1192 Bull. Chem. Soc. Jpn. Vol. 84, No. 11, 1192–1207 (2011)

Selected Papers

Symmetry-Itemized Enumeration of Cubane Derivatives as Three-Dimensional Entities by the Fixed-Point Matrix Method of the USCI Approach

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Cubane derivatives with chiral and achiral proligands are counted as three-dimensional (3D) structural isomers by the fixed-point matrix method of the unit-subduced-cycle-index (USCI) approach (S. Fujita, "Symmetry and Combinatorial Enumeration in Chemistry," Springer-Verlag, **1991**). The numbers of such 3D structural isomers are itemized with respect to their point-group symmetries, which are subgroups of the point group O_h for a cubane skeleton. For this purpose, the full list of unit subduced cycle indices with chirality fittingness (USCI-CFs) of O_h is constructed in a tabular form. Fixed-point vectors or fixed-point matrices, which are calculated by starting from USCI-CFs, are used to count 3D structural isomers in the form of isomer-counting matrices. A Maple program source for counting cubane derivatives as 3D structural isomers is given as an example of practical calculation.

Since the elaborate synthesis of cubane (IUPAC name: pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane) by Eaton and Cole,[1] syntheses of its derivatives have been studied extensively.[2–4] Because the cubane skeleton has so high symmetry (belonging to the O_h point group) as to generate many substitution derivatives, preliminary enumerations of possible derivatives and evaluations on their symmetries are desirable for the purpose of systematic synthetic studies.

Although Pólya's method[5] has been widely used to solve various problems of counting isomers,[6–13] it takes account of achiral ligands only, as pointed out by us.[14] This drawback has been avoided by the proligand method,[15–17] where the concepts of sphericities and chirality fittingness have been introduced to take account of chiral ligands along with achiral ligands. The merit of the proligand method has been emphasized in the enumeration of alkanes as 3D structural isomers.[18] In addition to the proligand method, several methods have been developed to evaluate the effects of chiral ligands as well as achiral ligands properly, i.e., the markaracter method,[19,20] the characteristic monomial method,[21,22] the extended superposition method as an application of elementary superposition,[23] and the double coset representation method.[24]

Although these newly-developed methods are capable of incorporating the effects of chiral ligands, they have been concerned with gross numbers of derivatives, which are itemized into achiral derivatives and pairs of enantiomers (chiral derivatives). That is to say, these methods are incapable of itemizing derivatives in terms of point-group symmetries. As a result, from the viewpoint of methodology, they can be regarded as simplified versions of the USCI (unit-subduced-cycle-index) approach,[25] which is, in turn, capable of categorizing derivatives by means of their point-group symmetries after the introduction of the concepts of *subduction of coset representations*, etc. As for pioneering works on enumerations based on marks, see,[26–28] although the concepts introduced by the USCI approach have not been taken into consideration.

The USCI approach is based on the concepts of *subduction of coset representations*, *sphericities*, and *chirality fittingness*, which are integrated to develop the concept of *unit subduced cycle indices without and with chirality fittingness* (USCIs and USCI-CFs).[25] The USCI approach supports four methods of combinatorial enumeration, i.e., (1) the fixed-point matrix (FPM) method based on generating functions derived from subduced cycle indices (SCIs) and mark Tables,[29–31] (2) the partial-cycle-index (PCI) method based on generating functions derived from partial cycle indices (PCIs),[32,33] (3) the elementary superposition method,[23] and (4) the partial superposition method.[32,33]

The task of this series of articles is to demonstrate the four methods of the USCI approach[25] and to compare them with one another as well as with the simplified methods by starting from the common cubane skeleton. In this article, we will describe the the fixed-point matrix (FPM) method of the USCI approach, where USCIs and USCI-CFs play an important role in evaluating fixed points so as to generate fixed-point matrices (FPMs).

Tables for the Point Group O_h

Mark Table and Inverse Mark Table for O_h. Coset Representations and Marks: Mark tables and their inverse matrices are essential to the USCI approach.[25] As for the O_h-group, they have been already reported for the enumeration of octahedral complexes.[34] Thus, the point group O_h has 33 subgroups up to conjugacy, which have been discussed in detail in terms of a nonredundant set of subgroups (SSG):[34]

Published on the web November 3, 2011; doi:10.1246/bcsj.20110195

Table 1. Mark Table of O_h $(M_{O_h})^{34}$

M_{O_h}	C_1	C_2	C_2'	C_s	C_s'	C_i	C_3	C_4	S_4	D_2	D_2'	C_{2v}	C_{2v}'	C_{2v}''	C_{2h}	C_{2h}'	D_3	C_{3v}	C_{3i}	D_4	C_{4v}	C_{4h}	D_{2d}	D_{2d}'	D_{2h}	D_{2h}'	T	D_{3d}	D_{4h}	O	T_h	T_d	O_h
$O_h(/C_1)$	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
$O_h(/C_2)$	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
$O_h(/C_2')$	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
$O_h(/C_s)$	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
$O_h(/C_s')$	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
$O_h(/C_i)$	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
$O_h(/C_3)$	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
$O_h(/C_4)$	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
$O_h(/S_4)$	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
$O_h(/D_2)$	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
$O_h(/D_2')$	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
$O_h(/C_{2v})$	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
$O_h(/C_{2v}')$	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
$O_h(/C_{2v}'')$	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
$O_h(/C_{2h})$	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
$O_h(/C_{2h}')$	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
$O_h(/D_3)$	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
$O_h(/C_{3v})$	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
$O_h(/C_{3i})$	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
$O_h(/D_4)$	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
$O_h(/C_{4v})$	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
$O_h(/C_{4h})$	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
$O_h(/D_{2d})$	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
$O_h(/D_{2d}')$	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
$O_h(/D_{2h})$	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
$O_h(/D_{2h}')$	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
$O_h(/T)$	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
$O_h(/D_{3d})$	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
$O_h(/D_{4h})$	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
$O_h(/O)$	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	0	2	0	0	2	0	0	0
$O_h(/T_h)$	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
$O_h(/T_d)$	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
$O_h(/O_h)$	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

$$\begin{aligned}\mathrm{SSG}_{O_h} = \{&C_1, C_2, C_2', C_s, C_s', C_i, C_3, C_4, S_4, D_2, D_2', C_{2v},\\ &C_{2v}', C_{2v}'', C_{2h}, C_{2h}', D_3, C_{3v}, C_{3i}, D_4, C_{4v}, C_{4h},\\ &D_{2d}, D_{2d}', D_{2h}, D_{2h}', T, D_{3d}, D_{4h}, O, T_h, T_d, O_h\} \quad (1)\end{aligned}$$

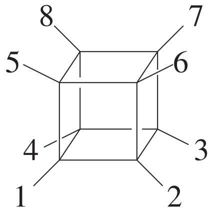
where the subgroups are aligned in the ascending order of their orders. The respective subgroups correspond to the coset representations $O_h(/G_i)$ $(G_i \in \mathrm{SSG}_{O_h})$, which generate the corresponding mark table, as reported in Table 1 of Ref. 34. For practices of calculations, the corresponding inverse matrix is also necessary, as reported in Table 2 of Ref. 34.

Because the reported inverse table (Table 2 of Ref. 34) contains typesetting errors in the $O_h(/C_s')$- and the $O_h(/D_2')$-column, the corrected inverse table (Table 2) is here represented along with the mark table (Table 1).

Assignment of Coset Representations to Orbits: The numbering of a cubane skeleton belonging to the O_h-point group is shown in **1** (Figure 1). This numbering is tentative but does not lose generality.

The 8 positions of the skeleton are restricted into respective subgroups contained in SSG_{O_h} (eq 1). During such processes of restriction, the numbers of fixed positions are counted to generate the following mark as a row vector (a fixed-point vector, FPV):

$$\begin{aligned}\mathrm{FPV}_1 = (&8, 0, 0, 0, 4, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,\\ &2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \quad (2)\end{aligned}$$



1

Figure 1. Numbering of the eight positions of cubane (**1**).

This vector is identical with the mark $M_{O_h(/C_{3v})}$, i.e., the $O_h(/C_{3v})$-row of Table 1, so that the orbit of the 8 positions of **1** is concluded to be governed by the coset representation $O_h(/C_{3v})$. According to Theorem 5.7 of Ref. 25, this assignment is formulated to calculate multiplicities of coset representations:

$$\begin{aligned}\mathrm{FPV}_1 \times M_{O_h}{}^{-1} = (&0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,\\ &1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \quad (3)\end{aligned}$$

where $M_{O_h}{}^{-1}$ is the inverse mark table (Table 2). This vector means that the multiplicity of the coset representation $O_h(/C_{3v})$ is equal to 1.

The $O_h(/C_{3v})$-row of Table 1 also corresponds to the eight faces of an octahedral skeleton of O_h. Note that the eight

Table 2. Inverse Mark Table of O_h $(M_{O_h}{}^{-1})^{34}$

$M_{O_h}{}^{-1}$	$(/C_1)$	$(/C_2)$	$(/C_2{}')$	$(/C_s)$	$(/C_s{}')$	$(/C_i)$	$(/C_3)$	$(/C_4)$	$(/S_4)$	$(/D_2)$	$(/D_2{}')$	$(/C_{2v})$	$(/C_{2v}{}')$	$(/C_{2v}{}'')$	$(/C_{2h})$	$(/C_{2h}{}')$	$(/D_3)$	$(/C_{3v})$	$(/C_{3i})$	$(/D_4)$	$(/C_{4v})$	$(/C_{4h})$	$(/D_{2d})$	$(/D_{2d}{}')$	$(/D_{2h})$	$(/D_{2h}{}')$	$(/T)$	$(/D_{3d})$	$(/D_{4h})$	$(/O)$	$(/T_h)$	$(/T_d)$	$(/O_h)$
																FACTOR = 1/48×																	
C_1	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	0	0	0
C_2	−3	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
$C_2{}'$	−6	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	0	0
C_s	−3	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	0
$C_s{}'$	−6	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
C_i	−1	0	0	0	0	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
C_3	−4	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	0	0	0
C_4	0	−6	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	0	0
S_4	0	−6	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	0
D_2	2	−6	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	0
$D_2{}'$	6	−6	−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
C_{2v}	6	−6	0	−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
$C_{2v}{}'$	6	−6	0	0	−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
$C_{2v}{}''$	12	0	−12	−12	−12	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C_{2h}	6	−6	0	−6	0	−6	0	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
$C_{2h}{}'$	12	0	−12	0	−12	−12	0	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
D_3	12	0	−24	0	0	0	−12	0	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C_{3v}	12	0	0	0	−24	0	−12	0	0	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C_{3i}	4	0	0	0	0	−8	−12	0	0	0	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0	0
D_4	0	12	0	0	0	0	0	−12	0	−12	−12	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0
C_{4v}	0	12	0	0	0	0	0	−12	0	0	0	−12	−12	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0
C_{4h}	0	12	0	0	0	0	0	−12	−12	0	0	0	0	0	−12	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0
D_{2d}	0	12	0	0	0	0	0	0	−12	−12	0	0	−12	0	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0
$D_{2d}{}'$	0	12	0	0	0	0	0	0	−12	0	−12	−12	0	0	0	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0
D_{2h}	−8	12	0	12	0	4	0	0	0	−4	0	−12	0	0	−12	0	0	0	0	0	0	0	0	0	8	0	0	0	0	0	0	0	0
$D_{2h}{}'$	−24	12	24	12	24	12	0	0	0	0	−12	0	−12	−24	−12	−24	0	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0
T	4	0	0	0	0	0	−12	0	0	−4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	0
D_{3d}	−24	0	24	0	24	24	24	0	0	0	0	0	0	0	0	−48	−24	−24	−24	0	0	0	0	0	0	0	0	48	0	0	0	0	0
D_{4h}	0	−48	0	0	0	0	0	24	24	24	24	24	24	0	24	0	0	0	0	−24	−24	−24	−24	−24	−24	−24	0	0	48	0	0	0	0
O	−12	0	24	0	0	0	12	0	0	12	0	0	0	0	0	0	−24	0	0	−24	0	0	0	0	0	0	−12	0	0	24	0	0	0
T_h	−4	0	0	0	0	8	12	0	0	4	0	0	0	0	0	0	0	0	−24	0	0	0	0	0	−8	0	−12	0	0	0	24	0	0
T_d	−12	0	0	0	24	0	12	0	0	12	0	0	0	0	0	0	0	−24	0	0	0	0	−24	0	0	0	−12	0	0	0	0	24	0
O_h	24	0	−24	0	−24	−24	−24	0	0	−24	0	0	0	0	0	48	24	24	24	24	0	0	24	0	24	0	24	−48	−48	−24	−24	−24	48

vertices of a cubane skeleton are truncated to generate such an octahedral skeleton.

On a similar line, the six faces of the cubane skeleton **1** construct an orbit assigned to the coset representation $O_h(/C_{4v})$, the mark of which is collected in the $O_h(/C_{4v})$-row of Table 1. The $O_h(/C_{4v})$-row of Table 1 also corresponds to the six vertices of an octahedral skeleton, which have been already discussed in Ref. 34. Geometrically speaking, the centers of the six faces of a cubane skeleton correspond to the six vertices of an octahedral skeleton.

The twelve edges of the cubane skeleton **1** construct an orbit governed by the coset representation $O_h(/C_{2v}'')$, the mark of which is collected in the $O_h(/C_{2v}'')$-row of Table 1. The $O_h(/C_{2v}'')$-row of Table 1 also corresponds to the twelve edges of an octahedral skeleton, which have been already discussed in Ref. 35. Geometrically speaking, each edge of a cubane skeleton is perpendicular to an edge of an octahedral skeleton, when the octahedral skeleton is placed in the cubane skeleton so as to maintain the O_h-symmetry.

Sphericities of Coset Representations: According to Chapter 8 of Ref. 25, coset representations $G(/G_i)$ are categorized into three cases, i.e., homospheric (G: achiral and G_i: achiral), enantiospheric (G: achiral and G_i: chiral), and hemispheric ones (G: chiral and G_i: chiral). As a result, orbits corresponding such coset representations are characterized by sphericity indices (SIs): a_d for homospheric orbits, c_d for enantiospheric orbits, and b_d for hemispheric orbits, where the subscript d represents the size of the orbit at issue, i.e., $d = |G|/|G_i|$.

USCI-CF Table for the Point Group O_h. Subduction of Coset Representations: According to the formulation of the USCI approach,[25] the mark table and its inverse are further used for the subduction of coset representations: $O_h(/G_i)\downarrow G_j$ (for $G_i, G_j \in \mathrm{SSG}_{O_h}$). For example, the subduction of $O_h(/C_{3v})$ into C_s' is conducted by selecting the values for $\mathrm{SSG}_{C_s'} = \{C_1, C_s'\}$ from the $O_h(/C_{3v})$-row of Table 1 (i.e., the first and 5th values in eq 2). Thereby, we obtain the corresponding mark:

$$M_{O_h(/C_{3v})\downarrow C_s'} = (8, 4) \tag{4}$$

which can be regarded as an FPV for the subgroup C_s'. Because the mark of C_s' and its inverse are obtained as follows:

$$M_{C_s'} = \begin{array}{c} \\ C_s'(/C_1) \\ C_s'(/C_s') \end{array} \!\!\begin{array}{c} \begin{array}{cc} C_1 & C_s' \end{array} \\ \begin{pmatrix} 2 & 0 \\ 1 & 1 \end{pmatrix} \end{array}, \quad {M_{C_s'}}^{-1} = \begin{pmatrix} \frac{1}{2} & 0 \\ -\frac{1}{2} & 1 \end{pmatrix} \tag{5}$$

the following multiplication:

$$M_{O_h(/C_{3v})\downarrow C_s'} \times {M_{C_s'}}^{-1} = (2, 4) \tag{6}$$

gives the multiplicities of $C_s'(/C_1)$ and $C_s'(/C_s')$. It follows that we obtain the following subduction:

$$O_h(/C_{3v}) \downarrow C_s' = 2C_s'(/C_1) + 4C_s'(/C_s') \tag{7}$$

This procedure is repeated to cover all the subgroups contained in $\mathrm{SSG}_{\mathrm{O}_h}$. Thereby, we obtain the subduction column of Table 3.

Each subduction has a geometric meaning which stems from the sphericities of the resulting orbits. Suppose, for example, that the group C_s' of eq 7 is concerned with the mirror plane containing the positions 1, 3, 5, and 7. Then, the subduction represented by eq 7 divides the 8 positions of the cubane skeleton **1** into four one-membered homospheric orbits ({1}, {3}, {5}, and {7}) and two two-membered enantiospheric orbits ({2,4} and {6,8}), as shown in Figure 2. Each homospheric orbit (governed by $C_s'(/C_s')$) can accommodate an achiral ligand such as H, X, Y, and Z, while each enantiospheric orbit (governed by $C_s'(/C_1')$) can accommodate a pair of enantiomeric ligands such as $\mathrm{p}/\bar{\mathrm{p}}$ and $\mathrm{q}/\bar{\mathrm{q}}$.

USCI-CF Table for the Point Group O_h: Because each coset representation generated by the subduction is characterized by a sphericity index (SI), the whole result of the subduction is characterized by a product of SIs, which is called *a unit subduced cycle index with chirality fittingness* (USCI-CF) according to Def. 9.3 of Ref. 25. For example, eq 7 means that the subduction $O_h(/C_{3v})\downarrow C_s'$ is characterized by a USCI-CF, $a_1^4c_2^2$, which corresponds to such a substitution pattern as shown in Figure 2. Similarly, the data collected in the subduction column of Table 3 provide USCI-CFs collected in the USCI-CF column of the same table. When sphericities are not taken into consideration, USCIs (without chirality fittingness) are obtained by putting $s_d = a_d = b_d = c_d$ according to Def. 9.2 of Ref. 25, as collected in the USCI column of Table 3.

The procedure exemplified by Table 3 for generating USCI-CIs (and USCIs) via subduction is repeated to cover all of the coset representations of O_h, the marks of which are collected in Table 1. Thereby, we are able to obtain the full list of the USCI-CFs of O_h, which is shown in Tables 4 and 5. Note that the data shown in Table 3 are collected in the $O_h(/C_{3v})$-rows of Tables 4 and 5. The corresponding USCIs (without chirality fittingness) can be obtained by putting $s_d = a_d = b_d = c_d$ in the data of Tables 4 and 5.

Symmetry-Itemized Enumeration

Fixed-Point Vectors for Symmetry-Itemized Enumeration. A subduced cycle index with chirality fittingness (SCI-CF), which is defined as a product of USCI-CFs (Def. 19.3 of Ref. 25), is capable of evaluating the number of fixed promolecules. Note that such an SCI-CF is identical with the corresponding USCI-CF when there is a single orbit, as found in **1**. Thus, the USCI-CFs appearing in the $O_h(/C_{3v})$-row of Tables 4 and 5 can be used as SCI-CFs for enumerations starting from **1**.

Suppose that substituents for the eight positions of **1** are selected from an inventory of proligands:

$$L' = \{\mathrm{H, A, W, X, Y, Z; p, \bar{p}; q, \bar{q}}\} \tag{8}$$

where H, A, W, X, Y, and Z are achiral proligands in isolation, while p, q, $\bar{\mathrm{p}}$, and $\bar{\mathrm{q}}$ are chiral proligands in isolation. Note that the pair of a letter (e.g., p) and its overlined counterpart (e.g., $\bar{\mathrm{p}}$) represents an enantiomeric pair.

According to Lemma 19.2 of Ref. 25, we use the following inventory functions:

$$a_d = \mathrm{H}^d + \mathrm{A}^d + \mathrm{W}^d + \mathrm{X}^d + \mathrm{Y}^d + \mathrm{Z}^d \tag{9}$$

$$b_d = \mathrm{H}^d + \mathrm{A}^d + \mathrm{W}^d + \mathrm{X}^d + \mathrm{Y}^d + \mathrm{Z}^d + \mathrm{p}^d + \bar{\mathrm{p}}^d + \mathrm{q}^d + \bar{\mathrm{q}}^d \tag{10}$$

$$c_d = \mathrm{H}^d + \mathrm{A}^d + \mathrm{W}^d + \mathrm{X}^d + \mathrm{Y}^d + \mathrm{Z}^d + 2\mathrm{p}^{d/2}\bar{\mathrm{p}}^{d/2} + 2\mathrm{q}^{d/2}\bar{\mathrm{q}}^{d/2} \tag{11}$$

It should be noted that the power $d/2$ appearing in eq 11 is an integer because the subscript d of c_d is always even in the light

Table 3. Subduction of $O_h(/C_{3v})$

Subgroup ($\downarrow G_j$)	Subduction ($O_h(/C_{3v})\downarrow G_j$)	USCI-CF	USCI	GEM (cf. eq 46)		
				Total ($\hat{N}_j$)	Chiral ($\hat{N}_j^{(e)}$)	Achiral ($\hat{N}_j^{(a)}$)
C_1	$8C_1(/C_1)$	b_1^8	s_1^8	1/48	1/48	0
C_2	$4C_2(/C_1)$	b_2^4	s_2^4	1/16	1/16	0
$C_2{}'$	$4C_2{}'(/C_1)$	b_2^4	s_2^4	1/8	1/8	0
C_s	$4C_s(/C_1)$	c_2^4	s_2^4	1/16	−1/16	1/8
$C_s{}'$	$2C_s{}'(/C_1) + 4C_s{}'(/C_s{}')$	$a_1^4c_2^2$	$s_1^4s_2^2$	1/8	−1/8	1/4
C_i	$4C_i(/C_1)$	c_2^4	s_2^4	1/48	−1/48	1/24
C_3	$2C_3(/C_1) + 2C_3(/C_3)$	$b_1^2b_3^2$	$s_1^2s_3^2$	1/6	1/6	0
C_4	$2C_4(/C_1)$	b_4^2	s_4^2	1/8	1/8	0
S_4	$2S_4(/C_1)$	c_4^2	s_4^2	1/8	−1/8	1/4
D_2	$2D_2(/C_1)$	b_4^2	s_4^2	0	0	0
$D_2{}'$	$2D_2{}'(/C_1)$	b_4^2	s_4^2	0	0	0
C_{2v}	$2C_{2v}(/C_1)$	c_4^2	s_4^2	0	0	0
$C_{2v}{}'$	$2C_{2v}{}'(/C_s) + 2C_{2v}{}'(/C_s{}')$	a_2^4	s_2^4	0	0	0
$C_{2v}{}''$	$C_{2v}{}''(/C_1) + 2C_{2v}{}''(/C_s{}')$	$a_2^2c_4$	$s_2^2s_4$	0	0	0
C_{2h}	$2C_{2h}(/C_1)$	c_4^2	s_4^2	0	0	0
$C_{2h}{}'$	$C_{2h}{}'(/C_1) + 2C_{2h}{}'(/C_s)$	$a_2^2c_4$	$s_2^2s_4$	0	0	0
D_3	$D_3(/C_1) + D_3(/C_3)$	b_2b_6	s_2s_6	0	0	0
C_{3v}	$2C_{3v}(/C_s) + 2C_{3v}(/C_{3v})$	$a_1^2a_3^2$	$s_1^2s_3^2$	0	0	0
C_{3i}	$C_{3i}(/C_1) + C_{3i}(/C_3)$	c_2c_6	s_2s_6	1/6	−1/6	1/3
D_4	$D_4(/C_1)$	b_8	s_8	0	0	0
C_{4v}	$2C_{4v}(/C_s{}')$	a_4^2	s_4^2	0	0	0
C_{4h}	$C_{4h}(/C_1)$	c_8	s_8	0	0	0
D_{2d}	$2D_{2d}(/C_s)$	a_4^2	s_4^2	0	0	0
$D_{2d}{}'$	$D_{2d}{}'(/C_1)$	c_8	s_8	0	0	0
D_{2h}	$D_{2h}(/C_1)$	c_8	s_8	0	0	0
$D_{2h}{}'$	$D_{2h}{}'(/C_s) + D_{2h}(/C_s{}')$	a_4^2	s_4^2	0	0	0
T	$2T(/C_3)$	b_4^2	s_4^2	0	0	0
D_{3d}	$D_{3d}(/C_s) + D_{3d}(/C_{3v})$	a_2a_6	s_2s_6	0	0	0
D_{4h}	$D_{4h}(/C_s{}')$	a_8	s_8	0	0	0
O	$O(/C_3)$	b_8	s_8	0	0	0
T_h	$T_h(/C_3)$	c_8	s_8	0	0	0
T_d	$2T_d(/C_{3v})$	a_4^2	s_4^2	0	0	0
O_h	$O_h\ (/C_{3v})$	a_8	s_8	0	0	0

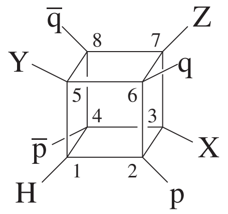


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Figure 2. Orbits generated by the subduction $O_h(/C_{3v})\downarrow C_s{}'$: Four one-membered homospheric orbits ({1}, {3}, {5}, and {7}) and two two-membered enantiospheric orbits ({2,4} and {6,8}), which are characterized by the USCI-CF, $a_1^4c_2^2$.

of the enantiosphericity of the corresponding orbit. These inventory functions are introduced into an SCI-CF to give a generating function, in which the coefficient of the term $\mathrm{H}^h\mathrm{A}^a\mathrm{W}^w\mathrm{Y}^y\mathrm{Z}^z\mathrm{p}^p\bar{\mathrm{p}}^{\bar{p}}\mathrm{q}^q\bar{\mathrm{q}}^{\bar{q}}$ indicates the number of fixed promolecules to be counted. Because H, A, etc. appear symmetrically, the term can be represented by the following partition:

$$[\theta] = [h, a, w, x, y, z; p, \bar{p}, q, \bar{q}] \tag{12}$$

where we put $h \geq a \geq w \geq \ldots \geq z$, $p \geq \bar{p}$, $p \geq q$, and $q \geq \bar{q}$ without losing generality.

For example, let us examine the SCI-CF (USCI-CF) for $O_h(/C_{3v})\downarrow C_s{}'$, i.e., $a_1^4c_2^2$, into which the inventory functions (eqs 9–11) are introduced. The resulting equation is expanded to give the following generating function:

$$\begin{aligned} g_{C_s{}'} &= (\mathrm{H}+\mathrm{A}+\mathrm{W}+\mathrm{X}+\mathrm{Y}+\mathrm{Z})^4 \\ &\quad \times (\mathrm{H}^2+\mathrm{A}^2+\mathrm{W}^2+\mathrm{X}^2+\mathrm{Y}^2+\mathrm{Z}^2+2\mathrm{p}\bar{\mathrm{p}}+2\mathrm{q}\bar{\mathrm{q}})^2 \\ &= \mathrm{H}^8+4\mathrm{H}^7\mathrm{A}+4\mathrm{H}^7\mathrm{W}+4\mathrm{H}^7\mathrm{X}+4\mathrm{H}^7\mathrm{Y}+4\mathrm{H}^7\mathrm{Z} \\ &\quad +8\mathrm{H}^6\mathrm{A}^2+12\mathrm{H}^6\mathrm{AW}+12\mathrm{H}^6\mathrm{AX}+12\mathrm{H}^6\mathrm{AY} \\ &\quad +12\mathrm{H}^6\mathrm{AZ}+8\mathrm{H}^6\mathrm{W}^2+12\mathrm{H}^6\mathrm{WX}+12\mathrm{H}^6\mathrm{WY} \\ &\quad +12\mathrm{H}^6\mathrm{WZ}+8\mathrm{H}^6\mathrm{X}^2+12\mathrm{H}^6\mathrm{XY}+12\mathrm{H}^6\mathrm{XZ}+8\mathrm{H}^6\mathrm{Y}^2 \\ &\quad +12\mathrm{H}^6\mathrm{YZ}+8\mathrm{H}^6\mathrm{Z}^2+4\mathrm{H}^6\mathrm{p}\bar{\mathrm{p}}+4\mathrm{H}^6\mathrm{q}\bar{\mathrm{q}}+\ldots \end{aligned} \tag{13}$$

Among these terms, for example, we focus our attention on $8\mathrm{H}^6\mathrm{A}^2$, which means that 8 promolecules with the formula $\mathrm{H}^6\mathrm{A}^2$ or the partition:

$$[\theta]_1 = [6, 2, 0, 0, 0, 0; 0, 0, 0, 0] \tag{14}$$

are fixed under the action of $C_s{}'$. This is symbolically represented as follows:

$$\rho_{[\theta]_1 C_s{}'} = 8 \tag{15}$$

Table 4. USCI-CF Table of O_h (Part 1)

	C_1	C_2	C_2'	C_s	C_s'	C_i	C_3	C_4	S_4	D_2	D_2'	C_{2v}	C_{2v}'	C_{2v}''	C_{2h}	C_{2h}'
$O_h(/C_1)$	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}
$O_h(/C_2)$	b_1^{24}	$b_1^8b_2^8$	b_2^{12}	c_2^{12}	c_2^{12}	c_2^{12}	b_3^8	$b_2^4b_4^4$	$c_2^4c_4^4$	b_2^{12}	$b_2^4b_4^4$	$c_2^4c_4^4$	$c_2^4c_4^4$	c_4^6	$c_2^4c_4^4$	c_4^6
$O_h(/C_2')$	b_1^{24}	b_2^{12}	$b_1^4b_2^{10}$	c_2^{12}	c_2^{12}	c_2^{12}	b_3^8	b_4^6	c_4^6	b_4^6	$b_2^4b_4^4$	c_4^6	c_4^6	$c_2^2c_4^5$	c_4^6	$c_2^2c_4^5$
$O_h(/C_s)$	b_1^{24}	b_2^{12}	b_2^{12}	$a_1^8c_2^8$	c_2^{12}	c_2^{12}	b_3^8	b_4^6	c_4^6	b_4^6	b_4^6	$a_2^8c_4^2$	c_4^6	$a_2^4c_4^4$	$a_2^4c_4^4$	c_4^6
$O_h(/C_s')$	b_1^{24}	b_2^{12}	b_2^{12}	c_2^{12}	$a_1^4c_2^{10}$	c_2^{12}	b_3^8	b_4^6	c_4^6	b_4^6	b_4^6	c_4^6	$a_2^4c_4^4$	$a_2^2c_4^5$	c_4^6	$a_2^2c_4^5$
$O_h(/C_i)$	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}
$O_h(/C_3)$	b_1^{16}	b_2^8	b_2^8	c_2^8	c_2^8	c_2^8	$b_1^4b_3^4$	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
$O_h(/C_4)$	b_1^{12}	$b_1^4b_2^4$	b_2^6	c_2^6	c_2^6	c_2^6	b_3^4	$b_1^4b_4^2$	$c_2^2c_4^2$	b_2^6	$b_2^2b_4^2$	$c_2^2c_4^2$	$c_2^2c_4^2$	c_4^3	$c_2^2c_4^2$	c_4^3
$O_h(/S_4)$	b_1^{12}	$b_1^4b_2^4$	b_2^6	c_2^6	c_2^6	c_2^6	b_3^4	$b_2^2b_4^2$	$a_1^4c_4^2$	b_2^6	$b_2^2b_4^2$	$c_2^2c_4^2$	$c_2^2c_4^2$	c_4^3	$c_2^2c_4^2$	c_4^3
$O_h(/D_2)$	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
$O_h(/D_2')$	b_1^{12}	$b_1^4b_2^4$	$b_1^4b_2^4$	c_2^6	c_2^6	c_2^6	b_3^4	$b_2^2b_4^2$	$c_2^2c_4^2$	b_2^6	$b_1^4b_4^2$	$c_2^2c_4^2$	$c_2^2c_4^2$	$c_2^2c_4^2$	$c_2^2c_4^2$	$c_2^2c_4^2$
$O_h(/C_{2v})$	b_1^{12}	$b_1^4b_2^4$	b_2^6	$a_1^8c_2^2$	c_2^6	c_2^6	b_3^4	$b_2^2b_4^2$	$c_2^2c_4^2$	b_2^6	$b_2^2b_4^2$	$a_1^4a_2^4$	$c_2^2c_4^2$	$a_2^4c_4$	$a_2^4c_2^2$	c_4^3
$O_h(/C_{2v}')$	b_1^{12}	$b_1^4b_2^4$	b_2^6	c_2^6	$a_1^4c_2^4$	c_2^6	b_3^4	$b_2^2b_4^2$	$c_2^2c_4^2$	b_2^6	$b_2^2b_4^2$	$c_2^2c_4^2$	$a_1^4c_4^2$	$a_2^2c_4^2$	$c_2^2c_4^2$	$a_2^2c_4^2$
$O_h(/C_{2v}'')$	b_1^{12}	b_2^6	$b_1^2b_2^5$	$a_1^4c_2^4$	$a_1^2c_2^5$	c_2^6	b_3^4	b_4^3	c_4^3	b_4^3	$b_2^2b_4^2$	$a_2^4c_4$	$a_2^2c_4^2$	$a_1^2a_2c_4^2$	$a_2^2c_4^2$	$a_2c_2c_4^2$
$O_h(/C_{2h})$	b_1^{12}	$b_1^4b_2^4$	b_2^6	$a_1^4c_2^4$	c_2^6	a_1^{12}	b_3^4	$b_2^2b_4^2$	$c_2^2c_4^2$	b_2^6	$b_2^2b_4^2$	$a_2^4c_2^2$	$c_2^2c_4^2$	$a_2^2c_4^2$	$a_1^4a_2^4$	a_2^6
$O_h(/C_{2h}')$	b_1^{12}	b_2^6	$b_1^2b_2^5$	c_2^6	$a_1^2c_2^5$	a_1^{12}	b_3^4	b_4^3	c_4^3	b_4^3	$b_2^2b_4^2$	c_4^3	$a_2^2c_4^2$	$a_2c_2c_4^2$	a_2^6	$a_1^2a_2^5$
$O_h(/D_3)$	b_1^8	b_2^4	$b_1^4b_2^2$	c_2^4	a_2^4	c_2^4	$b_1^2b_3^2$	b_4^2	c_4^2	b_4^2	b_2^4	c_4^2	c_4^2	$c_2^2c_4$	c_4^2	$c_2^2c_4$
$O_h(/C_{3v})$	b_1^8	b_2^4	b_2^4	c_2^4	$a_1^4c_2^2$	c_2^4	$b_1^2b_3^2$	b_4^2	c_4^2	b_4^2	b_4^2	c_4^2	a_2^4	$a_2^2c_4$	c_4^2	$a_2^2c_4$
$O_h(/C_{3i})$	b_1^8	b_2^4	b_2^4	c_2^4	c_2^4	a_1^8	$b_1^2b_3^2$	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
$O_h(/D_4)$	b_1^6	b_1^6	$b_1^2b_2^2$	c_2^3	c_2^3	c_2^3	b_3^2	$b_1^2b_2^2$	c_2^3	b_1^6	$b_1^2b_2^2$	c_2^3	c_2^3	c_2c_4	c_2^3	c_2c_4
$O_h(/C_{4v})$	b_1^6	$b_1^2b_2^2$	b_2^3	$a_1^4c_2$	$a_1^2c_2^2$	c_2^3	b_3^2	$b_1^2b_4$	c_2c_4	b_2^3	b_2b_4	$a_1^2a_2^2$	$a_1^2c_4$	a_2^3	$a_2^2c_2$	a_2c_4
$O_h(/C_{4h})$	b_1^6	$b_1^2b_2^2$	b_2^3	$a_1^2c_2^2$	c_2^3	a_1^6	b_3^2	$b_1^2b_4$	$a_1^2c_4$	b_2^3	b_2b_4	$a_2^2c_2$	c_2c_4	a_2c_4	$a_1^2a_2^2$	a_2^3
$O_h(/D_{2d})$	b_1^6	b_1^6	b_2^3	c_2^3	$a_1^2c_2^2$	c_2^3	b_3^2	b_2^3	$a_1^2c_2^2$	b_1^6	b_2^3	c_2^3	$a_1^2c_2^2$	a_2c_4	c_2^3	a_2c_4
$O_h(/D_{2d}')$	b_1^6	$b_1^2b_2^2$	$b_1^2b_2^2$	$a_1^4c_2$	c_2^3	c_2^3	b_3^2	b_2b_4	$a_1^2c_4$	b_2^3	$b_1^2b_4$	$a_1^2a_2^2$	c_2c_4	$a_2^2c_2$	$a_2^2c_2$	c_2c_4
$O_h(/D_{2h})$	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
$O_h(/D_{2h}')$	b_1^6	$b_1^2b_2^2$	$b_1^2b_2^2$	$a_1^2c_2^2$	$a_1^2c_2^2$	a_1^6	b_3^2	b_2b_4	c_2c_4	b_2^3	$b_1^2b_4$	$a_2^2c_2$	$a_1^2c_4$	$a_1^2c_4$	$a_1^2a_2^2$	$a_1^2a_2^2$
$O_h(/T)$	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
$O_h(/D_{3d})$	b_1^4	b_2^2	$b_1^2b_2$	c_2^2	$a_1^2c_2$	a_1^4	b_1b_3	b_4	c_4	b_4	b_2^2	c_4	a_2^2	a_2c_2	a_2^2	$a_1^2a_2$
$O_h(/D_{4h})$	b_1^3	b_1^3	b_1b_2	a_1^3	a_1c_2	a_1^3	b_3	b_1b_2	a_1c_2	b_1^3	b_1b_2	a_1^3	a_1c_2	a_1a_2	a_1^3	a_1a_2
$O_h(/O)$	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
$O_h(/T_h)$	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
$O_h(/T_d)$	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
$O_h(/O_h)$	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
Σ	$\frac{1}{48}$	$\frac{1}{16}$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{8}$	$\frac{1}{48}$	$\frac{1}{6}$	$\frac{1}{8}$	$\frac{1}{8}$	0	0	0	0	0	0	0

Eight fixed promolecules with $[\theta]_1$ (eq 15) are shown in Figure 3, where the ligand H corresponds to a vertex with no symbol and the ligand A is denoted by a solid circle, and where the hatched plane indicates the mirror plane of C_s' at issue (containing two remote edges). Each row shows a set of promolecules with a point-group symmetry shown in the rightmost part.

This procedure is repeated to cover all the subgroups contained in SSG_{O_h}. Thereby, we obtain $\rho_{[\theta]_1 G_j}$ for $G_j \in \mathrm{SSG}_{O_h}$, which are collected so as to give an FPV for symmetry-itemized enumeration:

$$\begin{aligned}\mathrm{FPV}_{[\theta]_1} &= (\rho_{[\theta]_1 C_1}, \ldots, \rho_{[\theta]_1 C_s'}, \ldots, \rho_{[\theta]_1 G_j}, \ldots, \rho_{[\theta]_1 O_h}) \\ &= (28, 4, 4, 4, 8, 4, 1, 0, 0, 0, 0, 0, 4, 2, 0, 2, \\ &\quad 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0) \end{aligned} \tag{16}$$

It should be noted that the value 4 for the C_{2v}' (at the 13th element of the $\mathrm{FPV}_{[\theta]_1}$) corresponds to **3**–**6** collected in the first row of Figure 3. On a similar line, the value 2 for the C_{2v}'' (at the 14th element of the $\mathrm{FPV}_{[\theta]_1}$) corresponds to **7** and **8** collected in the second row of Figure 3. On the other hand, the value 1 for the D_{3d} (at the 28th element of the $\mathrm{FPV}_{[\theta]_1}$) corresponds to either one (**9** or **10**) collected in the third row of Figure 3, depending on a threefold axis to be considered.

According to Theorem 19.4 (coupled with Theorem 15.4) in Ref. 25, the FPV is multiplied by the inverse $M_{O_h}{}^{-1}$ (Table 2) to give the following isomer-counting vector (ICV):

$$\begin{aligned}\mathrm{ICV}_{[\theta]_1} &= \mathrm{FPV}_{[\theta]_1} \times M_{O_h}{}^{-1} \\ &= (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, \\ &\quad 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0) \end{aligned} \tag{17}$$

which shows the multiplicity for each subgroup of SSG_{O_h}, i.e., the number of isomers assigned to the subgroup at issue. It follows that there exist one C_{2v}'-, one C_{2v}''-, and one D_{3d}-isomers with $[\theta]_1$, as shown in Figure 4. Note that they correspond to the respective rows of Figure 3 by taking account of conjugacy.

Fixed-Point Matrices for Symmetry-Itemized Enumeration. For the purpose of systematic enumeration, several FPVs can be collected as row vectors of a matrix, which is called *a fixed-point matrix* (FPM) (cf. Sections 15.2 and 19.2 of Ref. 25). For example, such an FPM as corresponding to the following partitions:

Table 5. USCI-CF Table of O_h (Part 2)

	D_3	C_{3v}	C_{3i}	D_4	C_{4v}	C_{4h}	D_{2d}	D_{2d}'	D_{2h}	D_{2h}'	T	D_{3d}	D_{4h}	O	T_h	T_d	O_h
$O_h(/C_1)$	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}
$O_h(/C_2)$	b_6^4	c_6^4	c_6^4	b_4^6	$c_4^2c_8^2$	$c_4^2c_8^2$	c_4^6	$c_4^2c_8^2$	c_4^6	$c_4^2c_8^2$	b_6^4	c_{12}^2	c_8^3	b_{12}^2	c_{12}^2	c_{12}^2	c_{24}
$O_h(/C_2')$	$b_3^4b_6^2$	c_6^4	c_6^4	$b_4^2b_8^2$	c_8^3	c_8^3	c_8^3	$c_4^2c_8^2$	c_8^3	$c_4^2c_8^2$	b_{12}^2	$c_6^2c_{12}$	c_8c_{16}	b_{12}^2	c_{24}	c_{24}	c_{24}
$O_h(/C_s)$	b_6^4	c_6^4	c_6^4	b_8^3	$a_4^4c_8$	$a_4^2c_8^2$	c_8^3	$a_4^4c_8$	a_4^6	$c_4^2c_8^2$	b_{12}^2	c_{12}^2	a_8^3	b_{24}	a_{12}^2	c_{24}	a_{24}
$O_h(/C_s')$	b_6^4	$a_3^4c_6^2$	c_6^4	b_8^3	$a_4^2c_8^2$	c_8^3	$a_4^2c_8^2$	c_8^3	c_8^3	$a_4^2c_8^2$	b_{12}^2	$a_6^2c_{12}$	a_8c_{16}	b_{24}	c_{24}	a_{12}^2	a_{24}
$O_h(/C_i)$	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}
$O_h(/C_3)$	$b_2^2b_6^2$	$c_2^2c_6^2$	$c_2^2c_6^2$	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_4c_{12}	c_{16}	b_8^2	c_8^2	c_8^2	c_{16}
$O_h(/C_4)$	b_6^2	c_6^2	c_6^2	$b_2^2b_4^2$	$c_2^2c_8$	$c_2^2c_8$	c_4^3	c_4c_8	c_4^3	c_4c_8	b_6^2	c_{12}	c_4c_8	b_6^2	c_{12}	c_{12}	c_{12}
$O_h(/S_4)$	b_6^2	c_6^2	c_6^2	b_4^3	c_4c_8	$a_2^2c_8$	$a_2^2c_4^2$	$a_2^2c_8$	c_4^3	c_4c_8	b_6^2	c_{12}	a_4c_8	b_{12}	c_{12}	a_6^2	a_{12}
$O_h(/D_2)$	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}
$O_h(/D_2')$	b_3^4	c_6^2	c_6^2	$b_2^2b_4^2$	c_4c_8	c_4c_8	c_4^3	$c_2^2c_8$	c_4^3	$c_2^2c_8$	b_6^2	c_6^2	c_4c_8	b_6^2	c_{12}	c_{12}	c_{12}
$O_h(/C_{2v})$	b_6^2	c_6^2	c_6^2	b_4^3	$a_2^2a_4^2$	$a_4^2c_4$	c_4^3	$a_2^2a_4^2$	a_2^6	$a_4^2c_4$	b_6^2	c_{12}	a_4^3	b_{12}	a_6^2	c_{12}	a_{12}
$O_h(/C_{2v}')$	b_6^2	a_3^4	c_6^2	b_4^3	$a_2^2c_8$	c_4c_8	$a_2^2c_4^2$	c_4c_8	c_4^3	$a_2^2c_8$	b_6^2	a_6^2	a_4c_8	b_{12}	c_{12}	a_6^2	a_{12}
$O_h(/C_{2v}'')$	$b_3^2b_6$	$a_3^2c_6$	c_6^2	b_4b_8	a_4^3	a_4c_8	a_4c_8	$a_4^2c_4$	a_4^3	$a_2^2c_8$	b_{12}	a_6c_6	a_4a_8	b_{12}	a_{12}	a_{12}	a_{12}
$O_h(/C_{2h})$	b_6^2	c_6^2	a_3^4	b_4^3	$a_4^2c_4$	$a_2^2a_4^2$	c_4^3	$a_4^2c_4$	a_2^6	$a_2^2a_4^2$	b_6^2	a_6^2	a_4^3	b_{12}	a_6^2	c_{12}	a_{12}
$O_h(/C_{2h}')$	$b_3^2b_6$	$a_3^2c_6$	a_3^4	b_4b_8	a_4c_8	a_4^3	a_4c_8	c_4c_8	a_4^3	$a_2^2a_4^2$	b_{12}	$a_3^2a_6$	a_4a_8	b_{12}	a_{12}	a_{12}	a_{12}
$O_h(/D_3)$	$b_1^2b_3^2$	c_2c_6	c_2c_6	b_4^2	c_8	c_8	c_8	c_4^2	c_8	c_4^2	b_4^2	c_2c_6	c_8	b_4^2	c_8	c_8	c_8
$O_h(/C_{3v})$	b_2b_6	$a_1^2a_3^2$	c_2c_6	b_8	a_4^2	c_8	a_4^2	c_8	c_8	a_4^2	b_4^2	a_2a_6	a_8	b_8	c_8	a_4^2	a_8
$O_h(/C_{3i})$	b_2b_6	c_2c_6	$a_1^2a_3^2$	b_8	c_8	a_4^2	c_8	c_8	a_4^2	a_4^2	b_4^2	a_2a_6	a_8	b_8	a_4^2	c_8	a_8
$O_h(/D_4)$	b_3^2	c_6	c_6	$b_1^2b_2^2$	c_2c_4	c_2c_4	c_2^3	c_2c_4	c_2^3	c_2c_4	b_3^2	c_6	c_2c_4	b_3^2	c_6	c_6	c_6
$O_h(/C_{4v})$	b_6	a_3^2	c_6	b_2b_4	$a_1^2a_4$	c_2a_4	a_2c_4	a_2a_4	a_2^3	a_2a_4	b_6	a_6	a_2a_4	b_6	a_6	a_6	a_6
$O_h(/C_{4h})$	b_6	c_6	a_3^2	b_2b_4	c_2a_4	$a_1^2a_4$	a_2c_4	a_2a_4	a_2^3	a_2a_4	b_6	a_6	a_2a_4	b_6	a_6	a_6	a_6
$O_h(/D_{2d})$	b_6	a_3^2	c_6	b_2^3	a_2c_4	a_2c_4	$a_1^2c_2^2$	a_2c_4	c_2^3	a_2c_4	b_3^2	a_6	a_2c_4	b_6	c_6	a_6	a_6
$O_h(/D_{2d}')$	b_3^2	c_6	c_6	b_2b_4	a_2a_4	a_2a_4	a_2c_4	$a_1^2a_4$	a_2^3	c_2a_4	b_6	c_6	a_2a_4	b_6	a_6	a_6	a_6
$O_h(/D_{2h})$	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
$O_h(/D_{2h}')$	b_3^2	a_3^2	a_3^2	b_2b_4	a_2a_4	a_2a_4	a_2c_4	c_2a_4	a_2^3	$a_1^2a_4$	b_6	a_3^2	a_2a_4	b_6	a_6	a_6	a_6
$O_h(/T)$	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
$O_h(/D_{3d})$	b_1b_3	a_1a_3	a_1a_3	b_4	a_4	a_4	a_4	c_4	a_4	a_2^2	b_4	a_1a_3	a_4	b_4	a_4	a_4	a_4
$O_h(/D_{4h})$	b_3	a_3	a_3	b_1b_2	a_1a_2	a_1a_2	a_1c_2	a_1a_2	a_1^3	a_1a_2	b_3	a_3	a_1a_2	b_3	a_3	a_3	a_3
$O_h(/O)$	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
$O_h(/T_h)$	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
$O_h(/T_d)$	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
$O_h(/O_h)$	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
Σ	0	0	$\frac{1}{6}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0

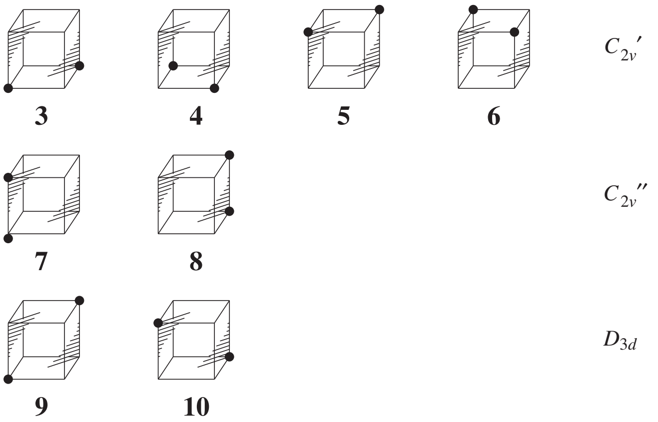
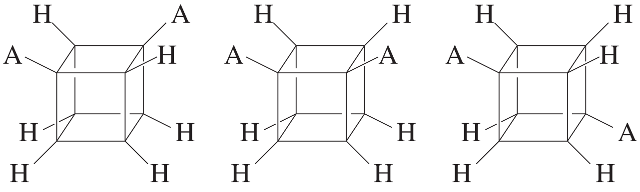


Figure 3. Eight promolecules with $[\theta]_1$ (eq 15), which are fixed on the action of C_s', where the hatched plane indicates the mirror plane at issue. Each row shows a set of promolecules with a point-group symmetry shown in the rightmost part.



11 ($C_{2v}{}'$, achiral) **12** ($C_{2v}{}''$, achiral) **13** (D_{3d}, achiral)

Figure 4. Cubane derivatives with H^6A^2 ([6,2,0,0,0,0; 0,0,0,0]).

$$[\theta]_2 = [8,0,0,0,0,0;0,0,0,0] \quad \text{(for H}^8\text{ etc.)} \tag{18}$$

$$[\theta]_3 = [7,1,0,0,0,0;0,0,0,0] \quad \text{(for H}^7\text{A etc.)} \tag{19}$$

$$[\theta]_4 = [7,0,0,0,0,0;1,0,0,0] \quad \text{(for H}^7\text{p etc.)} \tag{20}$$

$$[\theta]_1 = [6,2,0,0,0,0;0,0,0,0] \quad \text{(for H}^6\text{A}^2\text{ etc. described above)} \tag{21}$$

$$[\theta]_5 = [6,0,0,0,0,0;2,0,0,0] \quad \text{(for H}^6\text{p}^2\text{ etc.)} \tag{22}$$

$$[\theta]_6 = [6,1,1,0,0,0;0,0,0,0] \quad \text{(for H}^6\text{AW etc.)} \tag{23}$$

$$[\theta]_7 = [6,1,0,0,0,0;1,0,0,0] \quad \text{(for H}^6\text{Ap etc.)} \tag{24}$$

$$[\theta]_8 = [6,0,0,0,0,0;1,1,0,0] \quad \text{(for H}^6\text{p}\bar{\text{p}}\text{ etc.)} \tag{25}$$

$$[\theta]_9 = [6,0,0,0,0,0;1,0,1,0] \quad \text{(for H}^6\text{pq etc.)} \tag{26}$$

can be constructed from the data of generating functions (e.g., eq 13) by applying the procedure described above (cf. eq 16 for obtaining $\mathrm{FPV}_{[\theta]_1}$). Thereby, we obtain the following FPM:

$$\mathrm{FPM}_1 = \begin{array}{c} [\theta]_2 \\ [\theta]_3 \\ [\theta]_4 \\ [\theta]_1 \\ [\theta]_5 \\ [\theta]_6 \\ [\theta]_7 \\ [\theta]_8 \\ [\theta]_9 \end{array} \left(\begin{array}{*{33}{c}}
1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1 \\
8&0&0&0&4&0&2&0&0&0&0&0&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
8&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
28&4&4&4&8&4&1&0&0&0&0&0&4&2&0&2&1&1&1&0&0&0&0&0&0&0&0&1&0&0&0&0&0 \\
28&4&4&0&0&0&1&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
56&0&0&0&12&0&2&0&0&0&0&0&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
56&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
56&0&0&8&4&8&2&0&0&0&0&0&0&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
56&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{array} \right) \tag{27}$$

where the values collected in each column appear as the coefficients of the terms which correspond to the partitions $[\theta]_i$ ($i = 1$ to 9), appearing in the generating function of the point group of the column. Thus, the coefficients of respective terms in the generating function $g_{C_s{}'}$ (eq 13) appear in the $C_s{}'$-column (the 5th column) of the FPM_1 (eq 27).

Because the FPM (eq 27) contains FPVs as its row vectors, it is multiplied by the inverse $M_{O_h}{}^{-1}$ (Table 2) so as to give an isomer-counting matrix (ICM) which contains the resulting ICVs as its row vectors:

$$\mathrm{ICM}_1 = \mathrm{FPM}_1 \times M_{O_h}{}^{-1}$$

$$= \begin{array}{c} [\theta]_2 \\ [\theta]_3 \\ [\theta]_4 \\ [\theta]_1 \\ [\theta]_5 \\ [\theta]_6 \\ [\theta]_7 \\ [\theta]_8 \\ [\theta]_9 \end{array} \left(\begin{array}{*{33}{c}}
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1 \\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
0&0&0&0&0&0&\frac{1}{2}&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
0&0&0&0&0&0&0&0&0&0&0&0&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0 \\
0&\frac{1}{2}&\frac{1}{2}&0&0&0&0&0&0&0&0&0&0&0&0&0&\frac{1}{2}&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
1&0&0&0&0&0&\frac{1}{2}&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
0&0&0&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\
1&0&0&0&0&0&\frac{1}{2}&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{array} \right) \tag{28}$$

The process of SCIs → FPM → ICM is programmed in terms of the Maple language[36] to give a file (named "cubaneICM6-2.mpl"), the source list of which is attached below.

The value $\frac{1}{2}$ at the intersection between the $[\theta]_4$-row and C_3-column (the 7th column) in the ICM (eq 28) corresponds to the term $\frac{1}{2}(H^7p + H^7\bar{p})$, which indicates that an enantiomeric pair is counted once.

As an example of such pairs of enantiomers, Figure 5 shows cubane derivatives with H^6p^2 or $H^6\bar{p}^2$ ($[\theta]_5 =$ [6,0,0,0,0,0;2,0,0,0] or $[\theta]'_5 =$ [6,0,0,0,0,0;0,2,0,0]). They are itemized into one pair of C_2-, one pair of $C_2{}'$-, and one pair of D_3-derivatives in accord with the $[\theta]_5$-row of eq 28. Note that each value $\frac{1}{2}$ corresponds to the term $\frac{1}{2}(H^6p^2 + H^6\bar{p}^2)$, which is counted once as a pair of enantiomers (**14a**/**14b**, **15a**/**15b**, or **16a**/**16b**).

To illustrate the results of eq 28, derivatives with $H^6p\bar{p}$ ($[\theta]_8 =$ [6,0,0,0,0,0;1,1,0,0]) are depicted in Figure 6. They are itemized into one $C_s{}'$- (**17**), one C_s- (**18**), and one C_{3i}-derivative (**19**) in accord with the $[\theta]_8$-row of the ICM_1 (eq 28). Each of them indicates an extension of a *meso*-type compound.

For an additional example, let us consider an FPM corresponding to the following partitions:

$$[\theta]_{10} = [5,3,0,0,0,0,0,0,0,0] \quad \text{(for H}^5\text{A}^3\text{ etc.)} \tag{29}$$

$$[\theta]_{11} = [5,0,0,0,0,0,3,0,0,0] \quad \text{(for H}^5\text{p}^3\text{ etc.)} \tag{30}$$

$$[\theta]_{12} = [5,2,1,0,0,0,0,0,0,0] \quad \text{(for H}^5\text{A}^2\text{W etc.)} \tag{31}$$

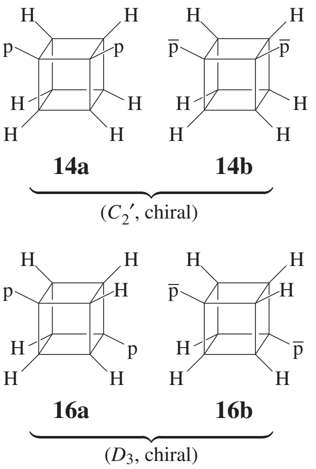


Figure 5. Cubane derivatives with H^6p^2 or $H^6\bar{p}^2$ ([6,0,0,0,0,0;2,0,0,0] or [6,0,0,0,0,0;0,2,0,0]), where p and $\bar{p}$ represents a pair of enantiomeric proligands. They are itemized into one pair of C_2-, one pair of C_2'-, and one pair of D_3-derivatives.

$$[\theta]_{13} = [5,2,0,0,0,0,1,0,0,0] \quad \text{(for } H^5A^2p \text{ etc.)} \tag{32}$$
$$[\theta]_{14} = [5,1,0,0,0,0,2,0,0,0] \quad \text{(for } H^5Ap^2 \text{ etc.)} \tag{33}$$
$$[\theta]_{15} = [5,0,0,0,0,0,2,1,0,0] \quad \text{(for } H^5p^2\bar{p} \text{ etc.)} \tag{34}$$

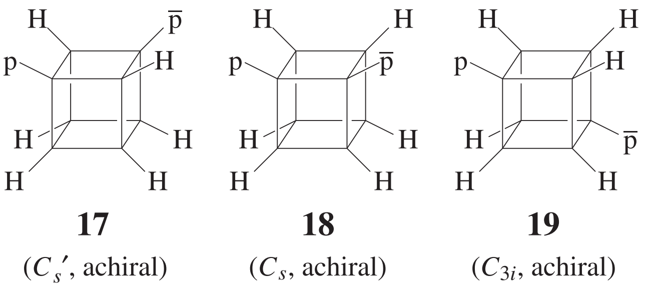


Figure 6. Cubane derivatives with $H^6p\bar{p}$ ([6,0,0,0,0,0; 1,1,0,0]), where p and $\bar{p}$ represents a pair of enantiomeric proligands. They are itemized into one C_s'-, one C_s-, and one C_{3i}-derivative.

$$[\theta]_{16} = [5,1,1,1,0,0,0,0,0,0] \quad \text{(for } H^5AWX \text{ etc.)} \tag{35}$$
$$[\theta]_{17} = [5,1,1,0,0,0,1,0,0,0] \quad \text{(for } H^5AWp \text{ etc.)} \tag{36}$$
$$[\theta]_{18} = [5,1,0,0,0,0,1,1,0,0] \quad \text{(for } H^5Ap\bar{p} \text{ etc.)} \tag{37}$$
$$[\theta]_{19} = [5,1,0,0,0,0,1,0,1,0] \quad \text{(for } H^5Apq \text{ etc.)} \tag{38}$$
$$[\theta]_{20} = [5,0,0,0,0,0,1,1,1,0] \quad \text{(for } H^5p\bar{p}q \text{ etc.)} \tag{39}$$

The FPM can be constructed from the data of generating functions (e.g., eq 13) by applying the procedure described above:

$$\mathrm{FPM}_2 = \left(\begin{array}{lccccccccccccccccccccccccccccccccc}
[\theta]_{10} & 56 & 0 & 0 & 0 & 12 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{11} & 56 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{12} & 168 & 0 & 0 & 0 & 20 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{13} & 168 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{14} & 168 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{15} & 168 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{16} & 336 & 0 & 0 & 0 & 24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{17} & 336 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{18} & 336 & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{19} & 336 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{20} & 336 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right) \tag{40}$$

The FPM (eq 40) is multiplied by the inverse ${M_{O_h}}^{-1}$ (Table 2) so as to give an isomer-counting matrix (ICM):

$$\mathrm{ICM}_2 = \mathrm{FPM}_2 \times {M_{O_h}}^{-1}$$
$$= \left(\begin{array}{lccccccccccccccccccccccccccccccccc}
[\theta]_{10} & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{11} & 1 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{12} & 1 & 0 & 0 & 0 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{13} & \frac{7}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{14} & \frac{7}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{15} & \frac{7}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{16} & 4 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{17} & 7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{18} & 5 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{19} & 7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
[\theta]_{20} & 7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right) \tag{41}$$

Figure 7 shows cubane derivatives with H^5A^2W ($[\theta]_{12} = [5,2,1,0,0,0,0,0]$). There are five C_s'-derivatives (**20**–**24**) and one C_1-derivative (**25a**/**25b**) in accord with the $[\theta]_{12}$-row of the ICM_2 (eq 41). Note that the value 1 for C_1 corresponds to one pair of enantiomers (**25a**/**25b**).

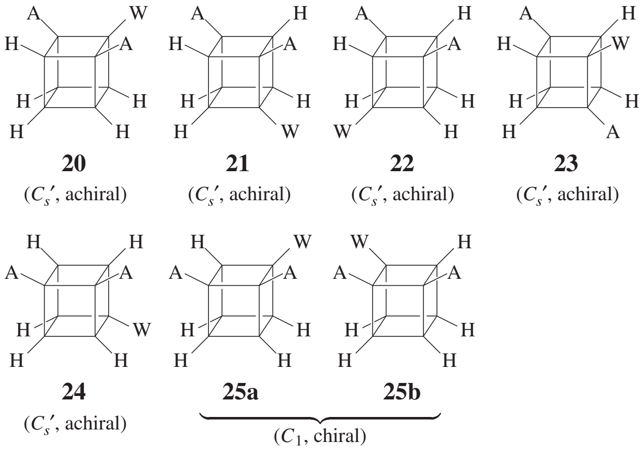


Figure 7. Cubane derivatives with H^5A^2W ([5,2,1,0,0,0,0,0]): Five $C_s{}'$-derivatives and one pair of C_1-derivatives.

Symmetry-Itemized and Gross Enumerations

Achiral Derivatives and Enantiomeric Pairs of Chiral Derivatives. According to the formulation of Ref. 33, the modified bisected mark (MBM) table and its inverse are obtained by simultaneous exchanges of rows and columns applied to the mark table and the inverse mark table. Thus, the inverse modified bisected mark (MBM) table of O_h (Table 6) is obtained as a lower triangular matrix by starting from the inverse mark table of O_h (Table 2), where the data of chiral subgroups are gathered in the upper-left part (the chiral section bordered by horizontal and vertical double straight lines). Further, the data of cyclic subgroups are gathered into the upper-left part of the chiral section:

$$\begin{array}{ll} U^{(c)} = \{C_1,\ C_2,\ C_2{}',\ C_3,\ C_4; & \text{(chiral cyclic subgroups)} \\ \qquad D_2,\ D_2{}',\ D_3,\ D_4,\ T,\ O\} & \text{(chiral noncyclic subgroups)} \end{array} \tag{42}$$

and the values for cyclic achiral subgroups are placed just after the chiral section as follows:

$$\begin{array}{ll} U^{(a)} = \{C_s,\ C_s{}',\ C_i,\ S_4,\ C_{3i}; & \text{(achiral cyclic subgroups)} \\ \left.\begin{array}{l} C_{2v},\ C_{2v}{}',\ C_{2v}{}'',\ C_{2h},\ C_{2h}{}', \\ C_{3v},\ C_{4v},\ C_{4h},\ D_{2d},\ D_{2d}{}', \\ D_{2h},\ D_{2h}{}',\ D_{3d},\ D_{4h},\ T_h, \\ T_d,\ O_h\} \end{array}\right\} & \text{(achiral noncyclic subgroups)} \end{array} \tag{43}$$

It should be noted that a modified mark table (and its inverse)[19] is generated from a mark table (and its inverse), where two rows are exchanged simultaneously in concordance with the corresponding column exchange so as to gather the data of cyclic subgroups contained in the non-redundant set of cyclic subgroups (SCSG):

$$\mathrm{SCSG}_{O_h} = \{C_1, C_2, C_2{}', C_s, C_s{}', C_i, C_3, C_4, S_4, C_{3i}\} \tag{44}$$

On the other hand, a bisected mark table (and its inverse)[33] is generated by gathering the data of chiral subgroups in a mark table (and its inverse). The two modes of modification are combined to provide such a modified bisected mark (MBM) table (and its inverse).[33]

Because Theorem 3 of Ref. 33 is concerned with the lower-left and the lower-right parts of an inverse MBM table of G, the G_j of the Theorem 3 is achiral cyclic subgroups. Hence, the misprinted expression "For chiral cyclic groups G_j" should be read as "For achiral cyclic groups G_j." Theorem 3 of Ref. 33 should be rewritten as follows.

Theorem 1 (Corrected Version of Theorem 3 of Ref. 33): For achiral cyclic group G_j, we have

$$\sum_{i=1}^{t} \bar{m}_{ji} = -\frac{\varphi(|G_j|)}{|N_G(G_j)|}$$

(for the lower-left part of the inverse MBM table) (45)

$$\sum_{i=t+1}^{s} \bar{m}_{ji} = \frac{2\varphi(|G_j|)}{|N_G(G_j)|}$$

(for the lower-right part of the inverse MBM table) (46)

for $j = t+1, t+2, \ldots, s'(\leq s)$. Otherwise, for achiral non-cyclic groups G_j $(j = s'+1, \ldots, s)$,

$$\sum_{i=1}^{t} \bar{m}_{ji} = \sum_{i=t+1}^{s} \bar{m}_{ji} = 0 \tag{47}$$

Note that the case of $i = t$ in the summation corresponds to the $(/O)$-column of Table 6, while the case of $i = t+1$ corresponds to the $(/C_s)$-column of Table 6. The nonzero cases of this theorem (eqs 45 and 46) are supported by the data appearing in the C_s-, $C_s{}'$-, C_i-, S_4-, and C_{3i}-rows of Table 6. The zero cases of this theorem (eq 47) are supported by the remaining data of achiral subgroups appearing in the bottom part of Table 6.

The sum N_j of the row of the subgroup G_j (tentatively fixed) in the MBM table of O_h (Table 6) is calculated as shown in the rightmost part. When G_j runs over all the subgroups of the SSG_{O_h} (eq 1), the values for subgroups other than cyclic subgroups vanish to zero according to eq 42 of Ref. 33.

The sum $N_j^{(e)}$ for G_j is calculated by summing up the values for $U^{(c)}$ (the columns corresponding to the chiral subgroups), as shown in the $N_j^{(e)}$-column of Table 6. According to eq 57 of Ref. 33, each element $N_j^{(e)}$ of a column vector $(N_j^{(e)})$ vanishes to zero if the element is concerned with a subgroup other than cyclic subgroups.

The sum $N_j^{(a)}$ for G_j is calculated by summing up the values for $U^{(a)}$ (the columns corresponding to the achiral subgroups), as shown in the $N_j^{(a)}$-column of Table 6. Each element $N_j^{(a)}$ of a column vector $(N_j^{(a)})$ vanishes to zero if the element is concerned with a subgroup other than cyclic subgroups. The values for the $N_j^{(a)}$ can be evaluated according to eq 63 of Ref. 33.

Let us consider a gross enumeration matrix (GEM) for gross enumerations (total, enantiomeric pairs, and achiral), where the j-th row as a row vector is represented as follows:

$$\mathrm{GEM}_j = (\hat{N}_j, \hat{N}_j^{(e)}, \hat{N}_j^{(a)}) \tag{48}$$

for G_j. Note that $(\hat{N}_j)$, $(\hat{N}_j^{(e)})$, and $(\hat{N}_j^{(a)})$ are generated by reordering the elements of (N_j), $(N_j^{(e)})$, and $(N_j^{(a)})$ into the original orders of elements, as shown in Table 3.

Because the FPM_1 (eq 27) contains FPVs as its row vectors, it is multiplied by the GEM (eq 48, Table 3) so as to give a gross isomer-counting matrix (GICM), where the three columns contain the numbers of total derivatives, enantiomeric pairs, and achiral derivatives, respectively:

Table 6. Inverse Modified Bisected Mark Table of O_h

	$(/C_1)$	$(/C_2)$	$(/C_2')$	$(/C_3)$	$(/C_4)$	$(/D_2)$	$(/D_2')$	$(/D_3)$	$(/D_4)$	$(/T)$	$(/O)$	$(/C_s)$	$(/C_s')$	$(/C_i)$	$(/S_4)$	$(/C_{3i})$	$(/C_{2v})$	$(/C_{2v}')$	$(/C_{2v}'')$	$(/C_{2h})$	$(/C_{2h}')$	$(/C_{3v})$	$(/C_{4v})$	$(/C_{4h})$	$(/D_{2d})$	$(/D_{2d}')$	$(/D_{2h})$	$(/D_{2h}')$	$(/D_{3d})$	$(/D_{4h})$	$(/T_h)$	$(/T_d)$	$(/O_h)$	N_j	$N_j^{(e)}$	$N_j^{(a)}$
																	FACTOR = 1/48×																			
C_1	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	0	0	0	1	1	0
C_2	−3	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	3	3	0
C_2'	−6	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	0	0	6	6	0
C_3	−4	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	0	8	8	0
C_4	0	−6	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	6	6	0
D_2	2	−6	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	0	0
D_2'	6	−6	−12	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	0
D_3	12	0	−24	−12	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	0
D_4	0	12	0	0	−12	−12	−12	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
T	4	0	0	−12	0	−4	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
O	−12	0	24	12	0	12	0	−24	−24	−12	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
C_s	−3	0	0	0	0	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	0	3	−3	6
C_s'	−6	0	0	0	0	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	6	−6	12
C_i	−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	0	0	0	0	0	0	0	1	−1	2
S_4	0	−6	0	0	0	0	0	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	6	−6	12
C_{3i}	4	0	0	−12	0	0	0	0	0	0	0	0	0	−8	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	−8	16
C_{2v}	6	−6	0	0	0	0	0	0	0	0	0	−12	0	0	0	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C_{2v}'	6	−6	0	0	0	0	0	0	0	0	0	0	−12	0	0	0	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C_{2v}''	12	0	−12	0	0	0	0	0	0	0	0	−12	−12	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C_{2h}	6	−6	0	0	0	0	0	0	0	0	0	−6	0	−6	0	0	0	0	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C_{2h}'	12	0	−12	0	0	0	0	0	0	0	0	0	−12	−12	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C_{3v}	12	0	0	−12	0	0	0	0	0	0	0	0	−24	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C_{4v}	0	12	0	0	−12	0	0	0	0	0	0	0	0	0	0	0	−12	−12	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0
C_{4h}	0	12	0	0	−12	0	0	0	0	0	0	0	0	0	−12	0	0	0	0	−12	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0
D_{2d}	0	12	0	0	0	−12	0	0	0	0	0	0	0	0	−12	0	0	−12	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0
D_{2d}'	0	12	0	0	0	0	−12	0	0	0	0	0	0	0	−12	0	−12	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0
D_{2h}	−8	12	0	0	0	−4	0	0	0	0	0	12	0	4	0	0	−12	0	0	−12	0	0	0	0	0	0	8	0	0	0	0	0	0	0	0	0
D_{2h}'	−24	12	24	0	0	0	−12	0	0	0	0	12	24	12	0	0	0	−12	−24	−12	−24	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0
D_{3d}	−24	0	24	24	0	0	0	−24	0	0	0	0	24	24	0	−24	0	0	0	0	−48	−24	0	0	0	0	0	0	48	0	0	0	0	0	0	0
D_{4h}	0	−48	0	0	24	24	24	0	−24	0	0	0	0	0	24	0	24	24	0	24	0	0	−24	−24	−24	−24	−24	−24	0	48	0	0	0	0	0	0
T_h	−4	0	0	12	0	4	0	0	0	−12	0	0	0	8	0	−24	0	0	0	0	0	0	0	0	0	0	−8	0	0	0	24	0	0	0	0	0
T_d	−12	0	0	12	0	12	0	0	0	−12	0	0	24	0	0	0	0	0	0	0	0	−24	0	0	−24	0	0	0	0	0	0	24	0	0	0	0
O_h	24	0	−24	−24	0	−24	0	24	24	24	−24	0	−24	−24	0	24	0	0	0	0	48	24	0	0	24	0	24	0	−48	−48	−24	−24	48	0	0	0

$$\mathrm{GICM}_1 = \mathrm{FPM}_1 \times \mathrm{GEM} = \begin{array}{c} [\theta]_2 \\ [\theta]_3 \\ [\theta]_4 \\ [\theta]_1 \\ [\theta]_5 \\ [\theta]_6 \\ [\theta]_7 \\ [\theta]_8 \\ [\theta]_9 \end{array} \begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & 1 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 3 & 0 & 3 \\ \frac{3}{2} & \frac{3}{2} & 0 \\ 3 & 0 & 3 \\ \frac{3}{2} & \frac{3}{2} & 0 \\ 3 & 0 & 3 \\ \frac{3}{2} & \frac{3}{2} & 0 \end{pmatrix} \tag{49}$$

Figure 4 shows the results of $[\theta]_1$, where all of isomers with $[\theta]_1$ (=[6,2,0,0,0,0;0,0,0,0]), which have been itemized into $C_{2v}{}'$, $C_{2v}{}''$, and the D_{3d}, are all achiral as calculated in eq 49. Figure 5 shows three cubane derivatives with $\mathrm{H}^6\mathrm{p}^2$ or $\mathrm{H}^6\bar{\mathrm{p}}^2$ ($[\theta]_5 = [6,0,0,0,0,0;2,0,0,0]$ or $[\theta]_5{}' = [6,0,0,0,0,0;0,2,0,0]$), which are all chiral, as calculated in eq 49. Figure 6 shows three cubane derivatives with $\mathrm{H}^6\mathrm{p}\bar{\mathrm{p}}$ ($[\theta]_8 = [6,0,0,0,0,0;1,1,0,0]$), which are all achiral, as calculated in eq 49.

In a similar way, the FPM_2 (eq 40) is multiplied by the GEM (eq 48, Table 3) so as to give a gross isomer-counting matrix (GICM):

$$\mathrm{GICM}_2 = \mathrm{FPM}_2 \times \mathrm{GEM} = \begin{array}{c} [\theta]_{10} \\ [\theta]_{11} \\ [\theta]_{12} \\ [\theta]_{13} \\ [\theta]_{14} \\ [\theta]_{15} \\ [\theta]_{16} \\ [\theta]_{17} \\ [\theta]_{18} \\ [\theta]_{19} \\ [\theta]_{20} \end{array} \begin{pmatrix} 3 & 0 & 3 \\ \frac{3}{2} & \frac{3}{2} & 0 \\ 6 & 1 & 5 \\ \frac{7}{2} & \frac{7}{2} & 0 \\ \frac{7}{2} & \frac{7}{2} & 0 \\ \frac{7}{2} & \frac{7}{2} & 0 \\ 10 & 4 & 6 \\ 7 & 7 & 0 \\ 9 & 5 & 4 \\ 7 & 7 & 0 \\ 7 & 7 & 0 \end{pmatrix} \tag{50}$$

Figure 7 shows cubane derivatives with $\mathrm{H}^5\mathrm{A}^2\mathrm{W}$ ($[\theta]_{12} = [5,2,1,0,0,0,0,0]$), where the five $C_s{}'$-derivatives (**20–24**) are achiral, while one pair of enantiomeric C_1-derivatives (**25a/25b**) is chiral, as calculated in the $[\theta]_{12}$-row of the GICM_2 (eq 50). It should be noted that the ligand inventory functions (eqs 9–11) imply $\frac{1}{2}(\mathrm{H}^5\mathrm{A}^2\mathrm{W} + \bar{\mathrm{H}}^5\bar{\mathrm{A}}^2\bar{\mathrm{W}}) = \mathrm{H}^5\mathrm{A}^2\mathrm{W}$ because the hypothetical enantiomeric ligand $\bar{\mathrm{H}}$ (or $\bar{\mathrm{A}}$ or $\bar{\mathrm{W}}$) is identical with an achiral ligand H (or A or W).

Generation of CI-CFs from USCI-CFs. Throughout the above discussions, the evaluation of FPVs (or FPMs) by using USCI-CFs (or SCI-CFs) and ligand inventory functions (e.g., eqs 9–11) precede the multiplication of the inverse mark table or the matrix of gross enumeration (GEM). According to Corollary 1.3 of Ref. 33, the order of the evaluation and the multiplication can be exchanged so as to generate the corresponding cycle index with chirality fittingness (CI-CF) by starting from USCI-CFs. The set of USCI-CFs (Table 3, or generally SCI-CFs), which is regarded as a row vector, is multiplied by the $(\hat{N}_j)$ column of the GEM (Table 3), so as to generate the corresponding CI-CF as follows:

$$\begin{aligned} &\text{CI-CF}(\mathbf{P}, \$_d) \\ &= \frac{1}{48}b_1^8 + \frac{1}{16}b_2^4 + \frac{1}{8}b_2^4 + \frac{1}{16}c_2^4 + \frac{1}{8}a_1^4c_2^2 + \frac{1}{48}c_2^4 \\ &\quad + \frac{1}{6}b_1^2b_3^2 + \frac{1}{8}b_4^2 + \frac{1}{8}c_4^2 + \frac{1}{6}c_2c_6 \\ &= \frac{1}{48}b_1^8 + \frac{3}{16}b_2^4 + \frac{1}{6}b_1^2b_3^2 + \frac{1}{8}b_4^2 + \frac{1}{12}c_2^4 \\ &\quad + \frac{1}{6}c_2c_6 + \frac{1}{8}a_1^4c_2^2 + \frac{1}{8}c_4^2 \end{aligned} \tag{51}$$

where $\mathbf{P}$ is the permutation representation of the substituted positions at issue. Obviously, the monomials contained in eq 51 are concerned with cyclic subgroups of O_h. Generating functions for gross enumeration can be derived by introducing ligand inventory functions (e.g., eqs 9–11) into the CI-CF (eq 51). The generating function obtained by the introduction of eqs 9–11 into eq 51 contains the data shown in the first column of the GICM_1 (eq 49) and that of the GICM_2 (eq 50).

As for the enumeration of enantiomeric pairs of chiral derivatives (Corollary 1.1 of Ref. 33), the set of USCI-CFs (Table 3, or generally SCI-CFs), is multiplied by the $(\hat{N}_j^{(e)})$ column of the GEM (Table 3), so as to generate the corresponding CI-CF as follows:

$$\begin{aligned} &\text{CI-CF}(e)(\mathbf{P}, \$_d) \\ &= \frac{1}{48}b_1^8 + \frac{1}{16}b_2^4 + \frac{1}{8}b_2^4 - \frac{1}{16}c_2^4 - \frac{1}{8}a_1^4c_2^2 - \frac{1}{48}c_2^4 \\ &\quad + \frac{1}{6}b_1^2b_3^2 + \frac{1}{8}b_4^2 - \frac{1}{8}c_4^2 - \frac{1}{6}c_2c_6 \\ &= \frac{1}{48}b_1^8 + \frac{3}{16}b_2^4 + \frac{1}{6}b_1^2b_3^2 + \frac{1}{8}b_4^2 - \frac{1}{12}c_2^4 \\ &\quad - \frac{1}{6}c_2c_6 - \frac{1}{8}a_1^4c_2^2 - \frac{1}{8}c_4^2 \end{aligned} \tag{52}$$

Note that the plus signs of the monomials for achiral cyclic subgroups in eq 51 are changed into minus to give eq 52. Generating functions for gross enumeration of enantiomeric pairs can be derived by introducing ligand inventory functions (e.g., eqs 9–11) into the CI-CF (eq 52). The generating function obtained by the introduction of eqs 9–11 into eq 52 contains the data shown in the second column of the GICM_1 (eq 49) and that of the GICM_2 (eq 50).

As for the enumeration of achiral derivatives (Corollary 1.2 of Ref. 33), the set of USCI-CFs (Table 3, or generally SCI-CFs), is multiplied by the $(\hat{N}_j^{(a)})$ column of the GEM (Table 3), so as to generate the corresponding CI-CF as follows:

$$\text{CI-CF}^{(a)}(\mathbf{P}, \$_d) = \frac{1}{8}c_2^4 + \frac{1}{4}a_1^4c_2^2 + \frac{1}{24}c_2^4 + \frac{1}{4}c_4^2 + \frac{1}{3}c_2c_6 \tag{53}$$

Note that the monomials for achiral cyclic subgroups remain in eq 53. Generating functions for gross enumeration of achiral derivatives can be derived by introducing ligand inventory functions (e.g., eqs 9–11) into the CI-CF (eq 53). The generating function obtained by the introduction of eqs 9–11 into eq 53 contains the data shown in the third column of the GICM_1 (eq 49) and that of the GICM_2 (eq 50).

Maple Program for Generating FPMs and ICMs

The Maple procedure named "coeff62SCI" is programmed to calculate the coefficient of the term $\mathrm{H}^h\mathrm{A}^a\mathrm{W}^w\mathrm{Y}^y\mathrm{Z}^z\mathrm{p}^p\bar{\mathrm{p}}^{\bar{p}}\mathrm{q}^q\bar{\mathrm{q}}^{\bar{q}}$ or the partition $[\theta] = [h, a, w, x, y, z; p, \bar{p}, q, \bar{q}]$. The Maple procedure named "cubaneFPV" is a procedure for calculating an FPV. The resulting FPVs are collected to give an FPM, which is multiplied by the inverse of the mark table to give an ICM.

```
#cubaneICM6-2.mpl
restart;
#read "c:/fujita0/cubaneVI/calc2/cubaneICM6-2.mpl";
#with H^k A^l W^m X^n Y^kk Z^ll p^h P^hh q^i Q^ii

SCIC1 := b1^8; SCIC2 := b2^4; SCIC2p := b2^4;
SCICs := c2^4; SCICsp := a1^4*c2^2;
SCICi := c2^4; SCIC3 := b1^2*b3^2; SCIC4 := b4^2; SCIS4 := c4^2;
SCID2 := b4^2; SCID2p := b4^2; SCIC2v := c4^2; SCIC2vp := a2^4;
SCIC2vpp := a2^2*c4; SCIC2h := c4^2;
SCIC2hp := a2^2*c4; SCID3 := b2*b6;
SCIC3v := a1^2*a3^2; SCIC3i := c2*c6; SCID4 := b8; SCIC4v := a4^2;
SCIC4h := c8; SCID2d := a4^2; SCID2dp := c8; SCID2h := c8;
SCID2hp := a4^2; SCIT := b4^2; SCID3d := a2*a6; SCID4h := a8;
SCIO := b8; SCITh := c8; SCITd := a4^2; SCIOh := a8;

# Maple procedure for calculating the coefficient of
# the term H^k A^l W^m X^n Y^kk Z^ll p^h P^hh q^i Q^ii
# (symmetry-itemized calculation)
coeff62SCI := proc(k::integer,
l::integer, m::integer, n::integer, kk::integer, ll::integer,
h::integer, hh::integer, i::integer, ii::integer, fSCI)
local N1g,N2g,N3g,N4g,N5g,N6g,N7g,N8g,N9g,SCI;
global N10g;
SCI := fSCI;
if(k=0) then N1g := expand(coeff(H*SCI,H));
else N1g := expand(coeff(SCI,H^k));end if;
if(l=0) then N2g := expand(coeff(A*N1g,A));
else N2g := expand(coeff(N1g,A^l));end if;
if(m=0) then N3g := expand(coeff(W*N2g,W));
else N3g := expand(coeff(N2g,W^m));end if;
if(n=0) then N4g := expand(coeff(X*N3g,X));
else N4g := expand(coeff(N3g,X^n));end if;
if(kk=0) then N5g := expand(coeff(Y*N4g,Y));
else N5g := expand(coeff(N4g,Y^kk));end if;
if(ll=0) then N6g := expand(coeff(Z*N5g,Z));
else N6g := expand(coeff(N5g,Z^ll));end if;
if(h=0) then N7g := expand(coeff(p*N6g,p));
else N7g := expand(coeff(N6g,p^h));end if;
if(hh=0) then N8g := expand(coeff(P*N7g,P));
else N8g := expand(coeff(N7g,P^hh));end if;
if(i=0) then N9g := expand(coeff(q*N8g,q));
else N9g := expand(coeff(N8g,q^i));end if;
if(ii=0) then N10g := expand(coeff(Q*N9g,Q));
else N10g := expand(coeff(N9g,Q^ii));end if;
end proc:

# Maple procedure for calculating a fixed point vector
cubaneFPV := proc(k::integer,
l::integer, m::integer, n::integer, kk::integer, ll::integer,
h::integer, hh::integer, i::integer, ii::integer)
global FPV;
FPV:= vector(33,[]):
printf("[%d,%d,%d,%d,%d,%d;%d,%d,%d,%d] n",
k, l, m, n, kk, ll, h, hh, i, ii);
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC1); FPV[1] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC2); FPV[2] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC2p); FPV[3] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCICs); FPV[4] := N10g;
```

```
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCICsp); FPV[5] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCICi); FPV[6] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC3); FPV[7] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC4); FPV[8] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIS4); FPV[9] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCID2); FPV[10] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCID2p); FPV[11] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC2v); FPV[12] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC2vp); FPV[13] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC2vpp); FPV[14] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC2h); FPV[15] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC2hp); FPV[16] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCID3); FPV[17] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC3v); FPV[18] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC3i); FPV[19] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCID4); FPV[20] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC4v); FPV[21] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIC4h); FPV[22] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCID2d); FPV[23] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCID2dp); FPV[24] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCID2h); FPV[25] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCID2hp); FPV[26] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIT); FPV[27] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCID3d); FPV[28] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCID4h); FPV[29] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIO); FPV[30] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCITh); FPV[31] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCITd); FPV[32] := N10g;
coeff62SCI(k,l,m,n,kk,ll,h,hh,i,ii,SCIOh); FPV[33] := N10g;
end proc:

InvMOh := evalm((1/48)*matrix(33,33,
 [[1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [-3,6,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [-6,0,12,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [-3,0,0,6,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [-6,0,0,0,12,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [-1,0,0,0,0,2,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [-4,0,0,0,0,0,12,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [ 0,-6,0,0,0,0,0,12,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [ 0,-6,0,0,0,0,0,0,12,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [ 2,-6,0,0,0,0,0,0,0,4,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [ 6,-6,-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],
 [ 6,-6,0,-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],
 [ 6,-6,0,0,-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],
 [12,0,-12,-12,-12,0,0,0,0,0,0,0,0,24,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [ 6,-6,0,-6,0,-6,0,0,0,0,0,0,0,0,12,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [12,0,-12,0,-12,-12,0,0,0,0,0,0,0,0,0,24,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [12,0,-24,0,0,0,-12,0,0,0,0,0,0,0,0,0,24,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [12,0,0,0,-24,0,-12,0,0,0,0,0,0,0,0,0,0,24,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [ 4,0,0,0,0,-8,-12,0,0,0,0,0,0,0,0,0,0,0,24,0,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [ 0,12,0,0,0,0,0,-12,0,-12,-12,0,0,0,0,0,0,0,0,24,0,0,0,0,0,0,0,0,0,0,0,0,0],
 [ 0,12,0,0,0,0,0,-12,0,0,0,-12,-12,0,0,0,0,0,0,0,24,0,0,0,0,0,0,0,0,0,0,0,0],
 [ 0,12,0,0,0,0,0,-12,-12,0,0,0,0,-12,0,0,0,0,0,0,0,24,0,0,0,0,0,0,0,0,0,0,0],
 [ 0,12,0,0,0,0,0,0,-12,-12,0,0,-12,0,0,0,0,0,0,0,0,0,24,0,0,0,0,0,0,0,0,0,0],
 [ 0,12,0,0,0,0,0,0,-12,0,-12,-12,0,0,0,0,0,0,0,0,0,0,0,24,0,0,0,0,0,0,0,0,0],
 [-8,12,0,12,0,4,0,0,0,-4,0,-12,0,0,-12,0,0,0,0,0,0,0,0,0,8,0,0,0,0,0,0,0,0],
 [-24,12,24,12,24,12,0,0,0,0,-12,0,-12,-24,-12,-24,
 0,0,0,0,0,0,0,0,0,24,0,0,0,0,0,0,0],
```

```
 [ 4,0,0,0,0,0,-12,0,0,-4,0,0,0,0,0,0,0,0,0,0,0,0,
 0,0,0,12,0,0,0,0,0,0],
 [-24,0,24,0,24,24,24,0,0,0,0,0,0,0,0,-48,-24,-24,-24,
 0,0,0,0,0,0,0,0,48,0,0,0,0,0],
 [ 0,-48,0,0,0,0,0,24,24,24,24,24,24,0,24,0,0,0,0,
 -24,-24,-24,-24,-24,-24,-24,0,0,48,0,0,0,0],
 [-12,0,24,0,0,0,12,0,0,12,0,0,0,0,0,0,-24,0,0,-24,
 0,0,0,0,0,0,-12,0,0,24,0,0,0],
 [-4,0,0,0,0,8,12,0,0,4,0,0,0,0,0,0,0,0,-24,0,0,0,
 0,0,-8,0,-12,0,0,0,24,0,0],
 [-12,0,0,0,24,0,12,0,0,12,0,0,0,0,0,0,0,-24,0,0,0,
 0,-24,0,0,0,-12,0,0,0,0,24,0],
 [24,0,-24,0,-24,-24,-24,0,0,-24,0,0,0,0,0,48,24,24,24,24,
 0,0,24,0,24,0,24,-48,-48,-24,-24,-24,48]]));

 a1 := H + A + W + X + Y + Z;
 a2 := H^2 + A^2 + W^2 + X^2 + Y^2 + Z^2;
 a3 := H^3 + A^3 + W^3 + X^3 + Y^3 + Z^3;
 a4 := H^4 + A^4 + W^4 + X^4 + Y^4 + Z^4;
 a6 := H^6 + A^6 + W^6 + X^6 + Y^6 + Z^6;
 a8 := H^8 + A^8 + W^8 + X^8 + Y^8 + Z^8;

 b1 := H + A + W + X + Y + Z + p + P + q + Q;
 b2 := H^2 + A^2 + W^2 + X^2 + Y^2 + Z^2 + p^2 + P^2 + q^2 + Q^2;
 b3 := H^3 + A^3 + W^3 + X^3 + Y^3 + Z^3 + p^3 + P^3 + q^3 + Q^3;
 b4 := H^4 + A^4 + W^4 + X^4 + Y^4 + Z^4 + p^4 + P^4 + q^4 + Q^4;
 b6 := H^6 + A^6 + W^6 + X^6 + Y^6 + Z^6 + p^6 + P^6 + q^6 + Q^6;
 b8 := H^8 + A^8 + W^8 + X^8 + Y^8 + Z^8 + p^8 + P^8 + q^8 + Q^8;

 c2 := H^2 + A^2 + W^2 + X^2 + Y^2 + Z^2 + 2*p*P + 2*q*Q;
 c4 := H^4 + A^4 + W^4 + X^4 + Y^4 + Z^4 + 2*p^2*P^2 + 2*q^2*Q^2;
 c6 := H^6 + A^6 + W^6 + X^6 + Y^6 + Z^6 + 2*p^3*P^3 + 2*q^3*Q^3;
 c8 := H^8 + A^8 + W^8 + X^8 + Y^8 + Z^8 + 2*p^4*P^4 + 2*q^4*Q^4;

#"H8";
cubaneFPV(8,0,0,0,0,0,0,0,0,0,0): v1 := evalm(FPV);
#"H7";
cubaneFPV(7,1,0,0,0,0,0,0,0,0,0): v2 := evalm(FPV);
cubaneFPV(7,0,0,0,0,0,1,0,0,0,0): v3 := evalm(FPV);
#"H6";
cubaneFPV(6,2,0,0,0,0,0,0,0,0,0): v4 := evalm(FPV);
cubaneFPV(6,0,0,0,0,0,2,0,0,0,0): v5 := evalm(FPV);
cubaneFPV(6,1,1,0,0,0,0,0,0,0,0): v6 := evalm(FPV);
cubaneFPV(6,1,0,0,0,0,1,0,0,0,0): v7 := evalm(FPV);
cubaneFPV(6,0,0,0,0,0,1,1,0,0,0): v8 := evalm(FPV);
cubaneFPV(6,0,0,0,0,0,1,0,1,0,0): v9 := evalm(FPV);

FPM := matrix([v1,v2,v3,v4,v5,v6,v7,v8,v9]);
ICM := evalm(FPM &* InvMOh);

#"H5";
cubaneFPV(5,3,0,0,0,0,0,0,0,0,0): v10 := evalm(FPV);
cubaneFPV(5,0,0,0,0,0,3,0,0,0,0): v11 := evalm(FPV);
cubaneFPV(5,2,1,0,0,0,0,0,0,0,0): v12 := evalm(FPV);
cubaneFPV(5,2,0,0,0,0,1,0,0,0,0): v13 := evalm(FPV);
cubaneFPV(5,1,0,0,0,0,2,0,0,0,0): v14 := evalm(FPV);
cubaneFPV(5,0,0,0,0,0,2,1,0,0,0): v15 := evalm(FPV);
cubaneFPV(5,1,1,1,0,0,0,0,0,0,0): v16 := evalm(FPV);
cubaneFPV(5,1,1,0,0,0,1,0,0,0,0): v17 := evalm(FPV);
```

```
cubaneFPV(5,1,0,0,0,0,1,1,0,0): v18 := evalm(FPV);
cubaneFPV(5,1,0,0,0,0,1,0,1,0): v19 := evalm(FPV);
cubaneFPV(5,0,0,0,0,0,1,1,1,0): v20 := evalm(FPV);

FPM2 := matrix([v10,v11,v12,v13,v14,v15,v16,v17,v18,v19,v20]);
ICM2 := evalm(FPM2 &* InvMOh);
```

Conclusion

Cubane derivatives with chiral and achiral proligands are counted as three-dimensional (3D) structural isomers by the fixed-point matrix (FPM) method of the unit-subduced-cycle-index (USCI) approach.[25] For the purpose of obtaining isomer numbers itemized with respect to their point-group symmetries, the full list of unit subduced cycle indices with chirality fittingness (USCI-CFs) is constructed in a tabular form. By starting from such USCI-CFs, fixed-point vectors (FPVs) or fixed-point matrices (FPMs) are calculated to evaluate the action of the point group O_h on a cubane skeleton. The FPVs or FPMs are multiplied by an inverse matrix of the mark table of O_h so as to generate isomer-counting matrices (ICMs), which collect the numbers of 3D structural isomers to be counted. A Maple program source for counting cubane derivatives as 3D structural isomers is given as an example of practical calculation.

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