned with $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1). Thereby, $\mathrm{SSG}^{octa}_{\boldsymbol{O}_h}$ for the mark table `tom_Oh_octa` is represented as follows:

$$
\begin{aligned}
\mathrm{SSG}^{octa}_{\boldsymbol{O}_h} = \{ & \overbrace{\underbrace{\boldsymbol{C}_1}_{1}}^{1}, \overbrace{\underbrace{\boldsymbol{C}_2}_{2}}^{2}, \overbrace{\underbrace{\boldsymbol{C}'_2}_{3}}^{3}, \overbrace{\underbrace{\boldsymbol{C}_s}_{4}}^{4}, \overbrace{\underbrace{\boldsymbol{C}_i}_{6}}^{5}, \overbrace{\underbrace{\boldsymbol{C}'_s}_{5}}^{6}, \overbrace{\underbrace{\boldsymbol{C}_3}_{7}}^{7}, \overbrace{\underbrace{\boldsymbol{D}_2}_{10}}^{8}, \overbrace{\underbrace{\boldsymbol{C}_{2v}}_{12}}^{9}, \overbrace{\underbrace{\boldsymbol{C}_{2h}}_{15}}^{10}, \\
& \overbrace{\underbrace{\boldsymbol{C}'_{2v}}_{13}}^{11}, \overbrace{\underbrace{\boldsymbol{S}_4}_{9}}^{12}, \overbrace{\underbrace{\boldsymbol{C}_4}_{8}}^{13}, \overbrace{\underbrace{\boldsymbol{D}'_2}_{11}}^{14}, \overbrace{\underbrace{\boldsymbol{C}''_{2v}}_{14}}^{15}, \overbrace{\underbrace{\boldsymbol{C}'_{2h}}_{16}}^{16}, \overbrace{\underbrace{\boldsymbol{C}_{3i}}_{19}}^{17}, \overbrace{\underbrace{\boldsymbol{D}_3}_{17}}^{18}, \overbrace{\underbrace{\boldsymbol{C}_{3v}}_{18}}^{19}, \overbrace{\underbrace{\boldsymbol{D}_4}_{20}}^{20}, \\
& \overbrace{\underbrace{\boldsymbol{D}_{2d}}_{23}}^{21}, \overbrace{\underbrace{\boldsymbol{C}_{4v}}_{21}}^{22}, \overbrace{\underbrace{\boldsymbol{D}'_{2d}}_{24}}^{23}, \overbrace{\underbrace{\boldsymbol{D}_{2h}}_{25}}^{24}, \overbrace{\underbrace{\boldsymbol{D}'_{2h}}_{26}}^{25}, \overbrace{\underbrace{\boldsymbol{C}_{4h}}_{22}}^{26}, \overbrace{\underbrace{\boldsymbol{D}_{3d}}_{28}}^{27}, \overbrace{\underbrace{\boldsymbol{T}}_{27}}^{28}, \overbrace{\underbrace{\boldsymbol{D}_{4h}}_{29}}^{29}, \overbrace{\underbrace{\boldsymbol{O}}_{30}}^{30}, \overbrace{\underbrace{\boldsymbol{T}_h}_{31}}^{31}, \overbrace{\underbrace{\boldsymbol{T}_d}_{32}}^{32}, \overbrace{\underbrace{\boldsymbol{O}_h}_{33}}^{33} \}
\end{aligned}
\tag{2}
$$

where the upper numbers are taken from the leftmost column of the mark table `tom_Oh_-octa`, while the lower numbers are taken from $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1).

The mark table `tom_Oh_octa` due to $\mathrm{SSG}^{octa}_{\boldsymbol{O}_h}$ (Eq. 2) can be converted into the mark table `test_sort` due to $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1) by using the GAP function `SortedTom` as follows:

```
gap> perm_octa := PermList
    ↪ ([1,2,3,4,6,5,7,10,12,15,13,9,8,11,14,16,19,17,18,20,23,21,24,25,26,22,28,27,29,30,31,32,33]
(5,6)(8,10,15,14,11,13)(9,12)(17,19,18)(21,23,24,25,26,22)(27,28)
gap> test_sort := SortedTom(tom_Oh_octa,perm_octa);;
gap> Display(test_sort);
 1: 48
 2: 24 8
 3: 24 . 4
 4: 24 . . 8
 5: 24 . . . 4
 6: 24 . . . . 24
(#omitted cf. Table 1)
```

where the permutation `perm_octa` is calculated by applying the GAP function `PermList` to a list derived from the lower numbering in Eq. 2. The resulting mark table is identical with Table 1, which will be calculated later as a standard mark table.

2.2.2 Mark Table Based on the Cubane Skeleton

On the other hand, the cubane skeleton **2** possesses a four-fold axis (based on a permutation: (1 2 3 4)(5 6 7 8)), a three-fold axis (based on a permutation: (2 4 5)(3 8 6)), and a mirror plane (based on a permutation (1 5)(2 6)(3 7)(4 8)(9 10)), where the 2-cycle (9 10) represents a mirror-permutation. These permutations construct a set (`gen2`) of generators for generating a combined-permutation representation (CPR) `Oh_cube`, which can be regarded as a permutation group isomorphic to the point group $\boldsymbol{O}_h$. The CPR `Oh_cube` is used to generate a mark table named `tom_Oh_cube` by means of the GAP function `TableOfMarks` as follows:

```
gap> gen2 := [(1,2,3,4)(5,6,7,8), (2,4,5)(3,8,6), (1,5)(2,6)(3,7)(4,8)(9,10)];; #generators for Oh_cube
gap> Oh_cube := Group(gen2); #cubane skeleton
Group([ (1,2,3,4)(5,6,7,8), (2,4,5)(3,8,6), (1,5)(2,6)(3,7)(4,8)(9,10) ])
gap> Display(Size(Oh_cube));
48
gap> tom_Oh_cube := TableOfMarks(Oh_cube);;
gap> Display(tom_Oh_cube);
 1: 48
 2: 24 8
 3: 24 . 4
 4: 24 . . 4
 5: 24 . . . 24
 6: 24 . . . . 8
(#omitted)
```

The mark table `tom_Oh_cube` calculated above is found to be based on the following $\mathrm{SSG}^{cube}_{\boldsymbol{O}_h}$ by using the GAP function `RepresentativeTom`:

$$\begin{aligned}\mathrm{SSG}^{cube}_{\boldsymbol{O}_h} = \{ & \overbrace{\underbrace{\boldsymbol{C}_1}_{1}}^{1}, \overbrace{\underbrace{\boldsymbol{C}_2}_{2}}^{2}, \overbrace{\underbrace{\boldsymbol{C}'_2}_{3}}^{3}, \overbrace{\underbrace{\boldsymbol{C}'_s}_{5}}^{4}, \overbrace{\underbrace{\boldsymbol{C}_i}_{6}}^{5}, \overbrace{\underbrace{\boldsymbol{C}_s}_{4}}^{6}, \overbrace{\underbrace{\boldsymbol{C}_3}_{7}}^{7}, \overbrace{\underbrace{\boldsymbol{C}_4}_{8}}^{8}, \overbrace{\underbrace{\boldsymbol{D}_2}_{10}}^{9}, \overbrace{\underbrace{\boldsymbol{C}_{2v}}_{12}}^{10}, \\ & \overbrace{\underbrace{\boldsymbol{C}'_{2v}}_{13}}^{11}, \overbrace{\underbrace{\boldsymbol{S}_4}_{9}}^{12}, \overbrace{\underbrace{\boldsymbol{C}'_{2h}}_{16}}^{13}, \overbrace{\underbrace{\boldsymbol{C}_{2h}}_{15}}^{14}, \overbrace{\underbrace{\boldsymbol{D}'_2}_{11}}^{15}, \overbrace{\underbrace{\boldsymbol{C}''_{2v}}_{14}}^{16}, \overbrace{\underbrace{\boldsymbol{C}_{3v}}_{18}}^{17}, \overbrace{\underbrace{\boldsymbol{C}_{3i}}_{19}}^{18}, \overbrace{\underbrace{\boldsymbol{D}_3}_{17}}^{19}, \overbrace{\underbrace{\boldsymbol{D}_4}_{20}}^{20}, \\ & \overbrace{\underbrace{\boldsymbol{D}_{2d}}_{23}}^{21}, \overbrace{\underbrace{\boldsymbol{C}_{4v}}_{21}}^{22}, \overbrace{\underbrace{\boldsymbol{D}_{2h}}_{25}}^{23}, \overbrace{\underbrace{\boldsymbol{C}_{4h}}_{22}}^{24}, \overbrace{\underbrace{\boldsymbol{D}'_{2h}}_{26}}^{25}, \overbrace{\underbrace{\boldsymbol{D}'_{2d}}_{24}}^{26}, \overbrace{\underbrace{\boldsymbol{D}_{3d}}_{28}}^{27}, \overbrace{\underbrace{\boldsymbol{T}}_{27}}^{28}, \overbrace{\underbrace{\boldsymbol{D}_{4h}}_{29}}^{29}, \overbrace{\underbrace{\boldsymbol{T}_d}_{32}}^{30}, \overbrace{\underbrace{\boldsymbol{T}_h}_{31}}^{31}, \overbrace{\underbrace{\boldsymbol{O}}_{30}}^{32}, \overbrace{\underbrace{\boldsymbol{O}_h}_{33}}^{33} \}\end{aligned} \tag{3}$$

The upper numbers are taken from the leftmost column of the mark table `tom_Oh_cube`, where the numbering is sequential from 1 to 33. On the other hand, the lower numbers taken from $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1) are reordered in Eq. 3 according to the appearance in the mark table `tom_Oh_cube`.

The data of Eq. 3 is converted into a permutation `perm_cube` by means of the GAP function `PermList`. The resulting permutation is used in the GAP function `SortedTom` to give a sorted mark table `test_sort` as follows:

```
gap> perm_cube := PermList
    ↪ ([1,2,3,5,6,4,7,8,10,12,13,9,16,15,11,14,18,19,17,20,23,21,25,22,26,24,28,27,29,32,31,30,33]);
(4,5,6)(9,10,12)(11,13,16,14,15)(17,18,19)(21,23,25,26,24,22)(27,28)(30,32)
gap> test_sort := SortedTom(tom_Oh_cube,perm_cube);;
gap> Display(test_sort);
 1: 48
 2: 24 8
 3: 24 . 4
 4: 24 . . 8
 5: 24 . . . 4
 6: 24 . . . . 24
(#omitted cf. Table 1)
```

The resulting mark table `test_sort` is found to be identical with the standard mark table based on $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1) which will be later obtained (Table 1).

2.2.3 Mark Table Based on the Cuboctahedral Skeleton

A set of generators `gen3` for the cuboctahedron **3** is based on a four-fold axis (based on a permutation: (1 2 3 4)(5 6 7 8)(9 10 11 12)), a three-fold axis (based on a permutation: (1 5 2)(3 8 10)(4 9 6)(7 12 11)), and a mirror plane (based on a permutation (1 9)(2 10)(3 11)(4 12)(13 14)), where the 2-cycle (13 14) represents a mirror-permutation. The application of the GAP function `Group` to `gen3` results in the construction of a CPR `Oh_cuboct`, which can be regarded as a permutation group isomorphic to the point group $\boldsymbol{O}_h$. The CPR `Oh_cuboct` is used to generate a mark table named `tom_Oh_cuboct` by means of the GAP function `TableOfMarks` as follows:

```
gap> gen3 := [(1,2,3,4)(5,6,7,8)(9,10,11,12), (1,5,2)(3,8,10)(4,9,6)(7,12,11),
> (1,9)(2,10)(3,11)(4,12)(13,14)];;
gap> Oh_cuboct := Group(gen3); #cuboctahedron
Group([ (1,2,3,4)(5,6,7,8)(9,10,11,12), (1,5,2)(3,8,10)(4,9,6)(7,12,11), (1,9)(2,10)(3,11)(4,12)(13,14) ])
gap> Display(Size(Oh_cuboct));
48
gap> tom_Oh_cuboct := TableOfMarks(Oh_cuboct);;
gap> Display(tom_Oh_cuboct);
 1: 48
 2: 24 8
 3: 24 . 4
 4: 24 . . 8
 5: 24 . . . 24
 6: 24 . . . . 4
(#omitted)
```

The mark table `tom_Oh_cuboct` calculated above is found to be based on the following $\mathrm{SSG}^{cuboct}_{\boldsymbol{O}_h}$ by using the GAP function `RepresentativeTom`:

$$\mathrm{SSG}^{cuboct}_{\boldsymbol{O}_h} = \{ \underbrace{\overbrace{\boldsymbol{C}_1}^{1}}_{1}, \underbrace{\overbrace{\boldsymbol{C}_2}^{2}}_{2}, \underbrace{\overbrace{\boldsymbol{C}'_2}^{3}}_{3}, \underbrace{\overbrace{\boldsymbol{C}_s}^{4}}_{4}, \underbrace{\overbrace{\boldsymbol{C}_i}^{5}}_{6}, \underbrace{\overbrace{\boldsymbol{C}'_s}^{6}}_{5}, \underbrace{\overbrace{\boldsymbol{C}_3}^{7}}_{7}, \underbrace{\overbrace{\boldsymbol{D}_2}^{8}}_{10}, \underbrace{\overbrace{\boldsymbol{C}_{2v}}^{9}}_{12}, \underbrace{\overbrace{\boldsymbol{C}_{2h}}^{10}}_{15},$$

$$\underbrace{\overbrace{\boldsymbol{C}'_{2v}}^{11}}_{13}, \underbrace{\overbrace{\boldsymbol{S}_4}^{12}}_{9}, \underbrace{\overbrace{\boldsymbol{D}'_2}^{13}}_{11}, \underbrace{\overbrace{\boldsymbol{C}_4}^{14}}_{8}, \underbrace{\overbrace{\boldsymbol{C}''_{2v}}^{15}}_{14}, \underbrace{\overbrace{\boldsymbol{C}'_{2h}}^{16}}_{16}, \underbrace{\overbrace{\boldsymbol{C}_{3i}}^{19}}_{19}, \underbrace{\overbrace{\boldsymbol{D}_3}^{17}}_{17}, \underbrace{\overbrace{\boldsymbol{C}_{3v}}^{18}}_{18}, \underbrace{\overbrace{\boldsymbol{D}_4}^{20}}_{20},$$

$$\overset{21}{\overbrace{\underbrace{\boldsymbol{D}_{2d}}_{23}}}, \overset{22}{\overbrace{\underbrace{\boldsymbol{D}'_{2h}}_{26}}}, \overset{23}{\overbrace{\underbrace{\boldsymbol{C}_{4h}}_{22}}}, \overset{24}{\overbrace{\underbrace{\boldsymbol{D}_{2h}}_{25}}}, \overset{25}{\overbrace{\underbrace{\boldsymbol{C}_{4v}}_{21}}}, \overset{26}{\overbrace{\underbrace{\boldsymbol{D}'_{2d}}_{24}}}, \overset{27}{\overbrace{\underbrace{\boldsymbol{D}_{3d}}_{28}}}, \overset{28}{\overbrace{\underbrace{\boldsymbol{T}}_{27}}}, \overset{29}{\overbrace{\underbrace{\boldsymbol{D}_{4h}}_{29}}}, \overset{30}{\overbrace{\underbrace{\boldsymbol{O}}_{30}}}, \overset{31}{\overbrace{\underbrace{\boldsymbol{T}_{h}}_{31}}}, \overset{32}{\overbrace{\underbrace{\boldsymbol{T}_{d}}_{32}}}, \overset{33}{\overbrace{\underbrace{\boldsymbol{O}_{h}}_{33}}}\} \quad (4)$$

The upper numbers are taken from the leftmost column of the mark table `tom_Oh_cuboct`, where the numbering is sequential from 1 to 33. On the other hand, the lower numbers taken from $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1) are reordered in Eq. 4 according to the appearance in the mark table `tom_Oh_cuboct`.

The data of Eq. 4 is converted into a permutation `perm_cuboct` by means of the GAP function `PermList`. The resulting permutation is used in the GAP function `SortedTom` to give a sorted mark table `test_sort` as follows:

```
gap> perm_cuboct := PermList
    ↪ ([1,2,3,4,6,5,7,10,12,15,13,9,11,8,14,16,19,17,18,20,23,26,22,25,21,24,28,27,29,30,31,32,33]);
(5,6)(8,10,15,14)(9,12)(11,13)(17,19,18)(21,23,22,26,24,25)(27,28)
gap> test_sort := SortedTom(tom_Oh_cuboct,perm_cuboct);;
gap> Display(test_sort);
 1: 48
 2: 24 8
 3: 24 . 4
 4: 24 . . 8
 5: 24 . . . 4
 6: 24 . . . . 24
(#omitted cf. Table 1)
```

The resulting mark table `test_sort` is found to be identical with the standard mark table based on $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1) which will be later obtained (Table 1).

2.2.4 Mark Table Based on the Truncated-octahedral Skeleton

A set of generators `gen4` for the truncated octahedron **4** is based on permutations stemmed from a four-fold axis, a three-fold axis and a mirror plane. Each permutation of degree 26 (= 24+2) controls the 24 vertices of **4**, accompanied with a mirror-permutation (a 2-cycle (25,26)). The application of the GAP function `Group` to `gen4` results in the construction of a CPR `Oh_troct`, which can be regarded as a permutation group isomorphic to the point group $\boldsymbol{O}_h$. The CPR `Oh_troct` is used to generate a mark table named `tom_Oh_troct` by means of the GAP function `TableOfMarks` as follows:

```
gap> gen4 := [(1,2,3,4)(5,6,7,8)(9,11,13,15)(10,12,14,16)(17,18,19,20)(21,22,23,24),
> (1,8,9)(4,16,5)(2,15,17)(3,20,10)(6,14,21)(7,24,11)(12,19,22)(13,23,18),
> (1,21)(2,22)(3,23)(4,24)(5,17)(6,18)(7,19)(8,20)(25,26)];;
gap> Oh_troct := Group(gen4); #truncated octahedron
Group([ (1,2,3,4)(5,6,7,8)(9,11,13,15)(10,12,14,16)(17,18,19,20)(21,22,23,24),
(1,8,9)(2,15,17)(3,20,10)(4,16,5)(6,14,21)(7,24,11)(12,19,22)(13,23,18),
(1,21)(2,22)(3,23)(4,24)(5,17)(6,18)(7,19)(8,20)(25,26) ])
gap> Display(Size(Oh_troct));
48
gap> tom_Oh_troct := TableOfMarks(Oh_troct);;
gap> Display(tom_Oh_troct);
 1: 48
 2: 24 8
```

```
 3: 24 . 4
 4: 24 . . 8
 5: 24 . . . 24
 6: 24 . . . . 4
(#omitted)
```

The mark table `tom_Oh_troct` calculated above is found to be based on the following $\mathrm{SSG}^{troct}_{\boldsymbol{O}_h}$ by using the GAP function `RepresentativeTom`:

$$
\begin{aligned}
\mathrm{SSG}^{troct}_{\boldsymbol{O}_h} = \{ & \underbrace{\overbrace{\boldsymbol{C}_1}^{1}}_{1}, \underbrace{\overbrace{\boldsymbol{C}_2}^{2}}_{2}, \underbrace{\overbrace{\boldsymbol{C}'_2}^{3}}_{3}, \underbrace{\overbrace{\boldsymbol{C}_s}^{4}}_{4}, \underbrace{\overbrace{\boldsymbol{C}_i}^{5}}_{6}, \underbrace{\overbrace{\boldsymbol{C}'_s}^{6}}_{5}, \underbrace{\overbrace{\boldsymbol{C}_3}^{7}}_{7}, \underbrace{\overbrace{\boldsymbol{D}_2}^{8}}_{10}, \underbrace{\overbrace{\boldsymbol{C}_{2v}}^{9}}_{12}, \underbrace{\overbrace{\boldsymbol{C}_{2h}}^{10}}_{15}, \\
& \underbrace{\overbrace{\boldsymbol{C}'_{2v}}^{11}}_{13}, \underbrace{\overbrace{\boldsymbol{S}_4}^{12}}_{9}, \underbrace{\overbrace{\boldsymbol{C}_4}^{13}}_{8}, \underbrace{\overbrace{\boldsymbol{D}'_2}^{14}}_{11}, \underbrace{\overbrace{\boldsymbol{C}'_{2h}}^{15}}_{16}, \underbrace{\overbrace{\boldsymbol{C}''_{2v}}^{16}}_{14}, \underbrace{\overbrace{\boldsymbol{C}_{3i}}^{17}}_{19}, \underbrace{\overbrace{\boldsymbol{D}_3}^{18}}_{17}, \underbrace{\overbrace{\boldsymbol{C}_{3v}}^{19}}_{18}, \underbrace{\overbrace{\boldsymbol{D}_4}^{20}}_{20}, \\
& \underbrace{\overbrace{\boldsymbol{D}_{2d}}^{21}}_{23}, \underbrace{\overbrace{\boldsymbol{C}_{4v}}^{22}}_{21}, \underbrace{\overbrace{\boldsymbol{D}'_{2d}}^{23}}_{24}, \underbrace{\overbrace{\boldsymbol{D}_{2h}}^{24}}_{25}, \underbrace{\overbrace{\boldsymbol{D}'_{2h}}^{25}}_{26}, \underbrace{\overbrace{\boldsymbol{C}_{4h}}^{26}}_{22}, \underbrace{\overbrace{\boldsymbol{D}_{3d}}^{27}}_{28}, \underbrace{\overbrace{\boldsymbol{T}}^{28}}_{27}, \underbrace{\overbrace{\boldsymbol{D}_{4h}}^{29}}_{29}, \underbrace{\overbrace{\boldsymbol{O}}^{30}}_{30}, \underbrace{\overbrace{\boldsymbol{T}_h}^{31}}_{31}, \underbrace{\overbrace{\boldsymbol{T}_d}^{32}}_{32}, \underbrace{\overbrace{\boldsymbol{O}_h}^{33}}_{33} \}
\end{aligned} \quad (5)
$$

The upper numbers are taken from the leftmost column of the mark table `tom_Oh_troct`, where the numbering is sequential from 1 to 33. On the other hand, the lower numbers taken from $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1) are reordered in Eq. 5 according to the appearance in the mark table `tom_Oh_troct`.

The data of Eq. 5 is converted into a permutation `perm_troct` by means of the GAP function `PermList`. The resulting permutation is used in the GAP function `SortedTom` to give a sorted mark table `test_sort` as follows:

```
gap> perm_troct := PermList
    ↪ ([1,2,3,4,6,5,7,10,12,15,13,9,8,11,16,14,19,17,18,20,23,21,24,25,26,22,28,27,29,30,31,32,33]);
(5,6)(8,10,15,16,14,11,13)(9,12)(17,19,18)(21,23,24,25,26,22)(27,28)
gap> test_sort := SortedTom(tom_Oh_troct,perm_troct);;
gap> Display(test_sort);
 1: 48
 2: 24 8
 3: 24 . 4
 4: 24 . . 8
 5: 24 . . . 4
 6: 24 . . . . 24
(#omitted cf. Table 1)
```

The resulting mark table `test_sort` is found to be identical with the standard mark table based on $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1) which will be later obtained (Table 1).

2.2.5 Mark Table Based on the Truncated-hexahedral Skeleton

A set of generators `gen5` for the truncated hexahedron **5** is based on permutations stemmed from a four-fold axis, a three-fold axis and a mirror plane. Note that the truncated hexahedron **5** is different from the truncated octahedron **5** in their concrete expressions of permutations whereas both of them have 24 vertices. Each permutation of degree 26 (= 24+2) controls the 24 vertices of **5**, accompanied with a mirror-permutation (a 2-cycle (25,26)). The application of the GAP function `Group` to `gen5` generates a CPR `Oh_trhex`, which can be regarded as a permutation group isomorphic to the point group $\boldsymbol{O}_h$. The CPR `Oh_trhex` is used to generate a mark table named `tom_Oh_trhex` by means of the GAP function `TableOfMarks` as follows:

```
gap> gen5 := [(1,3,5,7)(2,4,6,8)(9,10,11,12)(13,14,15,16)(17,19,21,23)(18,20,22,24),
> (1,9,2)(8,13,3)(4,12,18)(5,16,19)(6,24,14)(7,17,10)(11,23,20)(15,22,21),
> (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)];;
gap> Oh_trhex := Group(gen5); #truncated hexahedron
Group([ (1,3,5,7)(2,4,6,8)(9,10,11,12)(13,14,15,16)(17,19,21,23)(18,20,22,24),
(1,9,2)(3,8,13)(4,12,18)(5,16,19)(6,24,14)(7,17,10)(11,23,20)(15,22,21),
(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) ])
gap> Display(Size(Oh_trhex));
48
gap> tom_Oh_trhex := TableOfMarks(Oh_trhex);;
gap> Display(tom_Oh_trhex);
 1: 48
 2: 24 8
 3: 24 . 4
 4: 24 . . 4
 5: 24 . . . 24
 6: 24 . . . . 8
(#omitted)
```

The mark table `tom_Oh_trhex` calculated above is found to be based on the following $\mathrm{SSG}_{\boldsymbol{O}_h}^{trhex}$ by using the GAP function `RepresentativeTom`:

$$\begin{aligned}\mathrm{SSG}_{\boldsymbol{O}_h}^{trhex} = \{ & \overbrace{\underbrace{\boldsymbol{C}_1}_{1}}^{1}, \overbrace{\underbrace{\boldsymbol{C}_2}_{2}}^{2}, \overbrace{\underbrace{\boldsymbol{C}'_2}_{3}}^{3}, \overbrace{\underbrace{\boldsymbol{C}'_s}_{5}}^{4}, \overbrace{\underbrace{\boldsymbol{C}_i}_{6}}^{5}, \overbrace{\underbrace{\boldsymbol{C}_s}_{4}}^{6}, \overbrace{\underbrace{\boldsymbol{C}_3}_{7}}^{7}, \overbrace{\underbrace{\boldsymbol{C}_4}_{8}}^{8}, \overbrace{\underbrace{\boldsymbol{D}_2}_{10}}^{9}, \overbrace{\underbrace{\boldsymbol{C}_{2h}}_{15}}^{10}, \\ & \overbrace{\underbrace{\boldsymbol{C}'_{2v}}_{13}}^{11}, \overbrace{\underbrace{\boldsymbol{S}_4}_{9}}^{12}, \overbrace{\underbrace{\boldsymbol{C}''_{2v}}_{14}}^{13}, \overbrace{\underbrace{\boldsymbol{C}_{2v}}_{12}}^{14}, \overbrace{\underbrace{\boldsymbol{D}'_2}_{11}}^{15}, \overbrace{\underbrace{\boldsymbol{C}'_{2h}}_{16}}^{16}, \overbrace{\underbrace{\boldsymbol{C}_{3v}}_{18}}^{17}, \overbrace{\underbrace{\boldsymbol{C}_{3i}}_{19}}^{18}, \overbrace{\underbrace{\boldsymbol{D}_3}_{17}}^{19}, \overbrace{\underbrace{\boldsymbol{D}_4}_{20}}^{20}, \\ & \overbrace{\underbrace{\boldsymbol{D}_{2d}}_{23}}^{21}, \overbrace{\underbrace{\boldsymbol{C}_{4h}}_{22}}^{22}, \overbrace{\underbrace{\boldsymbol{D}_{2h}}_{25}}^{23}, \overbrace{\underbrace{\boldsymbol{C}_{4v}}_{21}}^{24}, \overbrace{\underbrace{\boldsymbol{D}'_{2d}}_{24}}^{25}, \overbrace{\underbrace{\boldsymbol{D}'_{2h}}_{26}}^{26}, \overbrace{\underbrace{\boldsymbol{D}_{3d}}_{28}}^{27}, \overbrace{\underbrace{\boldsymbol{T}}_{27}}^{28}, \overbrace{\underbrace{\boldsymbol{D}_{4h}}_{29}}^{29}, \overbrace{\underbrace{\boldsymbol{T}_d}_{32}}^{30}, \overbrace{\underbrace{\boldsymbol{T}_h}_{31}}^{31}, \overbrace{\underbrace{\boldsymbol{O}}_{30}}^{32}, \overbrace{\underbrace{\boldsymbol{O}_h}_{33}}^{33} \}\end{aligned} \quad (6)$$

The upper sequential numbers from 1 to 33 are taken from the leftmost column of the mark table `tom_Oh_trhex`, while the lower numbering is taken from $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1). Note that the latter numbering is reordered in Eq. 6 according to the appearance in the mark table `tom_Oh_trhex`.

The data of Eq. 6 is converted into a permutation `perm_trhex` by means of the GAP function `PermList`. The resulting permutation is used in the GAP function `SortedTom` to give a sorted mark table `test_sort` as follows:

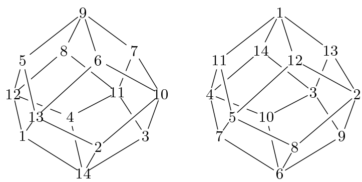
```
gap> perm_trhex := PermList
    ↪ ([1,2,3,5,6,4,7,8,10,15,13,9,14,12,11,16,18,19,17,20,23,22,25,21,24,26,28,27,29,32,31,30,33]);
```

```
(4,5,6)(9,10,15,11,13,14,12)(17,18,19)(21,23,25,24)(27,28)(30,32)
gap> test_sort := SortedTom(tom_Oh_trhex,perm_trhex);;
gap> Display(test_sort);
 1: 48
 2: 24 8
 3: 24 . 4
 4: 24 . . 8
 5: 24 . . . 4
 6: 24 . . . . 24
(#omitted cf. Table 1)
```

As the same name `test_sort` is used, the resulting mark table `test_sort` stemmed from the truncated hexahedron **5** is also found to be identical with the standard mark table based on SSG$_{\boldsymbol{O}_h}$ (Eq. 1) which will be later obtained (Table 1).

2.2.6 Mark Table Based on the Rhombic Dodecahedron

Let us next examine a rhombic dodecahedron **6**, which belongs to the point group $\boldsymbol{O}_h$ and has 14 vertices, 24 edges, and 12 faces. The 14 vertices are separated into eight vertices with valency 3 and six vertices with valency 4. Note that the eight vertices are capable of generating a hypothetical cubane skeleton, if they are linked directly; on the other hand, the six vertices are capable of generating a hypothetical octahedral skeleton, if they are linked directly. Figure 2 illustrates two modes of numbering of the rhombic dodecahedron, **6a** and **6b**.



6a **6b**

Figure 2. Rhombic dodecahedral skeletons with different modes of numbering. The skeleton **6** belongs to the point group $\boldsymbol{O}_h$. In the skeleton **6a** for the set of generators (`gen6`), the eight vertices with valency 3 are numbered from 1 to 8, while the six vertices with valency 4 are numbered from 9 to 14. In the skeleton **6b** for the set of generators (`gen7`), the six vertices with valency 4 are numbered from 1 to 6, while the eight vertices with valency 3 are numbered from 7 to 14.

As illustrated by the formula **6a**, the eight vertices related to a cubane skeleton are numbered in accord with the numbering of the cubane skeleton **2**; on the other hand, the six vertices related to an octahedral skeleton are numbered from 9 to 14 by adding 8 to the numbers from 1 to 6 of the octahedral skeleton **1**. Thereby, a set of generators (`gen6`) can be generated by referring to `gen2` of the cubane skeleton **2** and `gen1` of the octahedral skeleton **1**. The corresponding combined-permutation representation (CPR) `Oh_rhdod` is regarded as a permutation group isomorphic to the point group $\boldsymbol{O}_h$. The CPR `Oh_rhdod` is used to generate a mark table named `tom_Oh_rhdod` by means of the GAP function `TableOfMarks` as follows:

```
gap> gen6 := [(1,2,3,4)(5,6,7,8)(10,11,12,13), (2,4,5)(3,8,6)(9,10,11)(12,13,14),
> (1,5)(2,6)(3,7)(4,8)(9,14)(15,16)];; #generators for Oh_rhdod
gap> Oh_rhdod := Group(gen6); #rhombic dodecahedron skeleton
Group([ (1,2,3,4)(5,6,7,8)(10,11,12,13), (2,4,5)(3,8,6)(9,10,11)(12,13,14),
      (1,5)(2,6)(3,7)(4,8)(9,14)(15,16) ])
gap> Display(Size(Oh_rhdod));
48
gap> tom_Oh_rhdod := TableOfMarks(Oh_rhdod);;
gap> Display(tom_Oh_rhdod);
 1: 48
 2: 24 8
 3: 24 . 4
 4: 24 . . 4
 5: 24 . . . 24
 6: 24 . . . . 8
(#omitted)
```

The mark table `tom_Oh_rhdod` calculated above is found to be identical with the mark table `tom_Oh_cube`. It follows that $\mathrm{SSG}_{\boldsymbol{O}_h}^{rhdod}$ (Eq. 7) calculated by using the GAP function `RepresentativeTom` is identical with $\mathrm{SSG}_{\boldsymbol{O}_h}^{cube}$ (Eq. 3) as follows:

$$
\begin{aligned}
\mathrm{SSG}_{\boldsymbol{O}_h}^{rhdod} = \{ & \overbrace{\underbrace{\boldsymbol{C}_1}_{1}}^{1}, \overbrace{\underbrace{\boldsymbol{C}_2}_{2}}^{2}, \overbrace{\underbrace{\boldsymbol{C}'_2}_{3}}^{3}, \overbrace{\underbrace{\boldsymbol{C}'_s}_{5}}^{4}, \overbrace{\underbrace{\boldsymbol{C}_i}_{6}}^{5}, \overbrace{\underbrace{\boldsymbol{C}_s}_{4}}^{6}, \overbrace{\underbrace{\boldsymbol{C}_3}_{7}}^{7}, \overbrace{\underbrace{\boldsymbol{C}_4}_{8}}^{8}, \overbrace{\underbrace{\boldsymbol{D}_2}_{10}}^{9}, \overbrace{\underbrace{\boldsymbol{C}_{2v}}_{12}}^{10}, \\
& \overbrace{\underbrace{\boldsymbol{C}'_{2v}}_{13}}^{11}, \overbrace{\underbrace{\boldsymbol{S}_4}_{9}}^{12}, \overbrace{\underbrace{\boldsymbol{C}'_{2h}}_{16}}^{13}, \overbrace{\underbrace{\boldsymbol{C}_{2h}}_{15}}^{14}, \overbrace{\underbrace{\boldsymbol{D}'_2}_{11}}^{15}, \overbrace{\underbrace{\boldsymbol{C}''_{2v}}_{14}}^{16}, \overbrace{\underbrace{\boldsymbol{C}_{3v}}_{18}}^{17}, \overbrace{\underbrace{\boldsymbol{C}_{3i}}_{19}}^{18}, \overbrace{\underbrace{\boldsymbol{D}_3}_{17}}^{19}, \overbrace{\underbrace{\boldsymbol{D}_4}_{20}}^{20}, \\
& \overbrace{\underbrace{\boldsymbol{D}_{2d}}_{23}}^{21}, \overbrace{\underbrace{\boldsymbol{C}_{4v}}_{21}}^{22}, \overbrace{\underbrace{\boldsymbol{D}_{2h}}_{25}}^{23}, \overbrace{\underbrace{\boldsymbol{C}_{4h}}_{22}}^{24}, \overbrace{\underbrace{\boldsymbol{D}'_{2h}}_{26}}^{25}, \overbrace{\underbrace{\boldsymbol{D}'_{2d}}_{24}}^{26}, \overbrace{\underbrace{\boldsymbol{D}_{3d}}_{28}}^{27}, \overbrace{\underbrace{\boldsymbol{T}}_{27}}^{28}, \overbrace{\underbrace{\boldsymbol{D}_{4h}}_{29}}^{29}, \overbrace{\underbrace{\boldsymbol{T}_d}_{32}}^{30}, \overbrace{\underbrace{\boldsymbol{T}_h}_{31}}^{31}, \overbrace{\underbrace{\boldsymbol{O}}_{30}}^{32}, \overbrace{\underbrace{\boldsymbol{O}_h}_{33}}^{33} \}
\end{aligned} \qquad (7)
$$

The data of Eq. 7 is converted into a permutation `perm_rhdod` by means of the GAP function `PermList`. The resulting permutation is used in the GAP function `SortedTom` to `tom_Oh_rhdod`. Thereby, we are able to obtain a sorted mark table (`test_sort` for `tom_Oh_rhdod`), which is identical with `test_sort` for `tom_Oh_cube`. The resulting mark table `test_sort` for `tom_Oh_rhdod` is found to be identical with the standard mark table based on $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1) which will be later obtained (Table 1).

Let us next examine another mode **6b** of numbering for the rhombic dodecahedron. Then, the six vertices with valency 4 are numbered from 1 to 6 according to the numbering of the octahedron skeleton **1**, while the eight vertices with valency 3 are numbered from 7 to 14 in accord with the numbering of the cubane skeleton **2** by adding 6 to the numbers from 1 to 8 of the cubane skeleton **2**. Thereby, a set of generators (`gen7`) based on the formula **6b** can be generated by referring to `gen1` of the octahedral skeleton **1** and `gen2` of the cubic skeleton **2**. The corresponding combined-permutation representation (CPR) `Oh_rhdodN` is regarded as a permutation group isomorphic to the point group $\boldsymbol{O}_h$. The CPR `Oh_rhdodN` is used to generate a mark table named `tom_Oh_rhdodN` by means of the GAP function `TableOfMarks` as follows:

```
gap> gen7 := [(2,3,4,5)(7,8,9,10)(11,12,13,14), (1,2,3)(4,5,6)(8,10,11)(9,14,12),
> (1,6)(7,11)(8,12)(9,13)(10,14)(15,16)];; #generators for Oh_rhdodN
gap> Oh_rhdodN := Group(gen7); #rhombic dodecahedroN skeleton
Group([ (2,3,4,5)(7,8,9,10)(11,12,13,14), (1,2,3)(4,5,6)(8,10,11)(9,14,12),
      (1,6)(7,11)(8,12)(9,13)(10,14)(15,16) ])
gap> Display(Size(Oh_rhdodN));
48
gap> tom_Oh_rhdodN := TableOfMarks(Oh_rhdodN);;
gap> Display(tom_Oh_rhdodN);
 1: 48
 2: 24 8
 3: 24 . 4
 4: 24 . . 8
 5: 24 . . . 24
 6: 24 . . . . 4
(#omitted)
```

The mark table `tom_Oh_rhdodN` calculated above is found to be identical with the mark table `tom_Oh_octa`. It follows that $\mathrm{SSG}_{\boldsymbol{O}_h}^{rhdodN}$ (Eq. 8) calculated by using the GAP function `RepresentativeTom` is identical with $\mathrm{SSG}_{\boldsymbol{O}_h}^{octa}$ (Eq. 2) as follows:

$$
\begin{aligned}
\mathrm{SSG}_{\boldsymbol{O}_h}^{rhdodN} = \{ & \overbrace{\underbrace{\boldsymbol{C}_1}_{1}}^{1}, \overbrace{\underbrace{\boldsymbol{C}_2}_{2}}^{2}, \overbrace{\underbrace{\boldsymbol{C}'_2}_{3}}^{3}, \overbrace{\underbrace{\boldsymbol{C}_s}_{4}}^{4}, \overbrace{\underbrace{\boldsymbol{C}_i}_{6}}^{5}, \overbrace{\underbrace{\boldsymbol{C}'_s}_{5}}^{6}, \overbrace{\underbrace{\boldsymbol{C}_3}_{7}}^{7}, \overbrace{\underbrace{\boldsymbol{D}_2}_{10}}^{8}, \overbrace{\underbrace{\boldsymbol{C}_{2v}}_{12}}^{9}, \overbrace{\underbrace{\boldsymbol{C}_{2h}}_{15}}^{10}, \\
& \overbrace{\underbrace{\boldsymbol{C}'_{2v}}_{13}}^{11}, \overbrace{\underbrace{\boldsymbol{S}_4}_{9}}^{12}, \overbrace{\underbrace{\boldsymbol{C}_4}_{8}}^{13}, \overbrace{\underbrace{\boldsymbol{D}'_2}_{11}}^{14}, \overbrace{\underbrace{\boldsymbol{C}''_{2v}}_{14}}^{15}, \overbrace{\underbrace{\boldsymbol{C}'_{2h}}_{16}}^{16}, \overbrace{\underbrace{\boldsymbol{C}_{3i}}_{19}}^{17}, \overbrace{\underbrace{\boldsymbol{D}_3}_{17}}^{18}, \overbrace{\underbrace{\boldsymbol{C}_{3v}}_{18}}^{19}, \overbrace{\underbrace{\boldsymbol{D}_4}_{20}}^{20}, \\
& \overbrace{\underbrace{\boldsymbol{D}_{2d}}_{23}}^{21}, \overbrace{\underbrace{\boldsymbol{C}_{4v}}_{21}}^{22}, \overbrace{\underbrace{\boldsymbol{D}'_{2d}}_{24}}^{23}, \overbrace{\underbrace{\boldsymbol{D}_{2h}}_{25}}^{24}, \overbrace{\underbrace{\boldsymbol{D}'_{2h}}_{26}}^{25}, \overbrace{\underbrace{\boldsymbol{C}_{4h}}_{22}}^{26}, \overbrace{\underbrace{\boldsymbol{D}_{3d}}_{28}}^{27}, \overbrace{\underbrace{\boldsymbol{T}}_{27}}^{28}, \overbrace{\underbrace{\boldsymbol{D}_{4h}}_{29}}^{29}, \overbrace{\underbrace{\boldsymbol{O}}_{30}}^{30}, \overbrace{\underbrace{\boldsymbol{T}_h}_{31}}^{31}, \overbrace{\underbrace{\boldsymbol{T}_d}_{32}}^{32}, \overbrace{\underbrace{\boldsymbol{O}_h}_{33}}^{33} \}
\end{aligned}
\tag{8}
$$

It should be noted that the rhombic dodecahedron corresponds to different mark tables and different SSGs, when different sets of generators (i.e., `gen6` for **6a** and `gen7` for **6b**) are used during the calculation processes of the GAP system. That is to say, the set of generators (`gen6`) generates the mark table `tom_Oh_rhdod` and $\mathrm{SSG}_{\boldsymbol{O}_h}^{rhdod}$ (Eq. 7), while the other set of generators (`gen7`) generates the mark table `tom_Oh_rhdodN` and $\mathrm{SSG}_{\boldsymbol{O}_h}^{rhdodN}$ (Eq. 8).

The data of Eq. 8 is converted into a permutation `perm_rhdodN` by means of the GAP function `PermList`. The resulting permutation is used in the GAP function `SortedTom` to tom_Oh_rhdodN. Thereby, we are able to obtain a sorted mark table (test_sort for tom_Oh_rhdodN), which is identical with test_sort for tom_Oh_octa. The resulting mark table test_sort for tom_Oh_rhdodN is found to be identical with the standard mark table based on $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1) which will be later obtained (Table 1).

3 Concordant Construction of a Standard Mark Table and a USCI-CF Table for $\boldsymbol{O}_h$

As shown in the preceding section, the mark tables stemmed from the various skeletons of $\boldsymbol{O}_h$ (**1**–**5**) are different in their sequences of subgroups, where they obey the respective SSGs, i.e., $\mathrm{SSG}^{octa}_{\boldsymbol{O}_h}$ (Eq. 2) for **1**, $\mathrm{SSG}^{cube}_{\boldsymbol{O}_h}$ (Eq. 3) for **2**, $\mathrm{SSG}^{cuboct}_{\boldsymbol{O}_h}$ (Eq. 4) for **3**, $\mathrm{SSG}^{troct}_{\boldsymbol{O}_h}$ (Eq. 5) for **4**, and $\mathrm{SSG}^{trhex}_{\boldsymbol{O}_h}$ (Eq. 6) for **5**. In addition, the two modes of numbering for the rhombic-dodecahedral skeleton **6** give mark tables different in their sequences of subgroups, i.e., $\mathrm{SSG}^{rhdod}_{\boldsymbol{O}_h}$ (Eq. 7) for **6a** and $\mathrm{SSG}^{rhdodN}_{\boldsymbol{O}_h}$ (Eq. 8) for **6b**.

These mark tables with different appearances should be converted into a single format (called *a standard mark table*) based on $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1), even if the corresponding different sets of generators are used. This is because the mark table and the USCI-CF table reported in the previous article [15] are based on $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1).

The newly-developed functions MarkTableforUSCI and constructUSCITable [14] are capable of concordant construction of a mark table and a USCI-CF table by starting from a CPR based on any of $\boldsymbol{O}_h$-skeletons (**1**–**5** as well as **6**). To assure the concordance, a list of subgroups derived from each SSG (Eq. 2–Eq. 6 as well as Eqs. 7 and 8) is given as a list of sets of generators gen[1]–gen[33].

As shown in the Source Code named SubOh5-A.gap, for example, the CPR Oh_octa based on the octahedral skeleton **1** is characterized by the sets of generators gen[1]–gen[33], which are shown as the following list derived from $\mathrm{SSG}^{octa}_{\boldsymbol{O}_h}$ (Eq. 2). The set gen1 of generators for generating the CPR Oh_octa and the corresponding set gen1x of generators for specifying the point group $\boldsymbol{O}$ are written as an argument in the GAP function Group.

Source Code 1 (SubOh5-A.gap)

```
#Read("c:/fujita00/fujita2018/subductionOh/gap/SubOh5-A.gap");
LogTo("c:/fujita00/fujita2018/subductionOh/gap/SubOh5-Alog.txt");
Read("c:/fujita00/fujita2018/subductionOh/gap/USCICF.gapfunc");

gen1 := [(2,3,4,5), (1,2,3)(4,5,6), (1,6)(7,8)];; #generators for Oh_octa
Oh_octa := Group(gen1); #octahedral skeleton
```

```
Display(Size(Oh_octa));

gen1x := [(2,3,4,5), (1,2,3)(4,5,6)];; #generators for O
O_octa := AsSubgroup(Oh_octa,Group(gen1x));
Display(Size(O_octa));

#tom_Oh_octa := TableOfMarks(Oh_octa);;

#Subgroups of Oh given
gen := [];;
gen[1] := [ ];; #C1 --1
gen[2] := [ (2,4)(3,5) ];; #C2 --2
gen[3] := [ (1,3)(2,4)(5,6) ];; #C2' --3
gen[4] := [ (3,5)(7,8) ];; #Cs --4
gen[6] := [ (1,6)(2,4)(3,5)(7,8) ];; #Ci --5
gen[5] := [ (1,5)(3,6)(7,8) ];; #Cs'--6
gen[7] := [ (1,3,4)(2,6,5) ];; #C3 --7
gen[10] := [ (1,6)(3,5), (2,4)(3,5) ];; #D2 --8
gen[12] := [ (3,5)(7,8), (2,4)(3,5) ];; #C2v --9
gen[15] := [ (1,6)(7,8), (2,4)(3,5) ];; #C2h --10
gen[13] := [ (1,5)(3,6)(7,8), (1,6)(3,5) ];; #C2v' --11
gen[9] := [ (1,3,6,5)(2,4)(7,8), (1,6)(3,5) ];; #S4--12
gen[8] := [ (1,5,6,3), (1,6)(3,5) ];; #C4 --13
gen[11] := [ (1,3)(2,4)(5,6), (1,6)(3,5) ];; #D2' --14
gen[14] := [ (2,4)(7,8), (1,3)(2,4)(5,6) ];; #C2v'' --15
gen[16] := [ (1,6)(2,4)(3,5)(7,8), (1,3)(2,4)(5,6) ];; #C2h' -- 16
gen[19] := [ (1,6)(2,4)(3,5)(7,8), (1,3,4)(2,6,5) ];; #C3i -- 17
gen[17] := [ (1,5)(2,4)(3,6), (1,3,4)(2,6,5) ];; #D3 -- 18
gen[18] := [ (1,3)(5,6)(7,8), (1,3,4)(2,6,5) ];; #C3v -- 19
gen[20] := [ (1,6)(3,5), (2,4)(3,5), (1,5,6,3) ];; #D4 -- 20
gen[23] := [ (1,6)(3,5), (2,4)(3,5), (1,5)(3,6)(7,8) ];; #D2d -- 21
gen[21] := [ (3,5)(7,8), (1,5,6,3), (1,6)(3,5) ];; #C4v -- 22
gen[24] := [ (3,5)(7,8), (1,3)(2,4)(5,6), (1,6)(3,5) ];; #D2d' --23
gen[25] := [ (1,6)(3,5), (2,4)(3,5), (3,5)(7,8) ];; #D2h -- 24
gen[26] := [ (2,4)(7,8), (1,3)(2,4)(5,6), (1,6)(3,5) ];; #D2h' -- 25
gen[22] := [ (2,4)(7,8), (1,5,6,3), (1,6)(3,5) ];; #C4h -- 26
gen[28] := [ (1,6)(2,4)(3,5)(7,8), (1,5)(2,4)(3,6), (1,3,4)(2,6,5) ];; #D3d -- 27
gen[27] := [ (1,6)(3,5), (2,4)(3,5), (1,3,4)(2,6,5) ];; #T -- 28
gen[29] := [ (1,6)(3,5), (2,4)(3,5), (3,5)(7,8), (1,5,6,3) ];; #D4h -- 29
gen[30] := [ (1,6)(3,5), (2,4)(3,5), (1,3,4)(2,6,5), (1,5,6,3) ];; #O -- 30
gen[31] := [ (1,6)(3,5), (2,4)(3,5), (1,3,4)(2,6,5), (3,5)(7,8) ];; #Th -- 31
gen[32] := [ (1,6)(3,5), (2,4)(3,5), (1,3,4)(2,6,5), (1,5)(3,6)(7,8) ];; #Td -- 32
gen[33] := [ (2,3,4,5), (1,2,3)(4,5,6), (1,6)(7,8) ];; #Oh -- 33

#mark table sorted for USCI table
MarkTableOh := MarkTableforUSCI(Oh_octa,O_octa,33,gen,6,8);;
Display(MarkTableOh);

USCITableOh := constructUSCITable(Oh_octa,O_octa,33,gen,6,8);
Display("##USCI-CF table (USCITableOh) :");
Display(USCITableOh);

#Matrix form of mark table
Matrix_tomOhocta := MatTom(MarkTableOh);
Display(Matrix_tomOhocta);

Display("#Fixed point vector for octahedron");
FPVocta := calculateFPvector(Oh_octa,O_octa,33,gen,6,8);;
Display(FPVocta);

Display("#SCI-CF for octahedron");
l_SCICF_octa := constructSCICF(Oh_octa,O_octa,Matrix_tomOhocta,USCITableOh,FPVocta);;
Display(l_SCICF_octa);

Display("#list of PCI-CFs for octahedron");
l_PCICF_octa := l_SCICF_octa * Inverse(Matrix_tomOhocta);;
Display(l_PCICF_octa);

Display("#PCI-CFs for subgroups");
for i in [1..33] do
Print("PCI-CF[", i, "] := ", l_PCICF_octa[i], "\n");
od;
```

Table 1. Standard Mark Table of $\boldsymbol{O}_h$ (`MarkTableOh`)

```
 1: 48
 2: 24 8
 3: 24 . 4
 4: 24 . . 8
 5: 24 . . . 4
 6: 24 . . . . 24
 7: 16 . . . . . 4
 8: 12 4 . . . . . 4
 9: 12 4 . . . . . . 4
10: 12 12 . . . . . . . 12
11: 12 4 4 . . . . . . . 4
12: 12 4 . 8 . . . . . . . 4
13: 12 4 . . 4 . . . . . . . 4
14: 12 . 2 4 2 . . . . . . . . 2
15: 12 4 . 4 . 12 . . . . . . . . 4
16: 12 . 2 . 2 12 . . . . . . . . . 2
17: 8 . 4 . . . 2 . . . . . . . . . 2
18: 8 . . . 4 . 2 . . . . . . . . . . 2
19: 8 . . . . 8 2 . . . . . . . . . . . 2
20: 6 6 2 . . . . 2 . 6 2 . . . . . . . . 2
21: 6 2 . 4 2 . . 2 . . . 2 2 . . . . . . . 2
22: 6 2 . 2 . 6 . 2 2 . . . . . 2 . . . . . . 2
23: 6 6 . . 2 . . . 2 6 . . 2 . . . . . . . . . 2
24: 6 2 2 4 . . . . 2 . 2 2 . . . . . . . . . . . 2
25: 6 6 . 6 . 6 . . . 6 . 6 . . 6 . . . . . . . . . 6
26: 6 2 2 2 2 6 . . . . 2 . 2 2 2 2 . . . . . . . . . 2
27: 4 4 . . . . 4 . . 4 . . . . . . . . . . . . . . . . 4
28: 4 . 2 . 2 4 1 . . . . . . . . 2 1 1 1 . . . . . . . . 1
29: 3 3 1 3 1 3 . 1 1 3 1 3 1 1 3 1 . . . 1 1 1 1 1 3 1 . . 1
30: 2 2 2 . . . 2 2 . 2 2 . . . . . 2 . . 2 . . . . . . 2 . . 2
31: 2 2 . 2 . 2 2 . . 2 . 2 . . 2 . . . 2 . . . . . 2 . 2 . . . 2
32: 2 2 . . 2 . 2 . 2 2 . . 2 . . . . 2 . . . . 2 . . . 2 . . . . 2
33: 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1


LogTo();
```

Source Code 1 (named `SubOh5-A.gap`) is stored in an appropriate directory, in which the file `USCICF.gapfunc` containing the newly-developed functions `MarkTableforUSCI` and `constructUSCITable` is also stored. To execute the Source Code 1 (`SubOh5-A.gap`), the `Read` command shown in the top line is copied and pasted after the command prompt `gap>`. The calculation result is output into the log file named `SubOh5-Alog.txt`.

The newly-developed function `MarkTableforUSCI` generates the standard mark table (Table 1), which corresponds to $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1). Compare Table 1 with `tom_Oh_octa` shown in Subsubsection 2.2.1. Thereby, these mark tables are found to be different in the orders of rows and columns. Table 1 is identical with the sorted mark table `test_sort`, which has been calculated by using the GAP function `SortedTom` as shown in Subsubsection 2.2.1.

Such a standard mark table as Table 1 is linked with a USCI-CF table (Table 2), which is generated by the other newly-developed function `constructUSCITable` appearing in the above Source Code 1 (`SubOh5-A.gap`).

Table 2. USCI-CF Table of $\boldsymbol{O}_h$ (`USCITableOh`). Each symbol `a_d` corresponds to the sphericity index (SI) a_d for a d-membered homospheric orbit; `c_d` corresponds to the SI c_d for a d-membered enantiospheric orbit; and `b_d` corresponds to the SI b_d for a d-membered hemispheric orbit.

```
##USCI-CF table (USCITableOh) :
[ [b_1^48, b_2^24, b_2^24, c_2^24, c_2^24, c_2^24, b_3^16, b_4^12, c_4^12, b_4^12,
  b_4^12, c_4^12, c_4^12, c_4^12, c_4^12, c_4^12, b_6^8, c_6^8, c_6^8, b_8^6,
  c_8^6, c_8^6, c_8^6, c_8^6, c_8^6, c_8^6, b_12^4, c_12^4, c_16^3, b_24^2, c_24^2, c_24^2, c_48 ], #1 -- C1
 [b_1^24, b_1^8*b_2^8, b_2^12, c_2^12, c_2^12, c_2^12, b_3^8, b_2^4*b_4^4, c_2^4*c_4^4, b_2^12,
  b_2^4*b_4^4, c_2^4*c_4^4, c_2^4*c_4^4, c_4^6, c_2^4*c_4^4, c_4^6, b_6^4, c_6^4, c_6^4, b_4^6,
  c_4^2*c_8^2, c_4^2*c_8^2, c_4^6, c_4^2*c_8^2, c_4^6, c_4^2*c_8^2, b_6^4, c_12^2, c_8^3, b_12^2, c_12^2, c_12^2, c_24], #2--C2
 [b_1^24, b_2^12, b_1^4*b_2^10, c_2^12, c_2^12, c_2^12, b_3^8, b_4^6, c_4^6, b_4^6,
  b_2^4*b_4^4, c_4^6, c_4^6, c_2^2*c_4^5, c_4^6, c_2^2*c_4^5, b_3^4*b_6^2, c_6^4, c_6^4, b_4^2*b_8^2,
  c_8^3, c_8^3, c_8^3, c_4^2*c_8^2, c_8^3, c_4^2*c_8^2, b_12^2, c_6^2*c_12, c_8*c_16, b_12^2, c_24, c_24, c_24 ], #3 -- C2'
 [b_1^24, b_2^12, b_2^12, a_1^8*c_2^8, c_2^12, c_2^12, b_3^8, b_4^6, c_4^6, b_4^6,
  b_4^6, a_2^8*c_4^2, c_4^6, a_2^4*c_4^4, a_2^4*c_4^4, c_4^6, b_6^4, c_6^4, c_6^4, b_8^3,
  a_4^4*c_8, a_4^2*c_8^2, c_8^3, a_4^4*c_8, a_4^6, a_4^2*c_8^2, b_12^2, c_12^2, a_8^3, b_24, a_12^2, c_24, a_24 ], #4 -- Cs
 [b_1^24, b_2^12, b_2^12, c_2^12, a_1^4*c_2^10, c_2^12, b_3^8, b_4^6, c_4^6, b_4^6,
  b_4^6, c_4^6, a_2^4*c_4^4, a_2^2*c_4^5, c_4^6, a_2^2*c_4^5, b_6^4, a_3^4*c_6^2, c_6^4, b_8^3,
  a_4^2*c_8^2, c_8^3, a_4^2*c_8^2, c_8^3, c_8^3, a_4^2*c_8^2, b_12^2, a_6^2*c_12, a_8*c_16, b_24,c_24,a_12^2, a_24], #5 -- Cs'
 [b_1^24, b_2^12, b_2^12, c_2^12, c_2^12, a_1^24, b_3^8, b_4^6, c_4^6, b_4^6,
  b_4^6, c_4^6, c_4^6, c_4^6, a_2^12, a_2^12, b_6^4, c_6^4, a_3^8, b_8^3,
  c_8^3, a_4^6, c_8^3, c_8^3, a_4^6, a_4^6, b_12^2, a_6^4, a_8^3, b_24, a_12^2, c_24, a_24 ], #6 -- Ci
 [b_1^16, b_2^8, b_2^8, c_2^8, c_2^8, c_2^8, b_1^4*b_3^4, b_4^4, c_4^4, b_4^4,
  b_4^4, c_4^4, c_4^4, c_4^4, c_4^4, c_4^4, b_2^2*b_6^2, c_2^2*c_6^2, c_2^2*c_6^2, b_8^2,
  c_8^2, c_8^2, c_8^2, c_8^2, c_8^2, c_8^2, b_4^4, c_4*c_12, c_16, b_8^2, c_8^2, c_8^2, c_16 ], #7 -- C3
 [b_1^12, b_1^4*b_2^4, b_2^6, c_2^6, c_2^6, c_2^6, b_3^4, b_1^4*b_4^2, c_2^2*c_4^2, b_2^6,
  b_2^2*b_4^2, c_2^2*c_4^2, c_2^2*c_4^2, c_4^3, c_2^2*c_4^2, c_4^3, b_6^2, c_6^2, c_6^2, b_2^2*b_4^2,
  c_2^2*c_8, c_2^2*c_8, c_4^3, c_4*c_8, c_4^3, c_4*c_8, b_6^2, c_12, c_4*c_8, b_6^2, c_12, c_12, c_12 ], #8 -- C4
 [b_1^12, b_1^4*b_2^4, b_2^6, c_2^6, c_2^6, c_2^6, b_3^4, b_2^2*b_4^2, a_1^4*c_4^2, b_2^6,
  b_2^2*b_4^2, c_2^2*c_4^2, c_2^2*c_4^2, c_4^3, c_2^2*c_4^2, c_4^3, b_6^2, c_6^2, c_6^2, b_4^3,
  c_4*c_8, a_2^2*c_8, a_2^2*c_4^2, a_2^2*c_8, c_4^3, c_4*c_8, b_6^2, c_12, a_4*c_8, b_12, c_12, a_6^2, a_12 ], #9 -- S4
 [b_1^12, b_1^12, b_2^6, c_2^6, c_2^6, c_2^6, b_3^4, b_2^6, c_2^6, b_1^12,
  b_2^6, c_2^6, c_2^6, c_4^3, c_2^6, c_4^3, b_6^2, c_6^2, c_6^2, b_2^6,
  c_4^3, c_4^3, c_2^6, c_4^3, c_2^6, c_4^3, b_3^4, c_12, c_4^3, b_6^2, c_6^2, c_6^2, c_12 ], #10 -- D2
 [b_1^12, b_1^4*b_2^4, b_1^4*b_2^4, c_2^6, c_2^6, c_2^6, b_3^4, b_2^2*b_4^2, c_2^2*c_4^2, b_2^6,
  b_1^4*b_4^2, c_2^2*c_4^2, c_2^2*c_4^2, c_2^2*c_4^2, c_2^2*c_4^2, c_2^2*c_4^2, b_3^4, c_6^2, c_6^2, b_2^2*b_4^2,
  c_4*c_8, c_4*c_8, c_4^3, c_2^2*c_8, c_4^3, c_2^2*c_8, b_6^2, c_6^2, c_4*c_8, b_6^2, c_12, c_12, c_12 ], #11 -- D2'
 [b_1^12, b_1^4*b_2^4, b_2^6, a_1^8*c_2^2, c_2^6, c_2^6, b_3^4, b_2^2*b_4^2, c_2^2*c_4^2, b_2^6,
  b_2^2*b_4^2, a_1^4*a_2^4, c_2^2*c_4^2, a_2^4*c_4, a_2^4*c_2^2, c_4^3, b_6^2, c_6^2, c_6^2, b_4^3,
  a_2^2*a_4^2, a_4^2*c_4, c_4^3, a_2^2*a_4^2, a_2^6, a_4^2*c_4, b_6^2, c_12, a_4^3, b_12, a_6^2, c_12, a_12 ], #12 -- C2v
 [b_1^12, b_1^4*b_2^4, b_2^6, c_2^6, a_1^4*c_2^4, c_2^6, b_3^4, b_2^2*b_4^2, c_2^2*c_4^2, b_2^6,
  b_2^2*b_4^2, c_2^2*c_4^2, a_1^4*c_4^2, a_2^2*c_4^2, c_2^2*c_4^2, a_2^2*c_4^2, b_6^2, a_3^4, c_6^2, b_4^3,
  a_2^2*c_8, c_4*c_8, a_2^2*c_4^2, c_4*c_8, c_4^3, a_2^2*c_8, b_6^2, a_6^2, a_4*c_8, b_12, c_12, a_6^2, a_12 ], #13 --C2v'
 [b_1^12, b_2^6, b_1^2*b_2^5, a_1^4*c_2^4, a_1^2*c_2^5, c_2^6, b_3^4, b_4^3, c_4^3, b_4^3,
  b_2^2*b_4^2, a_2^4*c_4, a_2^2*c_4^2, a_1^2*a_2*c_4^2, a_2^2*c_4^2, a_2*c_2*c_4^2, b_3^2*b_6, a_3^2*c_6, c_6^2, b_4*b_8,
  a_4^3, a_4*c_8, a_4*c_8, a_4^2*c_4, a_4^3, a_2^2*c_8, b_12, a_6*c_6, a_4*a_8, b_12, a_12, a_12, a_12 ], #14 -- C2v''
 [b_1^12, b_1^4*b_2^4, b_2^6, a_1^4*c_2^4, c_2^6, a_1^12, b_3^4, b_2^2*b_4^2, c_2^2*c_4^2, b_2^6,
  b_2^2*b_4^2, a_2^4*c_2^2, c_2^2*c_4^2, a_2^2*c_4^2, a_1^4*a_2^4, a_2^6, b_6^2, c_6^2, a_3^4, b_4^3,
  a_4^2*c_4, a_2^2*a_4^2, c_4^3, a_4^2*c_4, a_2^6, a_2^2*a_4^2, b_6^2, a_6^2, a_4^3, b_12, a_6^2, c_12, a_12 ], #15 -- C2h
 [b_1^12, b_2^6, b_1^2*b_2^5, c_2^6, a_1^2*c_2^5, a_1^12, b_3^4, b_4^3, c_4^3, b_4^3,
  b_2^2*b_4^2, c_4^3, a_2^2*c_4^2, a_2*c_2*c_4^2, a_2^6, a_1^2*a_2^5, b_3^2*b_6, a_3^2*c_6, a_3^4, b_4*b_8,
  a_4*c_8, a_4^3, a_4*c_8, c_4*c_8, a_4^3, a_2^2*a_4^2, b_12, a_3^2*a_6, a_4*a_8, b_12, a_12, a_12, a_12 ], #16 -- C2h'
 [b_1^8, b_2^4, b_1^4*b_2^2, c_2^4, c_2^4, c_2^4, b_1^2*b_3^2, b_4^2, c_4^2, b_4^2,
  b_2^4, c_4^2, c_4^2, c_2^2*c_4, c_4^2, c_2^2*c_4, b_1^2*b_3^2, c_2*c_6, c_2*c_6, b_4^2,
  c_8, c_8, c_8, c_4^2, c_8, c_4^2, b_4^2, c_2*c_6, c_8, b_4^2, c_8, c_8, c_8 ], #17 -- D3
 [b_1^8, b_2^4, b_2^4, c_2^4, a_1^4*c_2^2, c_2^4, b_1^2*b_3^2, b_4^2, c_4^2, b_4^2,
  b_4^2, c_4^2, a_2^4, a_2^2*c_4, c_4^2, a_2^2*c_4, b_2*b_6, a_1^2*a_3^2, c_2*c_6, b_8,
  a_4^2, c_8, a_4^2, c_8, c_8, a_4^2, b_4^2, a_2*a_6, a_8, b_8, c_8, a_4^2, a_8 ], #18 -- C3v
 [b_1^8, b_2^4, b_2^4, c_2^4, c_2^4, a_1^8, b_1^2*b_3^2, b_4^2, c_4^2, b_4^2,
  b_4^2, c_4^2, c_4^2, c_4^2, a_2^4, a_2^4, b_2*b_6, c_2*c_6, a_1^2*a_3^2, b_8,
  c_8, a_4^2, c_8, c_8, a_4^2, a_4^2, b_4^2, a_2*a_6, a_8, b_8, a_4^2, c_8, a_8 ], #19 -- C3i
 [b_1^6, b_1^6, b_1^2*b_2^2, c_2^3, c_2^3, c_2^3, b_3^2, b_1^2*b_2^2, c_2^3, b_1^6,
  b_1^2*b_2^2, c_2^3, c_2^3, c_2*c_4, c_2^3, c_2*c_4, b_3^2, c_6, c_6,
  b_1^2*b_2^2, c_2*c_4, c_2*c_4, c_2^3, c_2*c_4, c_2^3,c_2*c_4, b_3^2, c_6, c_2*c_4, b_3^2, c_6, c_6, c_6 ], #20 -- D4
 [b_1^6, b_1^2*b_2^2, b_2^3, a_1^4*c_2, a_1^2*c_2^2, c_2^3, b_3^2, b_1^2*b_4, c_2*c_4, b_2^3,
  b_2*b_4, a_1^2*a_2^2, a_1^2*c_4, a_2^3, a_2^2*c_2, a_2*c_4, b_6, a_3^2, c_6, b_2*b_4,
  a_1^2*a_4, a_4*c_2, a_2*c_4, a_2*a_4, a_2^3, a_2*a_4, b_6, a_6, a_2*a_4, b_6, a_6, a_6, a_6 ], #21 -- C4v
 [b_1^6, b_1^2*b_2^2, b_2^3, a_1^2*c_2^2, c_2^3, a_1^6, b_3^2, b_1^2*b_4, a_1^2*c_4, b_2^3,
  b_2*b_4, a_2^2*c_2, c_2*c_4, a_2*c_4, a_1^2*a_2^2, a_2^3, b_6, c_6, a_3^2, b_2*b_4,
  a_4*c_2, a_1^2*a_4, a_2*c_4, a_2*a_4, a_2^3, a_2*a_4, b_6, a_6, a_2*a_4, b_6, a_6, a_6, a_6 ], #22 -- C4h
 [b_1^6, b_1^6, b_2^3, c_2^3, a_1^2*c_2^2, c_2^3, b_3^2, b_2^3, a_1^2*c_2^2, b_1^6,
  b_2^3, c_2^3, a_1^2*c_2^2, a_2*c_4, c_2^3, a_2*c_4, b_6, a_3^2, c_6, b_2^3,
  a_2*c_4, a_2*c_4, a_1^2*c_2^2, a_2*c_4, c_2^3, a_2*c_4, b_3^2, a_6, a_2*c_4, b_6, c_6, a_3^2, a_6 ], #23 -- D2d
 [b_1^6, b_1^2*b_2^2, b_1^2*b_2^2, a_1^4*c_2, c_2^3, c_2^3, b_3^2, b_2*b_4, a_1^2*c_4, b_2^3,
  b_1^2*b_4, a_1^2*a_2^2, c_2*c_4, a_2^2*c_2, a_2^2*c_2, c_2*c_4, b_3^2, c_6, c_6, b_2*b_4,
  a_2*a_4, a_2*a_4, a_2*c_4, a_1^2*a_4, a_2^3, a_4*c_2, b_6, c_6, a_2*a_4, b_6, a_6, a_6, a_6 ], #24 -- D2d'
 [b_1^6, b_1^6, b_2^3, a_1^6, c_2^3, a_1^6, b_3^2, b_2^3, c_2^3, b_1^6,
  b_2^3, a_1^6, c_2^3, a_2^3, a_1^6, a_2^3, b_6, c_6, a_3^2, b_2^3,
  a_2^3, a_2^3, c_2^3, a_2^3, a_1^6, a_2^3, b_3^2, a_6, a_2^3, b_6, a_3^2, c_6, a_6 ], #25 -- D2h
 [b_1^6, b_1^2*b_2^2, b_1^2*b_2^2, a_1^2*c_2^2, a_1^2*c_2^2, a_1^6, b_3^2, b_2*b_4, c_2*c_4, b_2^3,
  b_1^2*b_4, a_2^2*c_2, a_1^2*c_4, a_1^2*c_4, a_1^2*a_2^2, a_1^2*a_2^2, b_3^2, a_3^2, a_3^2, b_2*b_4,
  a_2*a_4, a_2*a_4, a_2*c_4, a_4*c_2, a_2^3, a_1^2*a_4, b_6, a_3^2, a_2*a_4, b_6, a_6, a_6, a_6 ], #26 -- D2h'
 [b_1^4, b_1^4, b_2^2, c_2^2, c_2^2, c_2^2, b_1^4, b_2^2, c_2^2, b_1^4,
  b_2^2, c_2^2, c_2^2, c_4, c_2^2, c_4, b_2^2, c_2^2, c_2^2, b_2^2,
  c_4, c_4, c_2^2, c_4, c_2^2, c_4, b_1^4, c_4, c_4, b_2^2, c_2^2, c_2^2, c_4 ], #27 -- T
 [b_1^4, b_2^2, b_1^2*b_2, c_2^2, a_1^2*c_2, a_1^4, b_1*b_3, b_4, c_4, b_4,
  b_2^2, c_4, a_2^2, a_2*c_2, a_2^2, a_1^2*a_2, b_1*b_3, a_1*a_3, a_1*a_3, b_4,
  a_4, a_4, a_4, c_4, a_4, a_2^2, b_4, a_1*a_3, a_4, b_4, a_4, a_4, a_4 ], #28 -- D3d
 [b_1^3, b_1^3, b_1*b_2, a_1^3, a_1*c_2, a_1^3, b_3, b_1*b_2, a_1*c_2, b_1^3,
  b_1*b_2, a_1^3, a_1*c_2, a_1*a_2, a_1^3, a_1*a_2, b_3, a_3, a_3, b_1*b_2,
  a_1*a_2, a_1*a_2, a_1*c_2, a_1*a_2, a_1^3, a_1*a_2, b_3, a_3, a_1*a_2, b_3, a_3, a_3, a_3 ], #29 -- D4h
 [b_1^2, b_1^2, b_1^2, c_2, c_2, c_2, b_1^2, b_1^2, c_2, b_1^2,
  b_1^2, c_2, c_2, c_2, c_2, c_2, b_1^2, c_2, c_2, b_1^2,
  c_2, c_2, c_2, c_2, c_2, c_2, b_1^2, c_2, c_2, b_1^2, c_2, c_2, c_2 ], #30 -- O
 [b_1^2, b_1^2, b_2, a_1^2, c_2, a_1^2, b_1^2, b_2, c_2, b_1^2,
  b_2, a_1^2, c_2, a_2, a_1^2, a_2, b_2, c_2, a_1^2, b_2,
  a_2, a_2, c_2, a_2, a_1^2, a_2, b_1^2, a_2, a_2, b_2, a_1^2, c_2, a_2 ], #31 -- Th
 [b_1^2, b_1^2, b_2, c_2, a_1^2, c_2, b_1^2, b_2, a_1^2, b_1^2,
  b_2, c_2, a_1^2, a_2, c_2, a_2, b_2, a_1^2, c_2, b_2,
  a_2, a_2, a_1^2, a_2, c_2, a_2, b_1^2, a_2, a_2, b_2, c_2, a_1^2, a_2 ], #32 -- Td
 [b_1, b_1, b_1, a_1, a_1, a_1, b_1, b_1, a_1, b_1,
  b_1, a_1, a_1, a_1, a_1, a_1, b_1, a_1, a_1, b_1,
  a_1, a_1, a_1, a_1, a_1, a_1, b_1, a_1, a_1, b_1, a_1, a_1, a_1 ] ] #33 -- Oh
```

Table 3. Matrix of Standard Mark Table of $\boldsymbol{O}_h$ (`Matrix_tomOh`)

```
[ [48, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [24, 8, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [24, 0, 4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [24, 0, 0, 8, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [24, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [24, 0, 0, 0, 0, 24, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [16, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [12, 4, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [12, 4, 0, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [12, 12, 0, 0, 0, 0, 0, 0, 0, 12, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [12, 4, 4, 0, 0, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [12, 4, 0, 8, 0, 0, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [12, 4, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [12, 0, 2, 4, 2, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [12, 4, 0, 4, 0, 12, 0, 0, 0, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [12, 0, 2, 0, 2, 12, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [8, 0, 4, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [8, 0, 0, 0, 4, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [8, 0, 0, 0, 0, 8, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [6, 6, 2, 0, 0, 0, 0, 2, 0, 6, 2, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [6, 2, 0, 4, 2, 0, 0, 2, 0, 0, 0, 2, 2, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [6, 2, 0, 2, 0, 6, 0, 2, 2, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [6, 6, 0, 0, 2, 0, 0, 0, 2, 6, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [6, 2, 2, 4, 0, 0, 0, 0, 2, 0, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [6, 6, 0, 6, 0, 6, 0, 0, 0, 6, 0, 6, 0, 0, 6, 0, 0, 0, 0, 0, 0, 0, 0, 0, 6, 0, 0, 0, 0, 0, 0, 0, 0],
  [6, 2, 2, 2, 2, 6, 0, 0, 0, 0, 2, 0, 2, 2, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0],
  [4, 4, 0, 0, 0, 0, 4, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0],
  [4, 0, 2, 0, 2, 4, 1, 0, 0, 0, 0, 0, 0, 0, 0, 2, 1, 1, 1, 0, 0, 0, 0,0, 0, 0, 0, 1, 0, 0, 0, 0, 0],
  [3, 3, 1, 3, 1, 3, 0, 1, 1, 3, 1, 3, 1, 1, 3, 1, 0, 0, 0, 1, 1, 1, 1, 1, 3, 1, 0, 0, 1, 0, 0, 0, 0],
  [2, 2, 2, 0, 0, 0, 2, 2, 0, 2, 2, 0, 0, 0, 0, 0, 2, 0, 0, 2, 0, 0, 0, 0, 0, 2, 0, 0, 2, 0, 0, 0, 0],
  [2, 2, 0, 2, 0, 2, 2, 0, 0, 2, 0, 2, 0, 0, 2, 0, 0, 0, 2, 0, 0, 0, 0, 0, 2, 0, 2, 0, 0, 0, 2, 0, 0],
  [2, 2, 0, 0, 2, 0, 2, 0, 2, 2, 0, 0, 2, 0, 0, 0, 0, 2, 0, 0, 0, 0, 2, 0, 0, 0, 2, 0, 0, 0, 0, 2, 0],
  [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1] ]
```

The USCI-CF table (`USCITableOh`) shown in Table 2 follows the convention of the GAP system for printing a matrix format, where a nested list of the GAP system is used. Each list in an inner pair of square brackets is a row vector of the matrix, and an outer pair of square brackets contains thirty-three of such row vectors to indicate the whole format of the matrix.

The standard mark table shown in Table 1 follows the convention of the GAP system for printing mark tables. A usual 33×33 matrix format is obtained as a nested list (Table 3) by using the GAP function `MatTom`, as shown in the last part of the above Source Code 1 (`SubOh5-A.gap`).

The concordant construction of a mark table and a USCI-CF table for $\boldsymbol{O}_h$ can be conducted by selecting the other $\boldsymbol{O}_h$-skeletons (**2**–**5** as well as **6**). For example, the set of generators `gen2` for generating the CPR `Oh_cube` for the cubane skeleton **2** (cf. Subsubsection 2.2.2) and the $\mathrm{SSG}_{\boldsymbol{O}_h}^{cube}$ (Eq. 3) are applied in a similar way to the above Source Code 1 (`SubOh5-A.gap`). The sets of generators `gen[1]`–`gen[33]` are specified according to the $\mathrm{SSG}_{\boldsymbol{O}_h}^{cube}$ (Eq. 3). The newly-developed functions `MarkTableforUSCI` and `constructUSCITable` are used as follows:

```
#mark table sorted for USCI table
MarkTableOhcube := MarkTableforUSCI(Oh_cube,O_cube,33,gen,8,10);;
Display(MarkTableOhcube);

USCITableOhcube := constructUSCITable(Oh_cube,O_cube,33,gen,8,10);
Display("##USCI-CF table (USCITableOhcube) :");
Display(USCITableOhcube);
```

The arguments '8' and '10' in these functions are based on the fact that the CPR for the cubane skeleton **2** has degree 10 ($= 8 + 2$), as found in the set of generators `gen2` (cf. Subsubsection 2.2.2). The resulting standard mark table (`MarkTableOhcube`) is identical with Table 1. In addition, the resulting USCI-CF table (`USCITableOhcube`) is identical with Table 2.

4 Generation of SCI-CFs

In general, a given skeleton has one or more orbits, where each orbit is governed by a coset representation. Each of the skeletons shown in Figure 1 has one orbit [12]. The six vertices of the octahedral skeleton **1** belong to one orbit, which corresponds to the coset representation $(\boldsymbol{C}_{4v}\backslash)\boldsymbol{O}_h$ (size: $|\boldsymbol{O}_h|/|\boldsymbol{C}_{4v}| = 48/8 = 6$); the eight vertices of the cubane skeleton **2** belong to one orbit, which corresponds to the coset representation $(\boldsymbol{C}_{3v}\backslash)\boldsymbol{O}_h$ (size: $|\boldsymbol{O}_h|/|\boldsymbol{C}_{3v}| = 48/6 = 8$); the twelve vertices of the cuboctahedron skeleton **3** belong to one orbit, which corresponds to the coset representation $(\boldsymbol{C}''_{2v}\backslash)\boldsymbol{O}_h$ (size: $|\boldsymbol{O}_h|/|\boldsymbol{C}_{2v}| = 48/4 = 12$); the twenty-four vertices of the truncated octahedron skeleton **4** belong to one orbit, which corresponds to the coset representation $(\boldsymbol{C}_s\backslash)\boldsymbol{O}_h$ (size: $|\boldsymbol{O}_h|/|\boldsymbol{C}_s| = 48/2 = 24$); and the twenty-four vertices of the truncated hexahedron skeleton **5** belong to one orbit, which corresponds to the coset representation $(\boldsymbol{C}'_s\backslash)\boldsymbol{O}_h$ (size: $|\boldsymbol{O}_h|/|\boldsymbol{C}'_s| = 48/2 = 24$).

As calculated in Source Code 1 (`SubOh5-A.gap`) for the octahedral skeleton **1**, for example, the fixed-point vector (`FPVocta`) is calculated by using the newly-developed function `calculateFPvector` [14]; and the list of SCI-CFs (`l_SCICF_octa`) is calculated by using the newly-developed function `constructSCICF` [14]. The corresponding outputs in the log file `SubOh5-Alog.gap` are as follows:

```
#Fixed point vector for octahedron --- #FPVocta :=
[ 6, 2, 0, 4, 2, 0, 0, 2, 0, 0, 0, 2, 2, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 ]
#SCI-CF for octahedron --- #l_SCICF_octa :=
[ b_1^6, b_1^2*b_2^2, b_2^3, c_2*a_1^4, c_2^2*a_1^2, c_2^3, b_3^2, b_1^2*b_4, c_2*c_4, b_2^3, b_2*b_4,
  a_1^2*a_2^2, c_4*a_1^2, a_2^3, c_2*a_2^2, c_4*a_2, b_6, a_3^2, c_6, b_2*b_4, a_1^2*a_4, c_2*a_4,
  c_4*a_2, a_2*a_4, a_2^3, a_2*a_4, b_6, a_6, a_2*a_4, b_6, a_6, a_6, a_6 ]
```

Because the octahedral skeleton **1** has one orbit governed by $(\boldsymbol{C}_{4v}\backslash)\boldsymbol{O}_h$, the $\boldsymbol{C}_{4v}$-row (the 21th-row) in the mark table (Table 1 or Table 3) is identical with the FPV calculated above; and the $\boldsymbol{C}_{4v}$-row (the 21th-row) in the USCI-CF table (Table 2) is identical with the list of SCI-CFs (`l_SCICF_octa`). Note that the point group $\boldsymbol{C}_{4v}$ appears as the 21th subgroup in Eq. 1. In a similar way, the fixed-point vectors and the lists of SCI-CFs for the other skeletons collected in Figure 1 appear in the corresponding rows of the mark table (Table 1 or Table 3) and of the USCI-CF table (Table 2).

On the other hand, the rhombic dodecahedron **6** shown in Figure 2 has two orbits. Thus, the eight vertices with valency 3 in **6** belong to one orbit governed by the coset representation $(\boldsymbol{C}_{3v}\backslash)\boldsymbol{O}_h$ (size: $|\boldsymbol{O}_h|/|\boldsymbol{C}_{3v}| = 48/6 = 8$), while the six vertices with valency 4 in **6** belong to the other orbit governed by the coset representation $(\boldsymbol{C}_{4v}\backslash)\boldsymbol{O}_h$ (size: $|\boldsymbol{O}_h|/|\boldsymbol{C}_{4v}| = 48/8 = 6$).

In spite of the presence of two orbits, the rhombic dodecahedron **6** can be treated in a similar way to Source Code 1 (`SubOh5-A.gap`) for treating the octahedral skeleton **1** with one orbit. Thus, the fixed-point vector (`FPVrhdod`) is calculated by using the newly-developed function `calculateFPvector`; and the list of SCI-CFs (`l_SCICF_rhdod`) is calculated by using the newly-developed function `constructSCICF`. The outputs in the corresponding log file are as follows:

```
#Fixed point vector for rhombic dodecahedron ---- FPVrhdod :=
[ 14, 2, 0, 4, 6, 0, 2, 2, 0, 0, 0, 2, 2, 0, 0, 0, 0, 2, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 ]
#SCI-CF for rhombic dodecahedron ---- l_SCICF_rhdod :=
[ b_1^14, b_1^2*b_2^6, b_2^7, c_2^5*a_1^4, c_2^4*a_1^6, c_2^7, b_1^2*b_3^4, b_1^2*b_4^3, c_2*c_4^3,
  b_2^3*b_4^2, b_2*b_4^3, c_4^2*a_1^2*a_2^2, c_4*a_1^2*a_2^4, c_4*a_2^5, c_2*c_4^2*a_2^2, c_4^2*a_2^3,
  b_2*b_6^2, a_1^2*a_3^4, c_2*c_6^2, b_2*b_4*b_8, a_1^2*a_4^3, c_2*c_8*a_4, c_4*a_2*a_4^2, c_8*a_2*a_4,
  c_8*a_2^3, a_2*a_4^3, b_4^2*b_6, a_2*a_6^2, a_2*a_4*a_8, b_6*b_8, c_8*a_6, a_4^2*a_6, a_8*a_6 ]
```

The fixed-point vector (`FPVrhdod`) multiplied by the inverse of the standard mark table (`Matrix_tomOh` shown in Table 3) indicates the presence of two orbits:

```
gap> Matrix_tomOhocta :=
> [ [48, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
> [24, 8, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
   (#omitted, cf. Table 3)
> [8, 0, 0, 0, 4, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
   (#the 18th C_3v-row, others omitted, cf. Table 3)
> [6, 2, 0, 4, 2, 0, 0, 2, 0, 0, 0, 2, 2, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
   (#the 21th C_4v-row, others omitted, cf. Table 3)
> [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1] ];;
gap>
gap> [14,2,0,4,6,0,2,2,0,0,0,2,2,0,0,0,0,2,0,0,2,0,0,0,0,0,0,0,0,0,0,0,0] * Inverse(Matrix_tomOhocta);
[ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 ]
gap>
```

Thus, the resulting vector has value 1 at element 18 ($\boldsymbol{C}_{3v}$) and at element 21 ($\boldsymbol{C}_{4v}$), which shows the appearance of the $(\boldsymbol{C}_{3v}\backslash)\boldsymbol{O}_h$-orbit and the $(\boldsymbol{C}_{4v}\backslash)\boldsymbol{O}_h$-orbit. This conclusion is confirmed by the fact that the sum of the 18th row and 21th row of the mark table (Table 1 or Table 3) is equal to the fixed-point vector (`FPVrhdod`).

The list of SCI-CFs for rhombic dodecahedron (`l_SCICF_rhdod`) calculated above can be alternatively obtained from the 18th row and the 21th row of the USCI-CF table shown in Table 2, where the i-th element of the former list is multiplied by the i-th element of the latter list to give `l_SCICF_rhdod[`i`]` ($i = 1, 2, \ldots, 33$).

5 Generation of PCI-CFs

Among the four methods supported by Fujita's USCI approach [1, 2], the present article deals with the partial-cycle-index (PCI) method [17,18], where the PCI method combined with CPRs is applied to $\boldsymbol{O}_h$-skeletons. The fixed-point matrix (FPM) method [5, 19, 20], the elementary-superposition (ES) method [21], and the partial-superposition (PS) method [17,21] have been developed as the other methods of Fujita's USCI approach. As for the symmetry-itemized enumeration based on $\boldsymbol{O}_h$-skeletons, cubane derivatives have been discussed as common targets by means of the FPM method [16], the PCI method [22], and the ES method [23].

5.1 PCI-CFs for the Octahedral Skeleton 1

As shown in the last part of Source Code 1 (`SubOh5-A.gap`) described above, the list of PCI-CFs (`l_PCICF_octa`) for the octahedral skeleton **1** has been obtained from the list of SCI-CFs (`l_SCICF_octa`), which is multiplied by the inverse of the mark table `Inverse(Matrix_tomOhocta)`. The output in the corresponding log file is as follows:

```
#list of PCI-CFs for octahedron --- l_PCICF_octa
[ 1/48*b_1^6-1/16*c_2*a_1^4-1/16*b_1^2*b_2^2-1/8*c_2^2*a_1^2+1/8*a_1^2*a_2^2-1/12*b_2^3-1/48*c_2^3
  +1/8*c_2*a_2^2+1/8*c_4*a_1^2+1/12*a_2^3+1/8*b_2*b_4-1/12*b_3^2+1/4*c_4*a_2-1/2*a_2*a_4+1/4*a_3^2
  +1/12*c_6+1/12*b_6-1/3*a_6,
  1/8*b_1^2*b_2^2-1/8*a_1^2*a_2^2-1/8*b_1^2*b_4-1/8*b_2^3-1/8*c_2*a_2^2-1/8*c_4*a_1^2+1/4*a_1^2*a_4
  +1/4*a_2^3+1/8*b_2*b_4-1/8*c_2*c_4+1/4*c_2*a_4+1/4*c_4*a_2-1/2*a_2*a_4, 1/4*b_2^3-1/4*a_2^3
  -1/4*b_2*b_4-1/4*c_4*a_2+1/2*a_2*a_4,
  1/8*c_2*a_1^4-1/4*a_1^2*a_2^2-1/8*c_2*a_2^2+1/4*a_2*a_4,
  1/4*c_2^2*a_1^2-1/4*c_4*a_1^2-1/4*a_2^3-1/4*c_4*a_2+1/2*a_2*a_4-1/2*a_3^2+1/2*a_6,
  1/24*c_2^3-1/8*c_2*a_2^2+1/12*a_2^3-1/4*c_4*a_2+1/4*a_2*a_4-1/6*c_6+1/6*a_6,
  1/4*b_3^2-1/4*a_3^2-1/4*c_6-1/4*b_6+1/2*a_6,
  1/4*b_1^2*b_4-1/4*a_1^2*a_4-1/4*b_2*b_4-1/4*c_2*a_4+1/2*a_2*a_4,
  1/4*c_2*c_4-1/4*c_2*a_4-1/4*c_4*a_2+1/4*a_2*a_4,
  1/12*b_2^3-1/12*a_2^3-1/4*b_2*b_4-1/4*c_4*a_2+1/2*a_2*a_4+1/6*b_6-1/6*a_6, 0,
  1/4*a_1^2*a_2^2-1/4*a_1^2*a_4-1/4*a_2^3+1/4*a_2*a_4,
  1/4*c_4*a_1^2-1/4*a_1^2*a_4-1/4*c_4*a_2+1/4*a_2*a_4, 1/2*a_2^3-1/2*a_2*a_4,
  1/4*c_2*a_2^2-1/4*a_2^3-1/4*c_2*a_4+1/4*a_2*a_4, 1/2*c_4*a_2-1/2*a_2*a_4, 0,
  1/2*a_3^2-1/2*a_6, 1/2*c_6-1/2*a_6, 1/2*b_2*b_4-1/2*a_2*a_4-1/2*b_6+1/2*a_6,
  1/2*a_1^2*a_4-1/2*a_2*a_4, 1/2*c_2*a_4-1/2*a_2*a_4, 1/2*c_4*a_2-1/2*a_2*a_4, 0,
  1/6*a_2^3-1/2*a_2*a_4+1/3*a_6, 0, 0, 0, a_2*a_4-a_6, 1/2*b_6-1/2*a_6, 0, 0, a_6 ]
```

The resulting list of PCI-CFs (`l_PCICF_octa`) consists of thirty-three elements, where the i-th element (`l_PCICF_octa[`i`]`) indicates the PCI-CF of the i-th subgroup of $\boldsymbol{O}_h$. The i-th element abbreviated as `PCI-CF[`i`]` is obtained by using the `do`–`od` iteration of the GAP system as follows:

```
#PCI-CFs for subgroups --- l_PCICF_octa[i]
PCI-CF[1] := 1/48*b_1^6-1/16*c_2*a_1^4-1/16*b_1^2*b_2^2-1/8*c_2^2*a_1^2+1/8*a_1^2*a_2^2-1/12*b_2^3
           -1/48*c_2^3+1/8*c_2*a_2^2+1/8*c_4*a_1^2+1/12*a_2^3+1/8*b_2*b_4-1/12*b_3^2+1/4*c_4*a_2
           -1/2*a_2*a_4+1/4*a_3^2+1/12*c_6+1/12*b_6-1/3*a_6
PCI-CF[2] := 1/8*b_1^2*b_2^2-1/8*a_1^2*a_2^2-1/8*b_1^2*b_4-1/8*b_2^3-1/8*c_2*a_2^2-1/8*c_4*a_1^2
           +1/4*a_1^2*a_4+1/4*a_2^3+1/8*b_2*b_4-1/8*c_2*c_4+1/4*c_2*a_4+1/4*c_4*a_2-1/2*a_2*a_4
PCI-CF[3] := 1/4*b_2^3-1/4*a_2^3-1/4*b_2*b_4-1/4*c_4*a_2+1/2*a_2*a_4
PCI-CF[4] := 1/8*c_2*a_1^4-1/4*a_1^2*a_2^2-1/8*c_2*a_2^2+1/4*a_2*a_4
PCI-CF[5] := 1/4*c_2^2*a_1^2-1/4*c_4*a_1^2-1/4*a_2^3-1/4*c_4*a_2+1/2*a_2*a_4-1/2*a_3^2+1/2*a_6
PCI-CF[6] := 1/24*c_2^3-1/8*c_2*a_2^2+1/12*a_2^3-1/4*c_4*a_2+1/4*a_2*a_4-1/6*c_6+1/6*a_6
PCI-CF[7] := 1/4*b_3^2-1/4*a_3^2-1/4*c_6-1/4*b_6+1/2*a_6
PCI-CF[8] := 1/4*b_1^2*b_4-1/4*a_1^2*a_4-1/4*b_2*b_4-1/4*c_2*a_4+1/2*a_2*a_4
PCI-CF[9] := 1/4*c_2*c_4-1/4*c_2*a_4-1/4*c_4*a_2+1/4*a_2*a_4
PCI-CF[10]  := 1/12*b_2^3-1/12*a_2^3-1/4*b_2*b_4-1/4*c_4*a_2+1/2*a_2*a_4+1/6*b_6-1/6*a_6
PCI-CF[11]  := 0
PCI-CF[12]  := 1/4*a_1^2*a_2^2-1/4*a_1^2*a_4-1/4*a_2^3+1/4*a_2*a_4
PCI-CF[13]  := 1/4*c_4*a_1^2-1/4*a_1^2*a_4-1/4*c_4*a_2+1/4*a_2*a_4
PCI-CF[14]  := 1/2*a_2^3-1/2*a_2*a_4
PCI-CF[15]  := 1/4*c_2*a_2^2-1/4*a_2^3-1/4*c_2*a_4+1/4*a_2*a_4
PCI-CF[16]  := 1/2*c_4*a_2-1/2*a_2*a_4
PCI-CF[17]  := 0
PCI-CF[18]  := 1/2*a_3^2-1/2*a_6
PCI-CF[19]  := 1/2*c_6-1/2*a_6
PCI-CF[20]  := 1/2*b_2*b_4-1/2*a_2*a_4-1/2*b_6+1/2*a_6
PCI-CF[21]  := 1/2*a_1^2*a_4-1/2*a_2*a_4
PCI-CF[22]  := 1/2*c_2*a_4-1/2*a_2*a_4
PCI-CF[23]  := 1/2*c_4*a_2-1/2*a_2*a_4
PCI-CF[24]  := 0
PCI-CF[25]  := 1/6*a_2^3-1/2*a_2*a_4+1/3*a_6
PCI-CF[26]  := 0
PCI-CF[27]  := 0
PCI-CF[28]  := 0
PCI-CF[29]  := a_2*a_4-a_6
PCI-CF[30]  := 1/2*b_6-1/2*a_6
PCI-CF[31]  := 0
PCI-CF[32]  := 0
PCI-CF[33]  := a_6
```

The i-th element `PCI-CF[`i`]` ($i = 1, 2, \cdots, 33$) corresponds to the respective subgroups numbered sequentially, as shown in Eq. 1. Hence, the above PCI-CFs (`PCI-CF[`i`]`) for the octahedral skeleton **1** can be written in usual notation (cf. Definition 19.6 of Ref. [1]), where the symbol `a_d` is replaced by the sphericity index (SI) a_d for a d-membered homospheric orbit; the symbol `c_d` is replaced by the SI c_d for a d-membered enantiospheric orbit; and the symbol `b_d` is replaced by the SI b_d for a d-membered hemispheric orbit:

$$\begin{aligned}\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_1, \$_d) = {} & \frac{1}{48}b_1^6 - \frac{1}{16}c_2a_1^4 - \frac{1}{16}b_1^2b_2^2 - \frac{1}{8}c_2^2a_1^2 + \frac{1}{8}a_1^2a_2^2 - \frac{1}{12}b_2^3 \\ & - \frac{1}{48}c_2^3 + \frac{1}{8}c_2a_2^2 + \frac{1}{8}c_4a_1^2 + \frac{1}{12}a_2^3 + \frac{1}{8}b_2b_4 \\ & - \frac{1}{12}b_3^2 + \frac{1}{4}c_4a_2 - \frac{1}{2}a_2a_4 + \frac{1}{4}a_3^2 + \frac{1}{12}c_6 + \frac{1}{12}b_6 - \frac{1}{3}a_6 \end{aligned} \tag{9}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_2, \$_d) = \frac{1}{8}b_1^2b_2^2 - \frac{1}{8}a_1^2a_2^2 - \frac{1}{8}b_1^2b_4 - \frac{1}{8}b_2^3 - \frac{1}{8}c_2a_2^2 - \frac{1}{8}c_4a_1^2 + \frac{1}{4}a_1^2a_4 + \frac{1}{4}a_2^3$$

$$+\frac{1}{8}b_2b_4-\frac{1}{8}c_2c_4+\frac{1}{4}c_2a_4+\frac{1}{4}c_4a_2-\frac{1}{2}a_2a_4 \tag{10}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_2',\$_d)=\frac{1}{4}b_2^3-\frac{1}{4}a_2^3-\frac{1}{4}b_2b_4-\frac{1}{4}c_4a_2+\frac{1}{2}a_2a_4 \tag{11}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_s,\$_d)=\frac{1}{8}c_2a_1^4-\frac{1}{4}a_1^2a_2^2-\frac{1}{8}c_2a_2^2+\frac{1}{4}a_2a_4 \tag{12}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_s',\$_d)=\frac{1}{4}c_2^2a_1^2-\frac{1}{4}c_4a_1^2-\frac{1}{4}a_2^3-\frac{1}{4}c_4a_2+\frac{1}{2}a_2a_4-\frac{1}{2}a_3^2+\frac{1}{2}a_6 \tag{13}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_i,\$_d)=\frac{1}{24}c_2^3-\frac{1}{8}c_2a_2^2+\frac{1}{12}a_2^3-\frac{1}{4}c_4a_2+\frac{1}{4}a_2a_4-\frac{1}{6}c_6+\frac{1}{6}a_6 \tag{14}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_3,\$_d)=\frac{1}{4}b_3^2-\frac{1}{4}a_3^2-\frac{1}{4}c_6-\frac{1}{4}b_6+\frac{1}{2}a_6 \tag{15}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_4,\$_d)=\frac{1}{4}b_1^2b_4-\frac{1}{4}a_1^2a_4-\frac{1}{4}b_2b_4-\frac{1}{4}c_2a_4+\frac{1}{2}a_2a_4 \tag{16}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{S}_4,\$_d)=\frac{1}{4}c_2c_4-\frac{1}{4}c_2a_4-\frac{1}{4}c_4a_2+\frac{1}{4}a_2a_4 \tag{17}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{D}_2,\$_d)=\frac{1}{12}b_2^3-\frac{1}{12}a_2^3-\frac{1}{4}b_2b_4-\frac{1}{4}c_4a_2+\frac{1}{2}a_2a_4+\frac{1}{6}b_6-\frac{1}{6}a_6 \tag{18}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{D}_2',\$_d)=0 \tag{19}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_{2v},\$_d)=\frac{1}{4}a_1^2a_2^2-\frac{1}{4}a_1^2a_4-\frac{1}{4}a_2^3+\frac{1}{4}a_2a_4 \tag{20}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_{2v}',\$_d)=\frac{1}{4}c_4a_1^2-\frac{1}{4}a_1^2a_4-\frac{1}{4}c_4a_2+\frac{1}{4}a_2a_4 \tag{21}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_{2v}'',\$_d)=\frac{1}{2}a_2^3-\frac{1}{2}a_2a_4 \tag{22}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_{2h},\$_d)=\frac{1}{4}c_2a_2^2-\frac{1}{4}a_2^3-\frac{1}{4}c_2a_4+\frac{1}{4}a_2a_4 \tag{23}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_{2h}',\$_d)=\frac{1}{2}c_4a_2-\frac{1}{2}a_2a_4 \tag{24}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{D}_3,\$_d)=0 \tag{25}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_{3v},\$_d)=\frac{1}{2}a_3^2-\frac{1}{2}a_6 \tag{26}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_{3i},\$_d)=\frac{1}{2}c_6-\frac{1}{2}a_6 \tag{27}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{D}_4,\$_d)=\frac{1}{2}b_2b_4-\frac{1}{2}a_2a_4-\frac{1}{2}b_6+\frac{1}{2}a_6 \tag{28}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_{4v},\$_d)=\frac{1}{2}a_1^2a_4-\frac{1}{2}a_2a_4 \tag{29}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{C}_{4h},\$_d)=\frac{1}{2}c_2a_4-\frac{1}{2}a_2a_4 \tag{30}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{D}_{2d},\$_d)=\frac{1}{2}c_4a_2-\frac{1}{2}a_2a_4 \tag{31}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{D}_{2d}',\$_d)=0 \tag{32}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{D}_{2h},\$_d)=\frac{1}{6}a_2^3-\frac{1}{2}a_2a_4+\frac{1}{3}a_6 \tag{33}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{D}_{2h}',\$_d)=0 \tag{34}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{T},\$_d)=0 \tag{35}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{D}_{3d}, \$_d) = 0 \tag{36}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{D}_{4h}, \$_d) = a_2a_4 - a_6 \tag{37}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{O}, \$_d) = \frac{1}{2}b_6 - \frac{1}{2}a_6 \tag{38}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{T}_h, \$_d) = 0 \tag{39}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{T}_d, \$_d) = 0 \tag{40}$$

$$\text{PCI-CF}_{\mathbf{1}}(\boldsymbol{O}_h, \$_d) = a_6 \tag{41}$$

5.2 PCI-CFs for the Cubane Skeleton 2

The above procedure of Source Code 1 (`SubOh5-A.gap`) for calculating PCI-CFs of the octahedral skeleton (Eqs. 9–41) via `l_SCICF_octa` and `l_PCICF_octa` is applicable to the other skeletons.

The use of the set of generators `gen2` in place of `gen1` of Source Code 1 (`SubOh5-A.gap`) provides us with the CPR `Oh_cube` for the cubane skeleton **2**. After the selection of the set of subgroups `gen[`i`]` ($i = 1, 2, \cdots, 33$) according to the $\text{SSG}_{\boldsymbol{O}_h}^{cube}$ (Eq. 3), the corresponding list of SCI-CFs (`l_SCICF_cube`) and the list of PCI-CFs (`l_PCICF_cube`) are calculated. Note that the list of SCI-CFs (`l_SCICF_cube`) is identical with the 18th $(\boldsymbol{C}_{3v}\backslash)\boldsymbol{O}_h$-row of the USCI-CF table (Table 2), because the cubane skeleton **2** contains one orbit governed by $(\boldsymbol{C}_{3v}\backslash)\boldsymbol{O}_h$. Thereby, the following PCI-CFs for the enumeration based on the cubane skeleton **2** are obtained:

$$\begin{aligned}\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}_1, \$_d) = {} & \frac{1}{48}b_1^8 - \frac{1}{8}c_2^2a_1^4 - \frac{1}{12}b_1^2b_3^2 - \frac{3}{16}b_2^4 - \frac{1}{12}c_2^4 + \frac{1}{4}a_1^2a_3^2 \\ & + \frac{1}{8}a_2^4 + \frac{1}{2}c_4a_2^2 + \frac{1}{4}b_2b_6 + \frac{1}{12}c_2c_6 + \frac{1}{4}b_4^2 + \frac{1}{4}c_4^2 - \frac{1}{2}a_2a_6 - \frac{3}{4}a_4^2 \\ & - \frac{1}{4}b_8 - \frac{1}{4}c_8 + \frac{1}{2}a_8\end{aligned} \tag{42}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}_2, \$_d) = \frac{1}{8}b_2^4 - \frac{1}{8}a_2^4 - \frac{3}{8}b_4^2 - \frac{3}{8}c_4^2 + \frac{3}{4}a_4^2 + \frac{1}{4}b_8 + \frac{3}{4}c_8 - a_8 \tag{43}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}'_2, \$_d) = \frac{1}{4}b_2^4 - \frac{1}{2}c_4a_2^2 - \frac{1}{2}b_2b_6 - \frac{1}{4}b_4^2 + \frac{1}{2}a_2a_6 + \frac{1}{2}a_4^2 + \frac{1}{2}b_8 - \frac{1}{2}a_8 \tag{44}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}_s, \$_d) = \frac{1}{8}c_2^4 - \frac{1}{4}c_4a_2^2 - \frac{3}{8}c_4^2 + \frac{1}{4}a_4^2 + \frac{1}{4}c_8 \tag{45}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}'_s, \$_d) = \frac{1}{4}c_2^2a_1^4 - \frac{1}{2}a_1^2a_3^2 - \frac{1}{4}a_2^4 - \frac{1}{2}c_4a_2^2 + \frac{1}{2}a_2a_6 + a_4^2 - \frac{1}{2}a_8 \tag{46}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}_i, \$_d) = \frac{1}{24}c_2^4 - \frac{1}{4}c_4a_2^2 - \frac{1}{6}c_2c_6 - \frac{1}{8}c_4^2 + \frac{1}{2}a_2a_6 + \frac{1}{4}a_4^2 + \frac{1}{4}c_8 - \frac{1}{2}a_8 \tag{47}$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}_3, \$_d) = {} & \frac{1}{4}b_1^2b_3^2 - \frac{1}{4}a_1^2a_3^2 - \frac{1}{4}b_2b_6 - \frac{1}{4}c_2c_6 - \frac{1}{4}b_4^2 + \frac{1}{2}a_2a_6 + \frac{1}{4}a_4^2 \\ & + \frac{1}{4}b_8 + \frac{1}{4}c_8 - \frac{1}{2}a_8\end{aligned} \tag{48}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}_4, \$_d) = \frac{1}{4}b_4^2 - \frac{1}{4}a_4^2 - \frac{1}{4}b_8 - \frac{1}{4}c_8 + \frac{1}{2}a_8 \tag{49}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{S}_4, \$_d) = \frac{1}{4}c_4^2 - \frac{1}{4}a_4^2 - \frac{1}{2}c_8 + \frac{1}{2}a_8 \tag{50}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{D}_2, \$_d) = 0 \tag{51}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{D}'_2, \$_d) = \frac{1}{4}b_4^2 - \frac{1}{4}a_4^2 - \frac{1}{4}b_8 - \frac{1}{4}c_8 + \frac{1}{2}a_8 \tag{52}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}_{2v}, \$_d) = \frac{1}{4}c_4^2 - \frac{1}{4}a_4^2 - \frac{1}{2}c_8 + \frac{1}{2}a_8 \tag{53}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}'_{2v}, \$_d) = \frac{1}{4}a_2^4 - \frac{3}{4}a_4^2 + \frac{1}{2}a_8 \tag{54}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}''_{2v}, \$_d) = \frac{1}{2}c_4a_2^2 - \frac{1}{2}a_4^2 \tag{55}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}_{2h}, \$_d) = \frac{1}{4}c_4^2 - \frac{1}{4}a_4^2 - \frac{1}{2}c_8 + \frac{1}{2}a_8 \tag{56}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}'_{2h}, \$_d) = \frac{1}{2}c_4a_2^2 - a_2a_6 - \frac{1}{2}a_4^2 + a_8 \tag{57}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{D}_3, \$_d) = \frac{1}{2}b_2b_6 - \frac{1}{2}a_2a_6 - \frac{1}{2}b_8 + \frac{1}{2}a_8 \tag{58}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}_{3v}, \$_d) = \frac{1}{2}a_1^2a_3^2 - \frac{1}{2}a_2a_6 - \frac{1}{2}a_4^2 + \frac{1}{2}a_8 \tag{59}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}_{3i}, \$_d) = \frac{1}{2}c_2c_6 - \frac{1}{2}a_2a_6 - \frac{1}{2}c_8 + \frac{1}{2}a_8 \tag{60}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{D}_4, \$_d) = 0 \tag{61}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}_{4v}, \$_d) = \frac{1}{2}a_4^2 - \frac{1}{2}a_8 \tag{62}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{C}_{4h}, \$_d) = \frac{1}{2}c_8 - \frac{1}{2}a_8 \tag{63}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{D}_{2d}, \$_d) = 0 \tag{64}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{D}'_{2d}, \$_d) = \frac{1}{2}c_8 - \frac{1}{2}a_8 \tag{65}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{D}_{2h}, \$_d) = 0 \tag{66}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{D}'_{2h}, \$_d) = \frac{1}{2}a_4^2 - \frac{1}{2}a_8 \tag{67}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{T}, \$_d) = \frac{1}{4}b_4^2 - \frac{1}{4}a_4^2 - \frac{1}{4}b_8 - \frac{1}{4}c_8 + \frac{1}{2}a_8 \tag{68}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{D}_{3d}, \$_d) = a_2a_6 - a_8 \tag{69}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{D}_{4h}, \$_d) = 0 \tag{70}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{O}, \$_d) = \frac{1}{2}b_8 - \frac{1}{2}a_8 \tag{71}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{T}_h, \$_d) = \frac{1}{2}c_8 - \frac{1}{2}a_8 \tag{72}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{T}_d, \$_d) = \frac{1}{2}a_4^2 - 1/2a_8 \tag{73}$$

$$\text{PCI-CF}_{\mathbf{2}}(\boldsymbol{O}_h, \$_d) = a_8 \tag{74}$$

The results of Eqs. 42–74 are consistent with Eqs. 6–38 of Ref. [22], where the 7th term $-\frac{1}{8}a_4^2$ in Eq. 7 of Ref. [22] (corresponding to Eq. 43 of the present article) should be read as $-\frac{1}{8}a_2^4$.

5.3 PCI-CFs for the Carboctahedron Skeleton 3

The use of the set of generators `gen3` in place of `gen1` of Source Code 1 (`SubOh5-A.gap`) provides us with the CPR `Oh_cubocta` for the cuboctahedron skeleton **3**. After the selection of the set of subgroups `gen[i]` ($i = 1, 2, \cdots, 33$) according to the $\mathrm{SSG}_{\boldsymbol{O}_h}^{cuboct}$ (Eq. 4), the corresponding list of SCI-CFs (`l_SCICF_cuboct`) and the list of PCI-CFs (`l_PCICF_cuboct`) are calculated. Note that the list of SCI-CFs (`l_SCICF_cuboct`) is identical with the 14th $(\boldsymbol{C}''_{2v}\backslash)\boldsymbol{O}_h$-row of the USCI-CF table (Table 2), because the cuboctahedron skeleton **3** contains one orbit governed by the coset representation $(\boldsymbol{C}''_{2v}\backslash)\boldsymbol{O}_h$. Thereby, the following PCI-CFs for the enumeration based on the carboctahedron skeleton **3** are obtained:

$$\begin{aligned}\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_1, \$_d) = {} & \frac{1}{48}b_1^12 - \frac{1}{16}c_2^4a_1^4 - \frac{1}{8}b_1^2b_2^5 - \frac{1}{8}c_2^5a_1^2 - \frac{1}{16}b_2^6 - \frac{1}{48}c_2^6 + \frac{1}{4}c_4^2a_1^2a_2 \\ & + \frac{1}{8}c_4a_2^4 + \frac{1}{8}b_2^2b_4^2 + \frac{1}{4}c_2c_4^2a_2 - \frac{1}{12}b_3^4 + \frac{1}{4}c_4^2a_2^2 + \frac{1}{4}b_3^2b_6 + \frac{1}{24}b_4^3 \\ & + \frac{1}{4}c_6a_3^2 - \frac{1}{2}c_8a_2^2 - \frac{1}{6}a_4^3 + \frac{1}{12}c_6^2 - \frac{1}{2}c_6a_6 - \frac{1}{6}b_{12} + \frac{1}{6}a_{12}\end{aligned} \tag{75}$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_2, \$_d) = {} & \frac{1}{8}b_2^6 - \frac{1}{8}c_4a_2^4 - \frac{1}{8}b_2^2b_4^2 - \frac{1}{4}c_4^2a_2^2 - \frac{1}{4}b_4^3 - \frac{1}{8}c_4^3 + \frac{1}{4}c_4a_4^2 + \frac{1}{4}c_8a_2^2 \\ & + \frac{1}{2}a_4^3 + \frac{1}{4}b_4b_8 + \frac{1}{2}c_8a_4 - a_4a_8\end{aligned} \tag{76}$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}'_2, \$_d) = {} & \frac{1}{4}b_1^2b_2^5 - \frac{1}{4}c_4^2a_1^2a_2 - \frac{1}{4}b_2^2b_4^2 - \frac{1}{4}c_2c_4^2a_2 - \frac{1}{2}b_3^2b_6 + \frac{1}{2}c_8a_2^2 \\ & + \frac{1}{2}c_6a_6 + \frac{1}{2}b_{12} - \frac{1}{2}a_{12}\end{aligned} \tag{77}$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_s, \$_d) = \frac{1}{8}c_2^4a_1^4 - \frac{1}{4}c_4^2a_1^2a_2 - \frac{1}{4}c_4a_2^4 - \frac{1}{8}c_4^2a_2^2 + \frac{1}{4}c_8a_2^2 + \frac{1}{4}a_4^3 \tag{78}$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}'_s, \$_d) = \frac{1}{4}c_2^5a_1^2 - \frac{1}{4}c_4^2a_1^2a_2 - \frac{1}{4}c_2c_4^2a_2 - \frac{1}{4}c_4^2a_2^2 - \frac{1}{2}c_6a_3^2 + \frac{1}{2}c_8a_2^2 + \frac{1}{2}c_6a_6 \tag{79}$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_i, \$_d) = {} & \frac{1}{24}c_2^6 - \frac{1}{4}c_2c_4^2a_2 - \frac{1}{8}c_4^2a_2^2 + \frac{1}{4}c_8a_2^2 + \frac{1}{12}a_4^3 \\ & - \frac{1}{6}c_6^2 + \frac{1}{2}c_6a_6 - \frac{1}{3}a_{12}\end{aligned} \tag{80}$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_3, \$_d) = \frac{1}{4}b_3^4 - \frac{1}{4}b_3^2b_6 - \frac{1}{4}c_6a_3^2 - \frac{1}{4}c_6^2 + \frac{1}{2}c_6a_6 \tag{81}$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_4, \$_d) = \frac{1}{4}b_4^3 - \frac{1}{4}a_4^3 - \frac{1}{4}b_4b_8 - \frac{1}{4}c_8a_4 + \frac{1}{2}a_4a_8 \tag{82}$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{S}_4, \$_d) = \frac{1}{4}c_4^3 - \frac{1}{4}c_4a_4^2 - \frac{1}{2}c_8a_4 + \frac{1}{2}a_4a_8 \tag{83}$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{D}_2, \$_d) = \frac{1}{12}b_4^3 - \frac{1}{12}a_4^3 - \frac{1}{4}b_4b_8 - \frac{1}{4}c_8a_4 + \frac{1}{2}a_4a_8 + \frac{1}{6}b_{12} - \frac{1}{6}a_{12} \quad (84)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{D}_2', \$_d) = \frac{1}{4}b_2^2b_4^2 - \frac{1}{4}c_4a_4^2 - \frac{1}{4}c_8a_2^2 - \frac{1}{4}b_4b_8 + \frac{1}{2}a_4a_8 \quad (85)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_{2v}, \$_d) = \frac{1}{4}c_4a_2^4 - \frac{1}{4}c_4a_4^2 - \frac{1}{2}a_4^3 + \frac{1}{2}a_4a_8 \quad (86)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_{2v}', \$_d) = \frac{1}{4}c_4^2a_2^2 - \frac{1}{4}c_8a_2^2 - \frac{1}{4}a_4^3 - \frac{1}{4}c_8a_4 + \frac{1}{2}a_4a_8 \quad (87)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_{2v}'', \$_d) = \frac{1}{2}c_4^2a_1^2a_2 - \frac{1}{2}c_8a_2^2 \quad (88)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_{2h}, \$_d) = \frac{1}{4}c_4^2a_2^2 - \frac{1}{4}c_8a_2^2 - \frac{1}{4}a_4^3 - \frac{1}{4}c_8a_4 + \frac{1}{2}a_4a_8 \quad (89)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_{2h}', \$_d) = \frac{1}{2}c_2c_4^2a_2 - \frac{1}{2}c_8a_2^2 - c_6a_6 + a_12 \quad (90)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{D}_3, \$_d) = \frac{1}{2}b_3^2b_6 - \frac{1}{2}c_6a_6 - \frac{1}{2}b_{12} + \frac{1}{2}a_{12} \quad (91)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_{3v}, \$_d) = \frac{1}{2}c_6a_3^2 - \frac{1}{2}c_6a_6 \quad (92)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_{3i}, \$_d) = \frac{1}{2}c_6^2 - \frac{1}{2}c_6a_6 \quad (93)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{D}_4, \$_d) = \frac{1}{2}b_4b_8 - \frac{1}{2}a_4a_8 - \frac{1}{2}b_{12} + \frac{1}{2}a_{12} \quad (94)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_{4v}, \$_d) = \frac{1}{2}a_4^3 - \frac{1}{2}a_4a_8 \quad (95)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{C}_{4h}, \$_d) = \frac{1}{2}c_8a_4 - \frac{1}{2}a_4a_8 \quad (96)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{D}_{2d}, \$_d) = \frac{1}{2}c_8a_4 - \frac{1}{2}a_4a_8 \quad (97)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{D}_{2d}', \$_d) = \frac{1}{2}c_4a_4^2 - \frac{1}{2}a_4a_8 \quad (98)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{D}_{2h}, \$_d) = \frac{1}{6}a_4^3 - \frac{1}{2}a_4a_8 + \frac{1}{3}a_{12} \quad (99)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{D}_{2h}', \$_d) = \frac{1}{2}c_8a_2^2 - \frac{1}{2}a_4a_8 \quad (100)$$

$$\text{PCI-CF}_{\mathbf{3}}(T, \$_d) = 0 \quad (101)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{D}_{3d}, \$_d) = c_6a_6 - a_{12} \quad (102)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{D}_{4h}, \$_d) = a_4a_8 - a_{12} \quad (103)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{O}, \$_d) = \frac{1}{2}b_{12} - \frac{1}{2}a_{12} \quad (104)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{T}_h, \$_d) = 0 \quad (105)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{T}_d, \$_d) = 0 \quad (106)$$

$$\text{PCI-CF}_{\mathbf{3}}(\boldsymbol{O}_h, \$_d) = a_{12} \quad (107)$$

5.4 PCI-CFs for the Truncated Octahedron Skeleton 4

For the purpose of providing the CPR `Oh_trocta` for the truncated octahedron skeleton **4**, the set of generators `gen4` is used in place of `gen1` of Source Code 1 (`SubOh5-A.gap`). After the selection of the set of subgroups `gen[`i`]` ($i = 1, 2, \cdots, 33$) according to the $\mathrm{SSG}_{\boldsymbol{O}_h}^{troct}$ (Eq. 5), the corresponding list of SCI-CFs (`l_SCICF_troct`) and the list of PCI-CFs (`l_PCICF_troct`) are calculated. Note that the list of SCI-CFs (`l_SCICF_troct`) is identical with the 4th $(\boldsymbol{C}_s\backslash)\boldsymbol{O}_h$-row of the USCI-CF table (Table 2), because the truncated octahedron skeleton **4** contains one orbit governed by the coset representation $(\boldsymbol{C}_s\backslash)\boldsymbol{O}_h$. Thereby, the following PCI-CFs for the enumeration based on the truncated octahedron skeleton **4** are obtained:

$$\begin{aligned}\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_1, \$_d) = {} & \frac{1}{48}b_1^{24} - \frac{1}{16}c_2^8a_1^8 - \frac{3}{16}b_2^{12} - \frac{7}{48}c_2^{12} + \frac{1}{8}c_4^2a_2^8 - \frac{1}{12}b_3^8 \\ & + \frac{3}{8}c_4^4a_2^4 + \frac{1}{6}b_4^6 + \frac{3}{8}c_4^6 - \frac{1}{6}a_4^6 + \frac{1}{3}c_6^4 + \frac{1}{4}b_6^4 - \frac{1}{2}c_8^2a_4^2 - \frac{1}{2}c_{12}^2 \\ & + \frac{1}{12}b_{12}^2 - \frac{1}{12}a_{12}^2 - \frac{1}{4}b_{24} - \frac{1}{4}c_{24} + \frac{1}{2}a_{24} \end{aligned} \tag{108}$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_2, \$_d) = {} & \frac{1}{8}b_2^{12} - \frac{1}{8}c_4^2a_2^8 - \frac{1}{8}c_4^4a_2^4 - \frac{3}{8}b_4^6 - \frac{1}{4}c_4^6 + \frac{1}{4}a_4^6 + \frac{1}{2}c_8a_4^4 + \frac{1}{2}c_8^2a_4^2 \\ & + \frac{1}{4}b_8^3 + \frac{1}{4}c_8^3 - a_8^3 \end{aligned} \tag{109}$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_2', \$_d) = {} & \frac{1}{4}b_2^{12} - \frac{1}{4}c_4^4a_2^4 - \frac{1}{4}b_4^6 - \frac{1}{4}c_4^6 - \frac{1}{2}b_6^4 + \frac{1}{2}c_8^2a_4^2 + \frac{1}{2}c_{12}^2 \\ & + \frac{1}{2}b_{24} - \frac{1}{2}a_{24} \end{aligned} \tag{110}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_s, \$_d) = \frac{1}{8}c_2^8a_1^8 - \frac{1}{4}c_4^2a_2^8 - \frac{3}{8}c_4^4a_2^4 + \frac{1}{4}a_4^6 + \frac{1}{4}c_8^2a_4^2 \tag{111}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_s', \$_d) = \frac{1}{4}c_2^{12} - \frac{1}{4}c_4^4a_2^4 - \frac{1}{2}c_4^6 - \frac{1}{2}c_6^4 + \frac{1}{2}c_8^2a_4^2 + \frac{1}{2}c_{12}^2 + \frac{1}{2}c_{24} - \frac{1}{2}a_{24} \tag{112}$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_i, \$_d) = {} & \frac{1}{24}c_2^{12} - \frac{1}{8}c_4^4a_2^4 - \frac{1}{4}c_4^6 + \frac{1}{12}a_4^6 - \frac{1}{6}c_6^4 + \frac{1}{4}c_8^2a_4^2 + \frac{1}{2}c_{12}^2 \\ & + \frac{1}{6}a_{12}^2 - \frac{1}{2}a_{24} \end{aligned} \tag{113}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_3, \$_d) = \frac{1}{4}b_3^8 - \frac{1}{2}c_6^4 - \frac{1}{4}b_6^4 + \frac{1}{2}c_{12}^2 - \frac{1}{4}b_{12}^2 + \frac{1}{4}a_{12}^2 + \frac{1}{4}b_{24} + \frac{1}{4}c_{24} - \frac{1}{2}a_{24} \tag{114}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_4, \$_d) = \frac{1}{4}b_4^6 - \frac{1}{4}c_8a_4^4 - \frac{1}{4}c_8^2a_4^2 - \frac{1}{4}b_8^3 + \frac{1}{2}a_8^3 \tag{115}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{S}_4, \$_d) = \frac{1}{4}c_4^6 - \frac{1}{4}c_8a_4^4 - \frac{1}{4}c_8^2a_4^2 - \frac{1}{4}c_8^3 + \frac{1}{2}a_8^3 \tag{116}$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{D}_2, \$_d) = {} & \frac{1}{12}b_4^6 - \frac{1}{12}a_4^6 - \frac{1}{4}b_8^3 - \frac{1}{4}c_8^3 + \frac{1}{2}a_8^3 - \frac{1}{12}b_{12}^2 + \frac{1}{12}a_{12}^2 + \frac{1}{4}b_{24} \\ & + \frac{1}{4}c_{24} - \frac{1}{2}a_{24} \end{aligned} \tag{117}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{D}_2', \$_d) = \frac{1}{4}b_4^6 - \frac{1}{4}c_8a_4^4 - \frac{1}{4}c_8^2a_4^2 - \frac{1}{4}b_8^3 + \frac{1}{2}a_8^3 \tag{118}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_{2v}, \$_d) = \frac{1}{4}c_4^2a_2^8 - \frac{1}{4}a_4^6 - \frac{1}{2}c_8a_4^4 + \frac{1}{2}a_8^3 \tag{119}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}'_{2v}, \$_d) = \frac{1}{4}c_4^6 - \frac{1}{4}c_8a_4^4 - \frac{1}{4}c_8^2a_4^2 - \frac{1}{4}c_8^3 + \frac{1}{2}a_8^3 \tag{120}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}''_{2}, \$_d) = \frac{1}{2}c_4^4a_2^4 - \frac{1}{2}c_8^2a_4^2 \tag{121}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_{2h}, \$_d) = \frac{1}{4}c_4^4a_2^4 - \frac{1}{4}a_4^6 - \frac{1}{2}c_8^2a_4^2 + \frac{1}{2}a_8^3 \tag{122}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}'_{2h}, \$_d) = \frac{1}{2}c_4^6 - \frac{1}{2}c_8^2a_4^2 - c_{12}^2 + a_{24} \tag{123}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{D}_{3}, \$_d) = \frac{1}{2}b_6^4 - \frac{1}{2}c_{12}^2 - \frac{1}{2}b_{24} + \frac{1}{2}a_{24} \tag{124}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_{3v}, \$_d) = \frac{1}{2}c_6^4 - \frac{1}{2}c_{12}^2 - \frac{1}{2}c_{24} + \frac{1}{2}a_{24} \tag{125}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_{3i}, \$_d) = \frac{1}{2}c_6^4 - \frac{1}{2}c_{12}^2 - \frac{1}{2}a_{12}^2 + \frac{1}{2}a_{24} \tag{126}$$

$$\text{PCI-CF}_{\mathbf{4}}(\mathbf{4_4}, \$_{\mathbf{d}}) = \frac{1}{2}b_8^3 - \frac{1}{2}a_8^3 - \frac{1}{2}b_{24} + \frac{1}{2}a_{24} \tag{127}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_{4v}, \$_d) = \frac{1}{2}c_8a_4^4 - \frac{1}{2}a_8^3 \tag{128}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{C}_{4h}, \$_d) = \frac{1}{2}c_8^2a_4^2 - \frac{1}{2}a_8^3 \tag{129}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{D}_{2d}, \$_d) = \frac{1}{2}c_8^3 - \frac{1}{2}a_8^3 - \frac{1}{2}c_{24} + \frac{1}{2}a_{24} \tag{130}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{D}'_{2d}, \$_d) = \frac{1}{2}c_8a_4^4 - \frac{1}{2}a_8^3 \tag{131}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{D}_{2h}, \$_d) = \frac{1}{6}a_4^6 - \frac{1}{2}a_8^3 - \frac{1}{6}a_{12}^2 + \frac{1}{2}a_{24} \tag{132}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{D}'_{2h}, \$_d) = \frac{1}{2}c_8^2a_4^2 - \frac{1}{2}a_8^3 \tag{133}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{T}, \$_d) = \frac{1}{4}b_{12}^2 - \frac{1}{4}a_{12}^2 - \frac{1}{4}b_{24} - \frac{1}{4}c_{24} + \frac{1}{2}a_{24} \tag{134}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{D}_{3d}, \$_d) = c_{12}^2 - a_{24} \tag{135}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{D}_{4h}, \$_d) = a_8^3 - a_{24} \tag{136}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{O}, \$_d) = \frac{1}{2}b_{24} - \frac{1}{2}a_{24} \tag{137}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{T}_{h}, \$_d) = \frac{1}{2}a_{12}^2 - \frac{1}{2}a_{24} \tag{138}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{T}_{d}, \$_d) = \frac{1}{2}c_{24} - \frac{1}{2}a_{24} \tag{139}$$

$$\text{PCI-CF}_{\mathbf{4}}(\boldsymbol{O}_{h}, \$_d) = a_{24} \tag{140}$$

5.5 PCI-CFs for the Truncated Hexahedral Skeleton 5

For the purpose of providing the CPR `Oh_trhex` for the truncated hexahedral skeleton **5**, the set of generators `gen5` is used in place of `gen1` of Source Code 1 (`SubOh5-A.gap`). After the selection of the set of subgroups `gen[i]` ($i = 1, 2, \cdots, 33$) according to the

$\mathrm{SSG}^{trhex}_{\boldsymbol{O}_h}$ (Eq. 6), the corresponding list of SCI-CFs (`l_SCICF_trhex`) and the list of PCI-CFs (`l_PCICF_trhex`) are calculated. Note that the list of SCI-CFs (`l_SCICF_trhex`) is identical with the 5th $(\boldsymbol{C}_s^{'}\backslash)\boldsymbol{O}_h$-row of the USCI-CF table (Table 2), because the truncated hexahedral skeleton **5** contains one orbit governed by the coset representation $(\boldsymbol{C}_s^{'}\backslash)\boldsymbol{O}_h$. Thereby, the following PCI-CFs for the enumeration based on the truncated hexahedral skeleton **5** are obtained:

$$\begin{aligned}\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_1, \$_d) &= \frac{1}{48}b_1^{24} - \frac{1}{8}c_2^10a_1^4 - \frac{3}{16}b_2^{12} - \frac{1}{12}c_2^{12} - \frac{1}{12}b_3^8 + \frac{1}{8}c_4^4a_2^4 + \frac{1}{2}c_4^5a_2^2 \\ &+ \frac{1}{6}b_4^6 + \frac{1}{4}c_4^6 + \frac{1}{4}c_6^2a_3^4 + \frac{1}{12}c_6^4 + \frac{1}{4}b_6^4 - \frac{1}{2}c_8^2a_4^2 - \frac{1}{6}c_8^3 - \frac{1}{2}c_{12}a_6^2 \\ &+ \frac{1}{12}b_{12}^2 - \frac{1}{4}a_{12}^2 - \frac{1}{12}c_{24} - \frac{1}{4}b_{24} + \frac{1}{2}a_{24} \end{aligned} \tag{141}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_2, \$_d) = \frac{1}{8}b_2^{12} - \frac{1}{8}c_4^4a_2^4 - \frac{3}{8}b_4^6 - \frac{3}{8}c_4^6 + \frac{3}{4}c_8^2a_4^2 + \frac{1}{4}b_8^3 + \frac{3}{4}c_8^3 - c_{16}a_8 \tag{142}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_2', \$_d) = \frac{1}{4}b_2^{12} - \frac{1}{2}c_4^5a_2^2 - \frac{1}{4}b_4^6 - \frac{1}{2}b_6^4 + \frac{1}{2}c_8^2a_4^2 + \frac{1}{2}c_{12}a_6^2 + \frac{1}{2}b_{24} - \frac{1}{2}a_{24} \tag{143}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_s, \$_d) = \frac{1}{8}c_2^{12} - \frac{1}{4}c_4^5a_2^2 - \frac{3}{8}c_4^6 + \frac{1}{4}c_8^2a_4^2 + \frac{1}{4}c_8^3 \tag{144}$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_s', \$_d) &= \frac{1}{4}c_2^{10}a_1^4 - \frac{1}{4}c_4^4a_2^4 - \frac{1}{2}c_4^5a_2^2 - \frac{1}{2}c_6^2a_3^4 + \frac{1}{2}c_8^2a_4^2 + \frac{1}{2}c_{12}a_6^2 \\ &+ \frac{1}{2}a_{12}^2 - \frac{1}{2}a_{24} \end{aligned} \tag{145}$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_i, \$_d) &= \frac{1}{24}c_2^{12} - \frac{1}{4}c_4^5a_2^2 - \frac{1}{8}c_4^6 - \frac{1}{6}c_6^4 + \frac{1}{4}c_8^2a_4^2 + \frac{1}{12}c_8^3 + \frac{1}{2}c_{12}a_6^2 \\ &+ \frac{1}{6}c_{24} - \frac{1}{2}a_{24} \end{aligned} \tag{146}$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_3, \$_d) &= \frac{1}{4}b_3^8 - \frac{1}{4}c_6^2a_3^4 - \frac{1}{4}c_6^4 - \frac{1}{4}b_6^4 + \frac{1}{2}c_{12}a_6^2 - \frac{1}{4}b_{12}^2 + \frac{1}{4}a_{12}^2 + \frac{1}{4}c_{24} \\ &+ \frac{1}{4}b_{24} - \frac{1}{2}a_{24} \end{aligned} \tag{147}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_4, \$_d) = \frac{1}{4}b_4^6 - \frac{1}{4}c_8^2a_4^2 - \frac{1}{4}b_8^3 - \frac{1}{4}c_8^3 + \frac{1}{2}c_{16}a_8 \tag{148}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{S}_4, \$_d) = \frac{1}{4}c_4^6 - \frac{1}{4}c_8^2a_4^2 - \frac{1}{2}c_8^3 + \frac{1}{2}c_{16}a_8 \tag{149}$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{D}_2, \$_d) &= \frac{1}{12}b_4^6 - \frac{1}{4}c_8^2a_4^2 - \frac{1}{4}b_8^3 - \frac{1}{12}c_8^3 - \frac{1}{12}b_{12}^2 + \frac{1}{2}c_{16}a_8 + \frac{1}{4}a_{12}^2 \\ &+ \frac{1}{12}c_{24} + \frac{1}{4}b_{24} - \frac{1}{2}a_{24} \end{aligned} \tag{150}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{D}_2', \$_d) = \frac{1}{4}b_4^6 - \frac{1}{4}c_8^2a_4^2 - \frac{1}{4}b_8^3 - \frac{1}{4}c_8^3 + \frac{1}{2}c_{16}a_8 \tag{151}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_{2v}, \$_d) = \frac{1}{4}c_4^6 - \frac{1}{4}c_8^2a_4^2 - \frac{1}{2}c_8^3 + \frac{1}{2}c_{16}a_8 \tag{152}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_{2v}', \$_d) = \frac{1}{4}c_4^4a_2^4 - \frac{3}{4}c_8^2a_4^2 + \frac{1}{2}c_{16}a_8 \tag{153}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_{2v}'', \$_d) = \frac{1}{2}c_4^5a_2^2 - \frac{1}{2}c_8^2a_4^2 \tag{154}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_{2h}, \$_d) = \frac{1}{4}c_4^6 - \frac{1}{4}c_8^2a_4^2 - \frac{1}{2}c_8^3 + \frac{1}{2}c_{16}a_8 \tag{155}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}'_{2h}, \$_d) = \frac{1}{2}c_4^5a_2^2 - \frac{1}{2}c_8^2a_4^2 - c_{12}a_6^2 + a_{24} \tag{156}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{D}_{3}, \$_d) = \frac{1}{2}b_6^4 - \frac{1}{2}c_{12}a_6^2 - \frac{1}{2}b_{24} + \frac{1}{2}a_{24} \tag{157}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_{3v}, \$_d) = \frac{1}{2}c_6^2a_3^4 - \frac{1}{2}c_{12}a_6^2 - \frac{1}{2}a_{12}^2 + \frac{1}{2}a_{24} \tag{158}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_{3i}, \$_d) = \frac{1}{2}c_6^4 - \frac{1}{2}c_{12}a_6^2 - \frac{1}{2}c_{24} + \frac{1}{2}a_{24} \tag{159}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{D}_{4}, \$_d) = \frac{1}{2}b_8^3 - \frac{1}{2}c_{16}a_8 - \frac{1}{2}b_{24} + \frac{1}{2}a_{24} \tag{160}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_{4v}, \$_d) = \frac{1}{2}c_8^2a_4^2 - \frac{1}{2}c_{16}a_8 \tag{161}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{C}_{4h}, \$_d) = \frac{1}{2}c_8^3 - \frac{1}{2}c_{16}a_8 \tag{162}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{D}_{2d}, \$_d) = \frac{1}{2}c_8^2a_4^2 - \frac{1}{2}c_{16}a_8 - \frac{1}{2}a_{12}^2 + \frac{1}{2}a_{24} \tag{163}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{D}'_{2d}, \$_d) = \frac{1}{2}c_8^3 - \frac{1}{2}c_{16}a_8 \tag{164}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{D}_{2h}, \$_d) = \frac{1}{6}c_8^3 - \frac{1}{2}c_{16}a_8 - \frac{1}{6}c_{24} + \frac{1}{2}a_{24} \tag{165}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{D}'_{2h}, \$_d) = \frac{1}{2}c_8^2a_4^2 - \frac{1}{2}c_{16}a_8 \tag{166}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{T}, \$_d) = \frac{1}{4}b_{12}^2 - \frac{1}{4}a_{12}^2 - \frac{1}{4}c_{24} - \frac{1}{4}b_{24} + \frac{1}{2}a_{24} \tag{167}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{D}_{3d}, \$_d) = c_{12}a_6^2 - a_{24} \tag{168}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{D}_{4h}, \$_d) = c_{16}a_8 - a_{24} \tag{169}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{O}, \$_d) = \frac{1}{2}b_{24} - \frac{1}{2}a_{24} \tag{170}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{T}_{h}, \$_d) = \frac{1}{2}c_{24} - \frac{1}{2}a_{24} \tag{171}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{T}_{d}, \$_d) = \frac{1}{2}a_{12}^2 - \frac{1}{2}a_{24} \tag{172}$$

$$\text{PCI-CF}_{\mathbf{5}}(\boldsymbol{O}_{h}, \$_d) = a_{24} \tag{173}$$

5.6 PCI-CFs for the Rhombic Dodecahedral Skeleton 6

The procedure shown in Source Code 1 (`SubOh5-A.gap`) is applicable to the rhombic dodecahedral skeleton **6**, which contains two orbits. For this purpose, the CPR `Oh_rhdod` for **6** is calculated by using the set of generators `gen6` (cf. Subsubsection 2.2.6) in place of `gen1` of Source Code 1 (`SubOh5-A.gap`). After the selection of the set of subgroups `gen[`i`]` ($i = 1, 2, \cdots, 33$) according to the $\text{SSG}_{\boldsymbol{O}_h}^{rhdod}$ (Eq. 7), the corresponding list of SCI-CFs (`l_SCICF_rhdod`) and the list of PCI-CFs (`l_PCICF_rhdod`) are calculated. As described above, the list of SCI-CFs for the rhombic dodecahedral skeleton (`l_SCICF_rhdod`) can be alternatively obtained from the 18th ($\boldsymbol{C}_{3v}\backslash)\boldsymbol{O}_h$-row and the 21th ($\boldsymbol{C}_{4v}\backslash)\boldsymbol{O}_h$-row of the USCI-CF table shown in Table 2. Thereby, the following PCI-CFs for the enumeration based on the truncated octahedron skeleton **5** are obtained:

$$\begin{aligned}\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_1,\$_d) &= \frac{1}{48}b_1^{14} - \frac{1}{8}c_2^4a_1^6 - \frac{1}{16}c_2^5a_1^4 - \frac{1}{16}b_1^2b_2^6 - \frac{1}{8}b_2^7 - \frac{1}{48}c_2^7 + \frac{1}{8}c_4a_1^2a_2^4 \\ &- \frac{1}{12}b_1^2b_3^4 + \frac{1}{8}c_4^2a_1^2a_2^2 + \frac{1}{4}c_4a_2^5 + \frac{1}{4}a_1^2a_3^4 + \frac{1}{24}b_2^3b_4^2 + \frac{1}{8}c_2c_4^2a_2^2 \\ &+ \frac{1}{4}c_4^2a_2^3 + \frac{1}{8}b_2b_4^3 - \frac{1}{6}c_8a_2^3 - \frac{1}{2}a_2a_4^3 + \frac{1}{4}b_2b_6^2 + \frac{1}{12}c_2c_6^2 + \frac{1}{12}b_4^2b_6 \\ &- \frac{1}{2}a_2a_6^2 - \frac{1}{4}a_4^2a_6 - \frac{1}{4}b_6b_8 - \frac{1}{12}c_8a_6 + \frac{1}{2}a_8a_6 \end{aligned} \quad (174)$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_2,\$_d) &= \frac{1}{8}b_1^2b_2^6 - \frac{1}{8}c_4a_1^2a_2^4 - \frac{1}{8}c_4^2a_1^2a_2^2 - \frac{1}{8}b_1^2b_4^3 - \frac{1}{8}b_2^3b_4^2 - \frac{1}{8}c_2c_4^2a_2^2 \\ &+ \frac{1}{4}a_1^2a_4^3 - \frac{1}{8}b_2b_4^3 - \frac{1}{8}c_2c_4^3 + \frac{1}{4}c_4a_2a_4^2 + \frac{1}{4}c_8a_2^3 + \frac{1}{4}a_2a_4^3 + \frac{1}{4}b_2b_4b_8 \\ &+ \frac{1}{4}c_2c_8a_4 + \frac{1}{4}c_8a_2a_4 - a_2a_4a_8 \end{aligned} \quad (175)$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_2',\$_d) &= \frac{1}{4}b_2^7 - \frac{1}{4}c_4a_2^5 - \frac{1}{4}c_4^2a_2^3 - \frac{1}{4}b_2b_4^3 + \frac{1}{2}a_2a_4^3 - \frac{1}{2}b_2b_6^2 \\ &+ \frac{1}{2}a_2a_6^2 + \frac{1}{2}b_6b_8 - \frac{1}{2}a_8a_6 \end{aligned} \quad (176)$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_s,\$_d) = \frac{1}{8}c_2^5a_1^4 - \frac{1}{4}c_4^2a_1^2a_2^2 - \frac{1}{4}c_4a_2^5 - \frac{1}{8}c_2c_4^2a_2^2 + \frac{1}{4}c_8a_2^3 + \frac{1}{4}a_2a_4^3 \quad (177)$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_s',\$_d) &= \frac{1}{4}c_2^4a_1^6 - \frac{1}{4}c_4a_1^2a_2^4 - \frac{1}{4}c_4a_2^5 - \frac{1}{2}a_1^2a_3^4 - \frac{1}{4}c_4^2a_2^3 + \frac{1}{2}a_2a_4^3 \\ &+ \frac{1}{2}a_2a_6^2 + \frac{1}{2}a_4^2a_6 - \frac{1}{2}a_8a_6 \end{aligned} \quad (178)$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_i,\$_d) &= \frac{1}{24}c_2^7 - \frac{1}{8}c_2c_4^2a_2^2 - \frac{1}{4}c_4^2a_2^3 + \frac{1}{12}c_8a_2^3 + \frac{1}{4}a_2a_4^3 - \frac{1}{6}c_2c_6^2 \\ &+ \frac{1}{2}a_2a_6^2 + \frac{1}{6}c_8a_6 - \frac{1}{2}a_8a_6 \end{aligned} \quad (179)$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_3,\$_d) &= \frac{1}{4}b_1^2b_3^4 - \frac{1}{4}a_1^2a_3^4 - \frac{1}{4}b_2b_6^2 - \frac{1}{4}c_2c_6^2 - \frac{1}{4}b_4^2b_6 + \frac{1}{2}a_2a_6^2 + \frac{1}{4}a_4^2a_6 \\ &+ \frac{1}{4}b_6b_8 + \frac{1}{4}c_8a_6 - \frac{1}{2}a_8a_6 \end{aligned} \quad (180)$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_4,\$_d) = \frac{1}{4}b_1^2b_4^3 - \frac{1}{4}a_1^2a_4^3 - \frac{1}{4}b_2b_4b_8 - \frac{1}{4}c_2c_8a_4 + \frac{1}{2}a_2a_4a_8 \quad (181)$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{S}_4,\$_d) = \frac{1}{4}c_2c_4^3 - \frac{1}{4}c_4a_2a_4^2 - \frac{1}{4}c_2c_8a_4 - \frac{1}{4}c_8a_2a_4 + \frac{1}{2}a_2a_4a_8 \quad (182)$$

$$\begin{aligned}\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{D}_2,\$_d) &= \frac{1}{12}b_2^3b_4^2 - \frac{1}{4}c_4a_2a_4^2 - \frac{1}{12}c_8a_2^3 - \frac{1}{4}b_2b_4b_8 - \frac{1}{12}b_4^2b_6 + \frac{1}{2}a_2a_4a_8 \\ &+ \frac{1}{4}a_4^2a_6 + \frac{1}{4}b_6b_8 + \frac{1}{12}c_8a_6 - \frac{1}{2}a_8a_6 \end{aligned} \quad (183)$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{D}_2',\$_d) = \frac{1}{4}b_2b_4^3 - \frac{1}{4}a_2a_4^3 - \frac{1}{4}b_2b_4b_8 - \frac{1}{4}c_8a_2a_4 + \frac{1}{2}a_2a_4a_8 \quad (184)$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_{2v},\$_d) = \frac{1}{4}c_4^2a_1^2a_2^2 - \frac{1}{4}a_1^2a_4^3 - \frac{1}{4}c_8a_2^3 - \frac{1}{4}c_8a_2a_4 + \frac{1}{2}a_2a_4a_8 \quad (185)$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_{2v}',\$_d) = \frac{1}{4}c_4a_1^2a_2^4 - \frac{1}{4}a_1^2a_4^3 - \frac{1}{4}c_4a_2a_4^2 - \frac{1}{4}a_2a_4^3 + \frac{1}{2}a_2a_4a_8 \quad (186)$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}''_{2v}, \$_d) = \frac{1}{2}c_4a_2^5 - \frac{1}{2}a_2a_4^3 \tag{187}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_{2h}, \$_d) = \frac{1}{4}c_2c_4^2a_2^2 - \frac{1}{4}c_8a_2^3 - \frac{1}{4}a_2a_4^3 - \frac{1}{4}c_2c_8a_4 + \frac{1}{2}a_2a_4a_8 \tag{188}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}'_{2h}, \$_d) = \frac{1}{2}c_4^2a_2^3 - \frac{1}{2}a_2a_4^3 - a_2a_6^2 + a_8a_6 \tag{189}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{D}_{3}, \$_d) = \frac{1}{2}b_2b_6^2 - \frac{1}{2}a_2a_6^2 - \frac{1}{2}b_6b_8 + \frac{1}{2}a_8a_6 \tag{190}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_{3v}, \$_d) = \frac{1}{2}a_1^2a_3^4 - \frac{1}{2}a_2a_6^2 - \frac{1}{2}a_4^2a_6 + \frac{1}{2}a_8a_6 \tag{191}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_{3i}, \$_d) = \frac{1}{2}c_2c_6^2 - \frac{1}{2}a_2a_6^2 - \frac{1}{2}c_8a_6 + \frac{1}{2}a_8a_6 \tag{192}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{D}_{4}, \$_d) = \frac{1}{2}b_2b_4b_8 - \frac{1}{2}a_2a_4a_8 - \frac{1}{2}b_6b_8 + \frac{1}{2}a_8a_6 \tag{193}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_{4v}, \$_d) = \frac{1}{2}a_1^2a_4^3 - \frac{1}{2}a_2a_4a_8 \tag{194}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{C}_{4h}, \$_d) = \frac{1}{2}c_2c_8a_4 - \frac{1}{2}a_2a_4a_8 \tag{195}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{D}_{2d}, \$_d) = \frac{1}{2}c_4a_2a_4^2 - \frac{1}{2}a_2a_4a_8 - \frac{1}{2}a_4^2a_6 + \frac{1}{2}a_8a_6 \tag{196}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{D}'_{2d}, \$_d) = \frac{1}{2}c_8a_2a_4 - \frac{1}{2}a_2a_4a_8 \tag{197}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{D}_{2h}, \$_d) = \frac{1}{6}c_8a_2^3 - \frac{1}{2}a_2a_4a_8 - \frac{1}{6}c_8a_6 + \frac{1}{2}a_8a_6 \tag{198}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{D}'_{2h}, \$_d) = \frac{1}{2}a_2a_4^3 - \frac{1}{2}a_2a_4a_8 \tag{199}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{T}, \$_d) = \frac{1}{4}b_4^2b_6 - \frac{1}{4}a_4^2a_6 - \frac{1}{4}b_6b_8 - \frac{1}{4}c_8a_6 + \frac{1}{2}a_8a_6 \tag{200}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{D}_{3d}, \$_d) = a_2a_6^2 - a_8a_6 \tag{201}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{D}_{4h}, \$_d) = a_2a_4a_8 - a_8a_6 \tag{202}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{O}, \$_d) = \frac{1}{2}b_6b_8 - \frac{1}{2}a_8a_6 \tag{203}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{T}_{h}, \$_d) = \frac{1}{2}c_8a_6 - \frac{1}{2}a_8a_6 \tag{204}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{T}_{d}, \$_d) = \frac{1}{2}a_4^2a_6 - \frac{1}{2}a_8a_6 \tag{205}$$

$$\text{PCI-CF}_{\mathbf{6}}(\boldsymbol{O}_{h}, \$_d) = a_8a_6 \tag{206}$$

6 Enumeration by the PCI-CF method

6.1 Backgrounds for General Procedure of Enumeration

Suppose that the n positions of a given skeleton ($n = 6$ for **1**, $n = 8$ for **2**, $n = 12$ for **3**, $n = 24$ for **4**, $n = 24$ for **5**, and $n = 14$ for **6**) are occupied by a set of n proligands selected from the following ligand inventory:

$$\boldsymbol{L} = \{\mathrm{A}_1, \mathrm{A}_2, \cdots, \mathrm{A}_m; \mathrm{p}_1/\overline{\mathrm{p}}_1, \mathrm{p}_2/\overline{\mathrm{p}}_2, \cdots, \mathrm{p}_\ell/\overline{\mathrm{p}}_\ell\}, \tag{207}$$

where the uppercase letters, A_i ($i = 1, 2, \cdots, m$), indicate achiral proligands, while a pair of lowercase letters without and with an overline, $\mathrm{p}_i/\overline{\mathrm{p}}_i$ ($i = 1, 2, \cdots, \ell$), indicates a pair of enantiomeric proligands when detached. Note that the non-negative integer m (or ℓ) can be selected dependently on the purpose of enumeration at issue, but independently of n. Then, the following inventory-functions are calculated by considering sphericities of orbits:

$$a_d = \sum_{i=1}^{m} \mathrm{A}_i^d \quad \text{(no lowercase terms)} \tag{208}$$

$$c_d = \sum_{i=1}^{m} \mathrm{A}_i^d + 2\sum_{i=1}^{\ell} \mathrm{p}_i^{d/2}\overline{\mathrm{p}}_i^{d/2} \tag{209}$$

$$b_d = \sum_{i=1}^{m} \mathrm{A}_i^d + \sum_{i=1}^{\ell} (\mathrm{p}_i^d + \overline{\mathrm{p}}_i^d), \tag{210}$$

where a_d indicates the mode of occupation for a d-membered homospheric orbit; c_d indicates the mode of occupation for a d-membered enantiospheric orbit; and b_d indicates the mode of occupation for a d-membered hemispheric orbit.

These inventory-functions are introduced into the right-hand side of each PCI-CF (Eqs. 9–41 for **1**, Eqs. 42–74 for **2**, Eqs. 75–107 for **3**, Eqs. 108–140 for **4**, Eqs. 141–173 for **5**, and Eqs. 174–206 for **6**). The resulting equation is expanded to give a generating function, in which the coefficient of the term $\prod_{i=1}^{m} \mathrm{A}_i^{a_i} \prod_{i=1}^{\ell} \mathrm{p}_i^{p_i}\overline{\mathrm{p}}_i^{\overline{p}_i}$ (representing the composition at issue) indicates the number of isomeric promolecules belonging to the corresponding subgroup. The composition is represented by the following partition:

$$[\theta] = [a_1, a_2, \cdots, a_m; p_1, \overline{p}_1, \cdots, p_\ell, \overline{p}_\ell], \tag{211}$$

where the respective elements represent non-negative integers which satisfy the following condition:

$$\sum_{i=1}^{m} a_i + \sum_{i=1}^{\ell} p_i + \sum_{i=1}^{\ell} \overline{p}_i = n. \tag{212}$$

Because of symmetric appearance of the terms, the restriction condition, $a_i \geq a_{i+1}$ as well as $p_i \geq p_{i+1}$ ($p_i \geq \overline{p}_i$), is postulated without losing generality.

6.2 Practices of Enumeration

The next task is to calculate generating functions from the PCI-CFs and the coefficients of respective compositions. The GAP functions developed to treat CI-CFs [12], e.g., `calcCoeffGen`, are capable of treat PCI-CFs as they are. In order to use the function `calcCoeffGen`, the file `CICFgenCC.gapfunc` (Appendix A of [12]) should be loaded along a similar way to Appendix B of [12].

In this article, generating functions are calculated from the PCI-CFs for the octahedral skeleton **1**, the cubane skeleton **2**, and the rhombic dodecahedral skeleton **6** as typical examples.

6.2.1 Enumeration of Octahedral Derivatives

As shown in the following Source Code 2 (`enum-octaX`), let us select six proligands for the octahedral skeleton **1** from the following ligand inventory:

$$\boldsymbol{L} = \{\mathrm{A}, \mathrm{B}, \mathrm{C}, \mathrm{D}, \mathrm{V}, \mathrm{W}; \mathrm{p}/\mathrm{P}, \mathrm{q}/\mathrm{Q}\}, \tag{213}$$

where A, B, $\cdots$, and W represent achiral proligands, while p/P or q/Q represents a pair of enantiomeric proligands when detached. The uppercase letters, P and Q, are used in place of the symbols, $\overline{\mathrm{p}}$ and $\overline{\mathrm{q}}$, to simplify the source code:

Source Code 2 (`enum-octaX.gap`)

```
#Read("c:/fujita00/fujita2018/subductionOh/gap/enum-octaX.gap");
LogTo("c:/fujita00/fujita2018/subductionOh/gap/enum-octaXlog.txt");

Read("c:/fujita00/fujita2018/subductionOh/gap/CICFgenCC.gapfunc"); #Loading of CICFgenCC.gapfunc

b_1 := Indeterminate(Rationals, "b_1"); b_2 := Indeterminate(Rationals, "b_2");
b_3 := Indeterminate(Rationals, "b_3"); b_4 := Indeterminate(Rationals, "b_4");
b_5 := Indeterminate(Rationals, "b_5"); b_6 := Indeterminate(Rationals, "b_6");
a_1 := Indeterminate(Rationals, "a_1"); a_2 := Indeterminate(Rationals, "a_2");
a_3 := Indeterminate(Rationals, "a_3"); a_4 := Indeterminate(Rationals, "a_4");
a_5 := Indeterminate(Rationals, "a_5"); a_6 := Indeterminate(Rationals, "a_6");
c_2 := Indeterminate(Rationals, "c_2"); c_4 := Indeterminate(Rationals, "c_4");
c_6 := Indeterminate(Rationals, "c_6");

PCICF := [ ];
PCICF[1] := 1/48*b_1^6-1/16*c_2*a_1^4-1/16*b_1^2*b_2^2-1/8*c_2^2*a_1^2+1/8*a_1^2*a_2^2-1/12*b_2^3
-1/48*c_2^3+1/8*c_2*a_2^2+1/8*c_4*a_1^2+1/12*a_2^3+1/8*b_2*b_4-1/12*b_3^2+1/4*c_4*a_2-1/2*a_2*a_4
+1/4*a_3^2+1/12*c_6+1/12*b_6-1/3*a_6;
PCICF[2] := 1/8*b_1^2*b_2^2-1/8*a_1^2*a_2^2-1/8*b_1^2*b_4-1/8*b_2^3-1/8*c_2*a_2^2-1/8*c_4*a_1^2
+1/4*a_1^2*a_4+1/4*a_2^3+1/8*b_2*b_4-1/8*c_2*c_4+1/4*c_2*a_4+1/4*c_4*a_2-1/2*a_2*a_4;
PCICF[3] := 1/4*b_2^3-1/4*a_2^3-1/4*b_2*b_4-1/4*c_4*a_2+1/2*a_2*a_4;
PCICF[4] := 1/8*c_2*a_1^4-1/4*a_1^2*a_2^2-1/8*c_2*a_2^2+1/4*a_2*a_4;
PCICF[5] := 1/4*c_2^2*a_1^2-1/4*c_4*a_1^2-1/4*a_2^3-1/4*c_4*a_2+1/2*a_2*a_4-1/2*a_3^2+1/2*a_6;

(#omitted)

PCICF[30] := 1/2*b_6-1/2*a_6;
PCICF[31] := 0;
PCICF[32] := 0;
```

```
PCICF[33] := a_6;

A := Indeterminate(Rationals, "A"); B := Indeterminate(Rationals, "B");
C := Indeterminate(Rationals, "C"); D := Indeterminate(Rationals, "D");
V := Indeterminate(Rationals, "V"); W := Indeterminate(Rationals, "W");
p := Indeterminate(Rationals, "p"); P := Indeterminate(Rationals, "P");
q := Indeterminate(Rationals, "q"); Q := Indeterminate(Rationals, "Q");

 aa_1 := A + B + C + D + V + W; aa_2 := A^2 + B^2 + C^2 + D^2 + V^2 + W^2;
 aa_3 := A^3 + B^3 + C^3 + D^3 + V^3 + W^3; aa_4 := A^4 + B^4 + C^4 + D^4 + V^4 + W^4;
 aa_5 := A^5 + B^5 + C^5 + D^5 + V^5 + W^5; aa_6 := A^6 + B^6 + C^6 + D^6 + V^6 + W^6;
 bb_1 := A + B + C + D + V + W + p + q + P + Q;
 bb_2 := A^2 + B^2 + C^2 + D^2 + V^2 + W^2 + p^2 + q^2 + P^2 + Q^2;
 bb_3 := A^3 + B^3 + C^3 + D^3 + V^3 + W^3 + p^3 + q^3 + P^3 + Q^3;
 bb_4 := A^4 + B^4 + C^4 + D^4 + V^4 + W^4 + p^4 + q^4 + P^4 + Q^4;
 bb_5 := A^5 + B^5 + C^5 + D^5 + V^5 + W^5 + p^5 + q^5 + P^5 + Q^5;
 bb_6 := A^6 + B^6 + C^6 + D^6 + V^6 + W^6 + p^6 + q^6 + P^6 + Q^6;
 cc_2 := A^2 + B^2 + C^2 + D^2 + V^2 + W^2 + 2*p*P + 2*q*Q;
 cc_4 := A^4 + B^4 + C^4 + D^4 + V^4 + W^4 + 2*p^2*P^2 + 2*q^2*Q^2;
 cc_6 := A^6 + B^6 + C^6 + D^6 + V^6 + W^6 + 2*p^3*P^3 + 2*q^3*Q^3;

f_1 := Value(PCICF[1],
[a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3, b_4, b_5, b_6, c_2, c_4, c_6],
[aa_1, aa_2, aa_3, aa_4, aa_5, aa_6, bb_1, bb_2, bb_3, bb_4, bb_5, bb_6, cc_2, cc_4, cc_6]);;

f_2 := Value(PCICF[2],
[a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3, b_4, b_5, b_6, c_2, c_4, c_6],
[aa_1, aa_2, aa_3, aa_4, aa_5, aa_6, bb_1, bb_2, bb_3, bb_4, bb_5, bb_6, cc_2, cc_4, cc_6]);;

f_3 := Value(PCICF[3],
[a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3, b_4, b_5, b_6, c_2, c_4, c_6],
[aa_1, aa_2, aa_3, aa_4, aa_5, aa_6, bb_1, bb_2, bb_3, bb_4, bb_5, bb_6, cc_2, cc_4, cc_6]);;

f_4 := Value(PCICF[4],
[a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3, b_4, b_5, b_6, c_2, c_4, c_6],
[aa_1, aa_2, aa_3, aa_4, aa_5, aa_6, bb_1, bb_2, bb_3, bb_4, bb_5, bb_6, cc_2, cc_4, cc_6]);;

f_5 := Value(PCICF[5],
[a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3, b_4, b_5, b_6, c_2, c_4, c_6],
[aa_1, aa_2, aa_3, aa_4, aa_5, aa_6, bb_1, bb_2, bb_3, bb_4, bb_5, bb_6, cc_2, cc_4, cc_6]);;

(#omitted)

f_30 := Value(PCICF[30],
[a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3, b_4, b_5, b_6, c_2, c_4, c_6],
[aa_1, aa_2, aa_3, aa_4, aa_5, aa_6, bb_1, bb_2, bb_3, bb_4, bb_5, bb_6, cc_2, cc_4, cc_6]);;

f_31 := 0;;
f_32 := 0;;

f_33 := Value(PCICF[33],
[a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3, b_4, b_5, b_6, c_2, c_4, c_6],
[aa_1, aa_2, aa_3, aa_4, aa_5, aa_6, bb_1, bb_2, bb_3, bb_4, bb_5, bb_6, cc_2, cc_4, cc_6]);;

list_partitions :=[];
calcCoeffGenocta := function(list_partitions)
local list_ligand_L, l_pp;
list_ligand_L := [A,B,C,D,V,W,p,P,q,Q];
l_pp := list_partitions;
Print("$", l_pp, "$ \n & ",
calcCoeffGen(f_1, list_ligand_L, list_partitions), " & ",
calcCoeffGen(f_2, list_ligand_L, list_partitions), " & ",
(#omitted)
calcCoeffGen(f_10, list_ligand_L, list_partitions), "\n", " & ",
0, " & ",
(#omitted)
calcCoeffGen(f_19, list_ligand_L, list_partitions), " & ",
calcCoeffGen(f_20, list_ligand_L, list_partitions), "\n", " & ",
calcCoeffGen(f_21, list_ligand_L, list_partitions), " & ",
(#omitted)
calcCoeffGen(f_33, list_ligand_L, list_partitions), " \\\\ \n");
end;
```

```
calcCoeffGenocta([6,0,0,0,0,0,0,0,0,0]); calcCoeffGenocta([5,1,0,0,0,0,0,0,0,0]);
calcCoeffGenocta([4,2,0,0,0,0,0,0,0,0]); calcCoeffGenocta([4,1,1,0,0,0,0,0,0,0]);
calcCoeffGenocta([3,3,0,0,0,0,0,0,0,0]); calcCoeffGenocta([3,2,1,0,0,0,0,0,0,0]);
calcCoeffGenocta([3,1,1,1,0,0,0,0,0,0]); calcCoeffGenocta([2,2,2,0,0,0,0,0,0,0]);
calcCoeffGenocta([2,2,1,1,0,0,0,0,0,0]); calcCoeffGenocta([2,1,1,1,1,0,0,0,0,0]);
calcCoeffGenocta([1,1,1,1,1,1,0,0,0,0]);

calcCoeffGenocta([5,0,0,0,0,0,1,0,0,0]); calcCoeffGenocta([4,1,0,0,0,0,1,0,0,0]);
calcCoeffGenocta([4,0,0,0,0,0,2,0,0,0]); calcCoeffGenocta([4,0,0,0,0,0,1,1,0,0]);
calcCoeffGenocta([3,2,0,0,0,0,1,0,0,0]); calcCoeffGenocta([3,1,1,0,0,0,1,0,0,0]);
calcCoeffGenocta([3,1,0,0,0,0,2,0,0,0]); calcCoeffGenocta([3,1,0,0,0,0,1,1,0,0]);
calcCoeffGenocta([3,0,0,0,0,0,3,0,0,0]); calcCoeffGenocta([3,0,0,0,0,0,2,1,0,0]);

LogTo();
```

The PCI-CFs of the octahedral skeleton (Eqs. 9–41) are adopted in the form of `PCICF[1]`–`PCICF[33]` in Source Code 2 (`enum-octaX.gap`), where each hyphen is omitted from `PCI-CF[1]`–`PCI-CF[33]` for the purpose of adapting to the GAP system. The ligand-inventory functions a_d (Eq. 208), c_d (Eq. 209), and b_d (Eq. 210) are represented to be `aa_1` etc., `cc_2` etc., and `bb_1` etc., which are introduced into the PCI-CFs by using the GAP function `Value`. The resulting generating functions `f_1`–`f_33` are treated by using the function `calcCoeffGen` defined in the file `CICFgenCC.gapfunc` (Appendix A of [12]). The function `calcCoeffGen` is used in the subroutine function `calcCoeffGenocta` for outputting enumeration results in a tabular form. During this process of tabulation, the composition $\mathrm{A}^A\mathrm{B}^B\mathrm{C}^C\mathrm{D}^D\mathrm{V}^V\mathrm{W}^W\mathrm{p}^p\mathrm{P}^P\mathrm{q}^q\mathrm{Q}^Q$ is represented by the following partition:

$$[\theta] = [A, B, C, D, V, W, p, P, q, Q], \tag{214}$$

which is used as the argument of the function `calcCoeffGen` and the subroutine function `calcCoeffGenocta`. Thereby, the coefficient of the term $\mathrm{A}^A\mathrm{B}^B\mathrm{C}^C\mathrm{D}^D\mathrm{V}^V\mathrm{W}^W\mathrm{p}^p\mathrm{P}^P\mathrm{q}^q\mathrm{Q}^Q$ appearing in each of the generating functions `f_1`–`f_33` is extracted to give the number of promolecules with the composition $\mathrm{A}^A\mathrm{B}^B\mathrm{C}^C\mathrm{D}^D\mathrm{V}^V\mathrm{W}^W\mathrm{p}^p\mathrm{P}^P\mathrm{q}^q\mathrm{Q}^Q$ and with the assigned subgroup of $\boldsymbol{O}_h$.

Table 4 collects the symmetry-itemized numbers of isomeric octahedral derivatives with achiral proligands only, where the symmetry-itemized values for each composition (the partition $[\theta]$) are shown in three rows in accord with the $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1).

For example, the partition $[4, 2, 0, 0, 0, 0, 0, 0, 0, 0]$ corresponding to the composition $\mathrm{A}^4\mathrm{B}^2$ generates one $\boldsymbol{C}''_{2v}$-derivative referred to as *cis* and one $\boldsymbol{D}_{4h}$-derivative referred to as *trans*. The partition $[3, 3, 0, 0, 0, 0, 0, 0, 0, 0]$ corresponding to the composition $\mathrm{A}^3\mathrm{B}^3$ generates one $\boldsymbol{C}_{2v}$-derivative referred to by a suffix *mer* (meridional) and one $\boldsymbol{C}_{3v}$-derivative referred to by a suffix *fac* (facial).

The values of Table 4, which are here calculated by the PCI method, are consistent

Table 4. Symmetry-Itemized Numbers of Isomeric Octahedral Derivatives With Achiral Proligands Only

$[\theta] \setminus \mathrm{SSG}_{\boldsymbol{O}_h} =$	$\boldsymbol{C}_1$ (1)	$\boldsymbol{C}_2$ (2)	$\boldsymbol{C}'_2$ (3)	$\boldsymbol{C}_s$ (4)	$\boldsymbol{C}'_s$ (5)	$\boldsymbol{C}_i$ (6)	$\boldsymbol{C}_3$ (7)	$\boldsymbol{C}_4$ (8)	$\boldsymbol{S}_4$ (9)	$\boldsymbol{D}_2$ (10)			
	$\boldsymbol{D}'_2$ (11)	$\boldsymbol{C}_{2v}$ (12)	$\boldsymbol{C}'_{2v}$ (13)	$\boldsymbol{C}''_{2v}$ (14)	$\boldsymbol{C}_{2h}$ (15)	$\boldsymbol{C}'_{2h}$ (16)	$\boldsymbol{D}_3$ (17)	$\boldsymbol{C}_{3v}$ (18)	$\boldsymbol{C}_{3i}$ (19)	$\boldsymbol{D}_4$ (20)			
	$\boldsymbol{C}_{4v}$ (21)	$\boldsymbol{C}_{4h}$ (22)	$\boldsymbol{D}_{2d}$ (23)	$\boldsymbol{D}'_{2d}$ (24)	$\boldsymbol{D}_{2h}$ (25)	$\boldsymbol{D}'_{2h}$ (26)	$\boldsymbol{T}$ (27)	$\boldsymbol{D}_{3d}$ (28)	$\boldsymbol{D}_{4h}$ (29)	$\boldsymbol{O}$ (30)	$\boldsymbol{T}_h$ (31)	$\boldsymbol{T}_d$ (32)	$\boldsymbol{O}_h$ (33)
[6, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	1
[5, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0]	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	1	0	0	0	0	0	0	0	0	0	0	0	0
[4, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0]	0	0	0	0	0	0	0	0	0	0			
	0	0	0	1	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	1	0	0	0	0
[4, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0]	0	0	0	1	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	1	0	0	0	0	0	0	0	0	0	0	0	0
[3, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0]	0	0	0	0	0	0	0	0	0	0			
	0	1	0	0	0	0	0	1	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[3, 2, 1, 0, 0, 0, 0, 0, 0, 0, 0]	0	0	0	1	1	0	0	0	0	0			
	0	1	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[3, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0]	1	0	0	3	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[2, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0]	1	0	0	0	0	0	0	0	0	0			
	0	0	0	3	0	0	0	0	0	0			
	0	0	0	0	1	0	0	0	0	0	0	0	0
[2, 2, 1, 1, 0, 0, 0, 0, 0, 0, 0]	2	0	0	2	1	0	0	0	0	0			
	0	1	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[2, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0]	6	0	0	3	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[1, 1, 1, 1, 1, 1, 0, 0, 0, 0, 0]	15	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0

with those of Table 5 of Ref. [15] obtained previously by means of the fixed-point matrix (FPM) method.

Table 5 collects the symmetry-itemized numbers of isomeric octahedral derivatives with achiral and chiral proligands, where the symmetry-itemized values for each composition (the partition $[\theta]$) are shown in three rows in accord with the $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1). The values in the row with an asterisk should be duplicated, because a pair of enantiomers is counted once under the point group $\boldsymbol{O}_h$. For example, the partition $[5,0,0,0,0,0,1,0,0,0]^*$ ($\mathrm{A}^5\mathrm{p}$), which is coupled with the partition $[5,0,0,0,0,0,0,1,0,0]^*$ ($\mathrm{A}^5\mathrm{P}$), corresponds to the term $\frac{1}{2}(\mathrm{A}^5\mathrm{p} + \mathrm{A}^5\mathrm{P})$, where a pair of p/P represents a pair of enantiomeric proligands.

The values of Table 5, which are here calculated by the PCI method, are consistent with those of Table 7 of Ref. [15] obtained previously by means of the fixed-point matrix (FPM) method.

6.2.2 Enumeration of Cubane Derivatives

For the purpose of enumerating cubane derivatives on the basis of the cubane skeleton **2**, Source Code 2 (`enum-octaX.gap`) can be used after appropriate modifications. The PCI-CFs of the cubane skeleton (Eqs. 42–74) are adopted in the form of `PCICF[1]`–`PCICF[33]` in Source Code 2 (`enum-octaX.gap`), where each hyphen is omitted from `PCI-CF[1]`–`PCI-CF[33]`.

Table 6 collects the symmetry-itemized numbers of isomeric cubane derivatives with achiral proligands only, where the symmetry-itemized values for each composition (the partition $[\theta]$) are shown in three rows in accord with the $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1).

The values of Table 6 are here calculated by the PCI method, where the CPRs are used under the GAP system. They are consistent with those of Table 1 of Ref. [22], which were obtained under Maple system without using the CPRs, although the PCI method was also applied.

6.2.3 Enumeration of Rhombic Dodecahedral Derivatives

Let us examine the enumeration based on the rhombic dodecahedral skeleton **6**, where Source Code 2 (`enum-octaX.gap`) can be used after appropriate modifications. The PCI-CFs of the rhombic dodecahedral skeleton (Eqs. 174–206) are adopted in the form of `PCICF[1]`–`PCICF[33]` in Source Code 2 (`enum-octaX.gap`), where each hyphen is omitted

Table 5. Symmetry-Itemized Numbers of Isomeric Octahedral Derivatives With Achiral and Chiral Proligands

$[\theta] \setminus \mathrm{SSG}_{\boldsymbol{O}_h} =$													
	$\boldsymbol{C}_1$ (1)	$\boldsymbol{C}_2$ (2)	$\boldsymbol{C}'_2$ (3)	$\boldsymbol{C}_s$ (4)	$\boldsymbol{C}'_s$ (5)	$\boldsymbol{C}_i$ (6)	$\boldsymbol{C}_3$ (7)	$\boldsymbol{C}_4$ (8)	$\boldsymbol{S}_4$ (9)	$\boldsymbol{D}_2$ (10)			
	$\boldsymbol{D}'_2$ (11)	$\boldsymbol{C}_{2v}$ (12)	$\boldsymbol{C}'_{2v}$ (13)	$\boldsymbol{C}''_{2v}$ (14)	$\boldsymbol{C}_{2h}$ (15)	$\boldsymbol{C}'_{2h}$ (16)	$\boldsymbol{D}_3$ (17)	$\boldsymbol{C}_{3v}$ (18)	$\boldsymbol{C}_{3i}$ (19)	$\boldsymbol{D}_4$ (20)			
	$\boldsymbol{C}_{4v}$ (21)	$\boldsymbol{C}_{4h}$ (22)	$\boldsymbol{D}_{2d}$ (23)	$\boldsymbol{D}'_{2d}$ (24)	$\boldsymbol{D}_{2h}$ (25)	$\boldsymbol{D}'_{2h}$ (26)	$\boldsymbol{T}$ (27)	$\boldsymbol{D}_{3d}$ (28)	$\boldsymbol{D}_{4h}$ (29)	$\boldsymbol{O}$ (30)	$\boldsymbol{T}_h$ (31)	$\boldsymbol{T}_d$ (32)	$\boldsymbol{O}_h$ (33)
[5, 0, 0, 0, 0, 0, 1, 0, 0, 0]*	0	0	0	0	0	0	0	1/2	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[4, 1, 0, 0, 0, 0, 1, 0, 0, 0]*	1/2	0	0	0	0	0	0	1/2	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[4, 0, 0, 0, 0, 0, 2, 0, 0, 0]*	0	0	1/2	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	1/2			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[4, 0, 0, 0, 0, 0, 1, 1, 0, 0]	0	0	0	0	1	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	1	0	0	0	0	0	0	0	0	0	0	0
[3, 2, 0, 0, 0, 0, 1, 0, 0, 0]*	1	1/2	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[3, 1, 1, 0, 0, 0, 1, 0, 0, 0]*	5/2	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[3, 1, 0, 0, 0, 0, 2, 0, 0, 0]*	1	1/2	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[3, 1, 0, 0, 0, 0, 1, 1, 0, 0]	1	0	0	1	2	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[3, 0, 0, 0, 0, 0, 3, 0, 0, 0]*	0	1/2	0	0	0	0	1/2	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[3, 0, 0, 0, 0, 0, 2, 1, 0, 0]*	1	1/2	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0

* The value should be duplicated.

Table 6. Symmetry-Itemized Numbers of Isomeric Cubane Derivatives With Achiral Proligands Only

$[\theta] \setminus \mathrm{SSG}_{\boldsymbol{O}_h} =$													
	$\boldsymbol{C}_1$ (1)	$\boldsymbol{C}_2$ (2)	$\boldsymbol{C}'_2$ (3)	$\boldsymbol{C}_s$ (4)	$\boldsymbol{C}'_s$ (5)	$\boldsymbol{C}_i$ (6)	$\boldsymbol{C}_3$ (7)	$\boldsymbol{C}_4$ (8)	$\boldsymbol{S}_4$ (9)	$\boldsymbol{D}_2$ (10)			
	$\boldsymbol{D}'_2$ (11)	$\boldsymbol{C}_{2v}$ (12)	$\boldsymbol{C}'_{2v}$ (13)	$\boldsymbol{C}''_{2v}$ (14)	$\boldsymbol{C}_{2h}$ (15)	$\boldsymbol{C}'_{2h}$ (16)	$\boldsymbol{D}_3$ (17)	$\boldsymbol{C}_{3v}$ (18)	$\boldsymbol{C}_{3i}$ (19)	$\boldsymbol{D}_4$ (20)			
	$\boldsymbol{C}_{4v}$ (21)	$\boldsymbol{C}_{4h}$ (22)	$\boldsymbol{D}_{2d}$ (23)	$\boldsymbol{D}'_{2d}$ (24)	$\boldsymbol{D}_{2h}$ (25)	$\boldsymbol{D}'_{2h}$ (26)	$\boldsymbol{T}$ (27)	$\boldsymbol{D}_{3d}$ (28)	$\boldsymbol{D}_{4h}$ (29)	$\boldsymbol{O}$ (30)	$\boldsymbol{T}_h$ (31)	$\boldsymbol{T}_d$ (32)	$\boldsymbol{O}_h$ (33)
$[8,0,0,0,0,0,0,0,0,0,0]$	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	1
$[7,1,0,0,0,0,0,0,0,0,0]$	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	1	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[6,2,0,0,0,0,0,0,0,0,0]$	0	0	0	0	0	0	0	0	0	0			
	0	0	1	1	0	0	0	0	0	0			
	0	0	0	0	0	0	0	1	0	0	0	0	0
$[6,1,1,0,0,0,0,0,0,0,0]$	0	0	0	0	2	0	0	0	0	0			
	0	0	0	0	0	0	0	1	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[5,3,0,0,0,0,0,0,0,0,0]$	0	0	0	0	2	0	0	0	0	0			
	0	0	0	0	0	0	0	1	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[5,2,1,0,0,0,0,0,0,0,0]$	1	0	0	0	5	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[5,1,1,1,0,0,0,0,0,0,0]$	4	0	0	0	6	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[4,4,0,0,0,0,0,0,0,0,0]$	0	0	1	0	1	0	0	0	0	0			
	0	0	0	0	0	0	0	1	0	0			
	1	0	0	0	0	1	0	0	0	0	0	1	0
$[4,3,1,0,0,0,0,0,0,0,0]$	3	0	0	0	5	0	0	0	0	0			
	0	0	0	0	0	0	0	2	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[4,2,2,0,0,0,0,0,0,0,0]$	4	0	2	1	4	0	0	0	0	0			
	0	0	3	1	0	1	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[4,2,1,1,0,0,0,0,0,0,0]$	13	0	0	0	9	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[4,1,1,1,1,0,0,0,0,0,0]$	32	0	0	0	6	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[3,3,2,0,0,0,0,0,0,0,0]$	7	0	0	0	9	0	0	0	0	0			
	0	0	0	0	0	0	0	1	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[3,3,1,1,0,0,0,0,0,0,0]$	18	0	0	0	10	0	0	0	0	0			
	0	0	0	0	0	0	0	2	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[3,2,2,1,0,0,0,0,0,0,0]$	28	0	0	0	14	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[3,2,1,1,1,0,0,0,0,0,0]$	64	0	0	0	12	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[3,1,1,1,1,1,0,0,0,0,0]$	140	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[2,2,2,2,0,0,0,0,0,0,0]$	40	0	6	3	12	1	0	0	0	0			
	0	0	6	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[2,2,2,1,1,0,0,0,0,0,0]$	96	0	0	0	18	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
$[2,2,1,1,1,1,0,0,0,0,0]$	204	0	0	0	12	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0

from PCI-CF[1]–PCI-CF[33].

For the sake of simplicity, a restricted set of proligands, {A, B, p, P}, is selected from the ligand inventory shown by Eq. 213. As a result, the composition $A^A B^B p^p P^P$ is represented by the following partition:

$$[\theta] = [A, B, p, P], \tag{215}$$

which is used as the argument of the function calcCoeffGen and the subroutine function calcCoeffGenocta. Thereby, the coefficient of the term $A^A B^B p^p P^P$ appearing in each of the generating functions f_1–f_33 is extracted to give the number of promolecules with the composition $A^A B^B p^p P^P$ and with the assigned subgroup of $\boldsymbol{O}_h$.

Table 7 collects the symmetry-itemized numbers of isomeric rhombic-dodecahedral derivatives with achiral proligands only, where the symmetry-itemized values for each composition (the partition $[\theta]$ shown by Eq. 215) are shown in three rows in accord with the $\mathrm{SSG}_{\boldsymbol{O}_h}$ (Eq. 1).

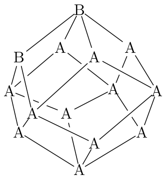
The $[13, 1, 0, 0]$-row of Table 7 indicates the presence of two rhombic dodecahedral derivatives with the composition $A^{13}B$, which belong to the point group $\boldsymbol{C}_{3v}$ and to the point group $\boldsymbol{C}_{4v}$. The $\boldsymbol{C}_{3v}$-derivative based on **6** is generated by the substitution B on a position of ligacy 3. This enumeration result can be related to the $[7, 1, 0, 0, 0, 0, 0, 0, 0, 0]$-row of Table 6, which shows the presence of one $\boldsymbol{C}_{3v}$-isomer in the case of the cubane skeleton **2**. On the other hand, the $\boldsymbol{C}_{4v}$-derivative based on **6** is generated by the substitution B on a position of ligacy 4. This enumeration result can be related to the $[5, 1, 0, 0, 0, 0, 0, 0, 0, 0]$-row of Table 4, which shows the presence of one $\boldsymbol{C}_{4v}$-isomer in the case of the octahedral skeleton **1**.

The $[12, 2, 0, 0]$-row of Table 7 indicates the presence of totally seven rhombic dodecahedral derivatives with the composition $A^{12}B^2$. They are depicted in Figure 3, i.e., two $\boldsymbol{C}'_s$-derivatives (**7** and **8**), one $\boldsymbol{C}'_{2v}$-derivative (**9**), two $\boldsymbol{C}''_{2v}$-derivatives (**10** and **11**), one $\boldsymbol{D}_{3d}$-derivative (**12**), and one $\boldsymbol{D}_{4h}$-derivative (**13**).

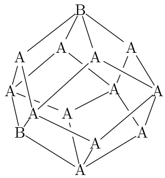
Among the derivatives shown in Figure 3, each of **9** ($\boldsymbol{C}'_{2v}$), **10** ($\boldsymbol{C}''_{2v}$), and **12** ($\boldsymbol{D}_{3d}$) is generated by placing two proligands B's on the respective positions of ligancy 3. Note that the eight positions of ligancy 3 in the rhombic dodecahedral skeleton **6** construct a hypothetical cubane skeleton. Hence, the three derivatives **9**, **10**, and **12** can be related to the $[6, 2, 0, 0, 0, 0, 0, 0, 0, 0]$-row of Table 6, which shows the presence of one $\boldsymbol{C}'_{2v}$-isomer, one $\boldsymbol{C}''_{2v}$-isomer, and one $\boldsymbol{D}_{3d}$-isomer in the case of the cubane skeleton **2**.

Table 7. Symmetry-Itemized Numbers of Isomeric Rhombic Dodecahedral Derivatives With Achiral Proligands Only

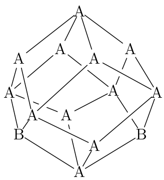
$[\theta] \setminus \mathrm{SSG}_{\boldsymbol{O}_h} =$													
	$\underbrace{\boldsymbol{C}_1}_{1}$	$\underbrace{\boldsymbol{C}_2}_{2}$	$\underbrace{\boldsymbol{C}'_2}_{3}$	$\underbrace{\boldsymbol{C}_s}_{4}$	$\underbrace{\boldsymbol{C}'_s}_{5}$	$\underbrace{\boldsymbol{C}_i}_{6}$	$\underbrace{\boldsymbol{C}_3}_{7}$	$\underbrace{\boldsymbol{C}_4}_{8}$	$\underbrace{\boldsymbol{S}_4}_{9}$	$\underbrace{\boldsymbol{D}_2}_{10}$			
	$\underbrace{\boldsymbol{D}'_2}_{11}$	$\underbrace{\boldsymbol{C}_{2v}}_{12}$	$\underbrace{\boldsymbol{C}'_{2v}}_{13}$	$\underbrace{\boldsymbol{C}''_{2v}}_{14}$	$\underbrace{\boldsymbol{C}_{2h}}_{15}$	$\underbrace{\boldsymbol{C}'_{2h}}_{16}$	$\underbrace{\boldsymbol{D}_3}_{17}$	$\underbrace{\boldsymbol{C}_{3v}}_{18}$	$\underbrace{\boldsymbol{C}_{3i}}_{19}$	$\underbrace{\boldsymbol{D}_4}_{20}$			
	$\underbrace{\boldsymbol{C}_{4v}}_{21}$	$\underbrace{\boldsymbol{C}_{4h}}_{22}$	$\underbrace{\boldsymbol{D}_{2d}}_{23}$	$\underbrace{\boldsymbol{D}'_{2d}}_{24}$	$\underbrace{\boldsymbol{D}_{2h}}_{25}$	$\underbrace{\boldsymbol{D}'_{2h}}_{26}$	$\underbrace{\boldsymbol{T}}_{27}$	$\underbrace{\boldsymbol{D}_{3d}}_{28}$	$\underbrace{\boldsymbol{D}_{4h}}_{29}$	$\underbrace{\boldsymbol{O}}_{30}$	$\underbrace{\boldsymbol{T}_h}_{31}$	$\underbrace{\boldsymbol{T}_d}_{32}$	$\underbrace{\boldsymbol{O}_h}_{33}$
[14, 0, 0, 0]	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	1
[13, 1, 0, 0]	0	0	0	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0	1	0	0			
	1	0	0	0	0	0	0	0	0	0	0	0	0
[12, 2, 0, 0]	0	0	0	0	2	0	0	0	0	0			
	0	0	1	2	0	0	0	0	0	0			
	0	0	0	0	0	0	0	1	1	0	0	0	0
[11, 3, 0, 0]	2	0	0	2	7	0	0	0	0	0			
	0	1	2	0	0	0	0	2	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0
[10, 4, 0, 0]	10	1	2	2	12	0	0	0	0	0			
	0	0	1	4	0	1	0	3	0	0			
	1	0	0	0	0	1	0	0	1	0	0	1	0
[9, 5, 0, 0]	24	2	0	6	25	0	0	0	0	0			
	0	0	2	0	0	0	0	2	0	0			
	3	0	0	0	0	0	0	0	0	0	0	0	0
[8, 6, 0, 0]	40	1	4	4	29	0	0	0	0	0			
	0	1	2	6	1	1	0	2	0	0			
	1	0	1	0	0	1	0	1	0	0	0	0	1
[7, 7, 0, 0]	48	2	0	8	32	0	0	0	0	0			
	0	2	4	0	0	0	0	6	0	0			
	0	0	0	0	0	0	0	0	0	0	0	0	0



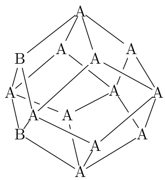
7 ($\boldsymbol{C}'_s$)



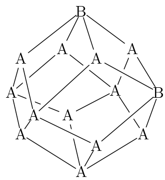
8 ($\boldsymbol{C}'_s$)



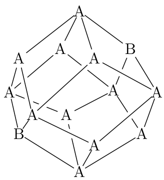
9 ($\boldsymbol{C}'_{2v}$)



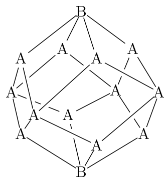
10 ($\boldsymbol{C}''_{2v}$)



11 ($\boldsymbol{C}''_{2v}$)



12 ($\boldsymbol{D}_{3d}$)



13 ($\boldsymbol{D}_{4h}$)

Figure 3. Isomeric rhombic-dodecahedral derivatives with the composition $A^{12}B^{2}$.

On the other hand, each of **11** ($\boldsymbol{C}''_{2v}$) and **13** ($\boldsymbol{D}_{4h}$) is generated by placing two proligands B's on the respective positions of ligancy 4. Note that the six positions of ligancy 4 in the rhombic dodecahedral skeleton **6** construct a hypothetical octahedral skeleton. Hence, the two derivatives **11** and **13** can be related to the $[4, 2, 0, 0, 0, 0, 0, 0, 0, 0]$-row of Table 4 which shows the presence of one $\boldsymbol{C}''_{2v}$-isomer and one $\boldsymbol{D}_{4h}$-isomer in the case of the octahedral skeleton **1**.

As for the remaining two derivatives, **7** ($\boldsymbol{C}'_s$) and **8** ($\boldsymbol{C}'_s$), each of them is generated by placing one B on a position of ligancy 3 and the other B on a position of ligancy 4.

7 Conclusion

Permutation groups derived by respective sets of generators based on various $\boldsymbol{O}_h$-skeletons (octahedron, cube, cuboctahedron, truncated octahedron, truncated hexahedron, and rhombic dodecahedron) have been confirmed to be isomorphic to the point group $\boldsymbol{O}_h$, where the generators are represented by combined-permutation representations (CPRs) which correspond to symmetry operations of the point group $\boldsymbol{O}_h$. Although mark tables (tables of marks) of the permutation groups are different from each other when they are produced by the GAP system, they can be sorted to give a standard mark table for the point group $\boldsymbol{O}_h$. Concordant construction of a standard mark table and a USCI-CF (unit-subduced-cycle-index-with-chirality-fittingness) table for $\boldsymbol{O}_h$ is discussed by starting from each of the above $\boldsymbol{O}_h$-skeletons. After SCI-CFs (subduced cycle indices with chirality fittingness) is generated, a set of PCI-CFs (partial cycle indices with chirality fittingness) is generated to conduct symmetry-itemized enumeration by starting from each of the $\boldsymbol{O}_h$-skeletons according to the PCI method of Fujita's USCI approach [1,2].

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