

Combinatorial Enumeration of Cubane Derivatives as Three-Dimensional Entities. I. Gross Enumeration by the Proligand Method

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Abstract

Cubane derivatives with chiral and achiral proligands are counted as 3D structural isomers and as steric isomers in the light of the proligand method developed by us (S. Fujita, *Theor. Chem. Acc.*, **113**, 73–79, (2005); **113**, 80–86, (2005); and **115**, 37–53, (2006)). The results are further applied to count achiral derivatives as well as enantiomeric pairs of chiral derivatives. By taking account of the sphericities of cycles, the proligand method is capable of counting cubane derivatives with chiral and achiral proligands, where the chirality of each proligand is judged in isolation. Pólya's theorem is concluded to lack such sphericities of cycles, so that it is restricted to counting cubane derivatives with achiral proligands only. A Maple program source for counting cubane derivatives as 3D structural isomers etc. is given as an example of practical calculation.

1 Introduction

Cubane (**1**) is a trivial name of pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane (the IUPAC name), which corresponds to the numbering shown in the formula **1a** of Figure 1. Cubane itself, in which all the substituents are hydrogen atoms, was synthesized by Eaton and Cole [1]. Thereafter, Eaton

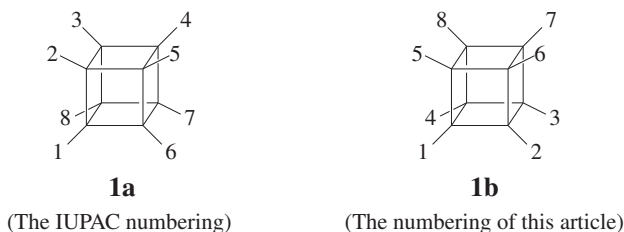


Figure 1: Numbering of the eight positions of cubane (1)

et al. have actively continued studies on cubane derivatives so that they reported systematic substitution on the cubane skeleton [2, 3] and synthesis of octanitrocubane and related compounds [4] as powerful explosives. Because the cubane skeleton belongs to the O_h point group, there exist many substitution derivatives in addition to such derivatives as have been synthesized. It is desirable to enumerate them in order to obtain a perspective of these derivatives.

A large repertoire of methods for isomer enumeration, which has been described in review articles [5–7] or books [8–12], would be applicable to enumerate cubane derivatives. It is to be emphasized, however, the calculation of the derivative number for a given set of substituents requires new techniques as discussed in [13], because the cubane skeleton has high symmetry (O_h). In particular, more sophisticated treatments become necessary, when chiral ligands in isolation (in addition to achiral ligands) are taken into consideration.

Recently, we have developed the proligand method [14–16] as a new technique for combinatorial enumeration, where the concept *sphericities of cycles* has been defined as a key for treating chiral proligands after the term *proligand* was defined as an abstract ligand with and without chirality sense in isolation. The proligand method was compared with Pólya's method, where the latter was concluded to be deficient in the concept *sphericities of cycles* [17]. The proligand method has been applied to the combinatorial enumeration of alkanes and substituted alkanes [18–21]. Related enumerations itemized from various viewpoints have been also reported in [22–25] (concerning uninuclear vs. binuclear etc.) and in [21–29] (concerning internal branching and so on).

The purpose of the present series is to compare various methods of combinatorial enumeration, where we use the cubane skeleton of high symmetry (O_h) as a common starting structure and we emphasize three-dimensional structures of enumerated isomers as well as those of ligands to be substituted. In this paper, the proligand method is applied to isomer enumerations of cubane derivatives, where both achiral and chiral ligands (more abstractly, proligands) are taken into consideration. Thereby, the versatility of the proligand method is emphasized even in the cubane skeleton of high symmetry (O_h).

2 Cubane Derivatives as 3D-structural Isomers

2.1 Cycle Index with Chirality Fittingness of O_h

According to Def. 3 of [30], the term *3D-structural isomers* is used in the present article to refer to a set of (self-)enantiomeric pairs which are characterized by the same molecular formula,

where each (self-)enantiomeric pair (an achiral entity or a pair of enantiomers) coincides with itself under proper rotations as well as improper rotations (reflections and inversions). Note that a self-enantiomeric pair corresponds to an achiral entity in the present terminology, while an enantiomeric pair corresponds to a pair of enantiomers (chiral entities of opposite chirality senses) in the same way as the conventional terminology of stereochemistry. Thus the number of 3D-structural isomers per molecular formula (or equivalent) is referred to the size of such a set of 3D-structural isomers, where an chiral molecule and its enantiomer are paired to be counted once.

Let us consider the numbering of a cubane skeleton shown in **1b** (Figure 1 right), which belongs to the \mathbf{O}_h -point group of order 48:

$$\begin{aligned} \mathbf{O}_h = & \left\{ I, C_{2(1)}, C_{2(2)}, C_{2(3)}; C_{3(1)}, C_{3(3)}, C_{3(2)}, C_{3(4)}, C_{3(1)}^2, C_{3(4)}^2, C_{3(3)}^2, C_{3(2)}^2, \right. \\ & C'_{2(6)}, C'_{2(1)}, C'_{2(4)}, C'_{2(2)}, C'_{2(5)}, C'_{2(3)}, C_{4(3)}^3, C_{4(3)}, C_{4(1)}^3, C_{4(1)}, C_{4(2)}, C_{4(2)}^3; \\ & i, \sigma_{h(3)}, \sigma_{h(2)}, \sigma_{h(1)}, S_{6(1)}^5, S_{6(3)}^5, S_{6(2)}^5, S_{6(4)}^5, S_{6(1)}, S_{6(4)}, S_{6(3)}, S_{6(2)}, \\ & \left. \sigma_{d(1)}, \sigma_{d(6)}, \sigma_{d(2)}, \sigma_{d(4)}, \sigma_{d(3)}, \sigma_{d(5)}, S_{4(3)}, S_{4(3)}^3, S_{4(1)}, S_{4(1)}^3, S_{4(2)}^3, S_{4(2)} \right\}, \quad (1) \end{aligned}$$

where the proper rotations are categorized as follows: I (identity element); $C_{2(j)}$ ($j = 1, 2$, or 3) is a two-fold rotation around a four-fold axis through the centers of the top and bottom faces, through the centers of the right and left faces, or through the centers of the front and back faces; a pair of $C_{3(i)}$ and $C_{3(i)}^2$ ($j = 1, 2, 3$, or 4) represents three-fold rotations around a three-fold axis through vertices 1 and 6, through vertices 7 and 4, through vertices 2 and 8, or through vertices 5 and 3; a pair of $C_{4(j)}$ and $C_{4(j)}^3$ ($j = 1, 2$, or 3) is four-fold rotations around the four-fold axis being the same as specified for the two-fold rotations, $C_{2(j)}$ ($j = 1, 2, 3$); and $C'_{2(j)}$ ($j = 1, 2, \dots$, or 6) is a two-fold rotation around a two-fold axis bisecting two diagonally faced edges of a pair; while the improper rotations are categorized as follows: i (inversion); $\sigma_{h(j)}$ ($j = 1, 2$, or 3) is a reflection due to the mirror plane containing $C_{2(k)}$ - and $C_{2(l)}$ -axes ($j \neq k$ and $j \neq l$); a pair of $S_{6(i)}$ and $S_{6(i)}^5$ ($j = 1, 2, 3$, or 4) represents six-fold rotoreflections along with the three-fold axis concerning a pair of $C_{3(i)}$ and $C_{3(i)}^2$ ($j = 1, 2, 3$, or 4); $\sigma_{d(j)}$ ($j = 1, 2, \dots$, or 6) is a reflection due to the mirror plane containing a pair of two diagonally faced edges; and a pair of $S_{4(j)}$ and $S_{4(j)}^3$ ($j = 1, 2$, or 3) is a four-fold rotoreflections around the four-fold rotoreflection axis being the same as specified for the two-fold rotations, $C_{2(j)}$ ($j = 1, 2, 3$).

Each symmetry operation shown in Eq. 1 is operated on the substitution positions (numbered as 1 to 8) so as to result in the generation of a permutation, which is shown in the form of a product of cycles in Table 1. The resulting set of permutations can be regarded as a coset representation \mathbf{O}_h/C_{3v} , as formulated in [31, 32].

According Lemmas 1 and 2 of [14], each cycle is recognized to be hemispheric, enantiospheric, or homospheric so that such a k -cycle is assigned to a sphericity index (SI) as follows: a hemispheric k -cycle in a rotation operation is assigned to an SI b_k (k : even or odd), an enantiospheric k -cycle in a rotoreflection operation is assigned to an SI c_k (k : even), or a homospheric k -cycle in a rotoreflection operation is assigned to an SI a_k (k : odd). Thereby, the product of SIs is ascribed to the product of cycles, as shown in Table 1.

Equation 2 reported in [14] is calculated to specify the present case of cubane derivatives as 3D-structural isomers, where the products of SIs listed in Table 1 are added and divided by the order of the point group \mathbf{O}_h ($|\mathbf{O}_h| = 48$) to give the following cycle index with chirality

Table 1: Products of Sphericity Indices for the Elements of \mathbf{O}_h

proper rotations			improper rotations		
element	permutation	product of		permutation	product of
element	(cycles)	SIs		(cycles)	SIs
I	(1)(2)(3)(4)(5)(6)(7)(8)	b_1^8	i	$\overline{(1\ 7)(2\ 8)(3\ 5)(4\ 6)}$	c_2^4
$C_{2(1)}$	(1 6)(2 5)(3 8)(4 7)	b_2^4	$\sigma_{h(3)}$	$\overline{(1\ 4)(2\ 3)(5\ 8)(6\ 7)}$	c_2^4
$C_{2(2)}$	(1 8)(2 7)(3 6)(4 5)	b_2^4	$\sigma_{h(2)}$	$\overline{(1\ 2)(3\ 4)(5\ 6)(7\ 8)}$	c_2^4
$C_{2(3)}$	(1 3)(2 4)(5 7)(6 8)	b_2^4	$\sigma_{h(1)}$	$\overline{(1\ 5)(2\ 6)(3\ 7)(4\ 8)}$	c_2^4
$C_{3(1)}$	(4)(6)(1 8 3)(2 5 7)	$b_1^2 b_3^2$	$S_{6(1)}^5$	$\overline{(4\ 6)(1\ 2\ 3\ 7\ 8\ 5)}$	$c_2 c_6$
$C_{3(3)}$	(2)(8)(1 3 6)(4 7 5)	$b_1^2 b_3^2$	$S_{6(3)}^5$	$\overline{(2\ 8)(1\ 5\ 6\ 7\ 3\ 4)}$	$c_2 c_6$
$C_{3(2)}$	(1)(7)(2 4 5)(3 8 6)	$b_1^2 b_3^2$	$S_{6(2)}^5$	$\overline{(1\ 7)(2\ 6\ 5\ 8\ 4\ 3)}$	$c_2 c_6$
$C_{3(4)}$	(3)(5)(1 6 8)(2 7 4)	$b_1^2 b_3^2$	$S_{6(4)}^5$	$\overline{(3\ 5)(1\ 4\ 8\ 7\ 6\ 2)}$	$c_2 c_6$
$C_{3(1)}^2$	(4)(6)(1 3 8)(2 7 5)	$b_1^2 b_3^2$	$S_{6(1)}$	$\overline{(4\ 6)(1\ 5\ 8\ 7\ 3\ 2)}$	$c_2 c_6$
$C_{3(4)}^2$	(3)(5)(1 8 6)(2 4 7)	$b_1^2 b_3^2$	$S_{6(4)}$	$\overline{(3\ 5)(1\ 2\ 6\ 7\ 8\ 4)}$	$c_2 c_6$
$C_{3(3)}^2$	(2)(8)(1 6 3)(4 5 7)	$b_1^2 b_3^2$	$S_{6(3)}$	$\overline{(2\ 8)(1\ 4\ 3\ 7\ 6\ 5)}$	$c_2 c_6$
$C_{3(2)}^2$	(1)(7)(2 5 4)(3 6 8)	$b_1^2 b_3^2$	$S_{6(2)}$	$\overline{(1\ 7)(2\ 3\ 4\ 8\ 5\ 6)}$	$c_2 c_6$
$C'_{2(6)}$	(1 5)(2 8)(3 7)(4 6)	b_2^4	$\sigma_{d(1)}$	$\overline{(3)(4)(6)(8)(1\ 3)(5\ 7)}$	$a_1^2 c_2^2$
$C'_{2(1)}$	(1 7)(2 6)(3 5)(4 8)	b_2^4	$\sigma_{d(6)}$	$\overline{(1)(3)(5)(7)(2\ 4)(6\ 8)}$	$a_1^2 c_2^2$
$C'_{2(4)}$	(1 7)(2 8)(3 4)(5 6)	b_2^4	$\sigma_{d(2)}$	$\overline{(1)(4)(6)(7)(2\ 5)(3\ 8)}$	$a_1^2 c_2^2$
$C'_{2(2)}$	(1 7)(2 3)(4 6)(5 8)	b_2^4	$\sigma_{d(4)}$	$\overline{(2)(3)(5)(8)(1\ 6)(4\ 7)}$	$a_1^2 c_2^2$
$C'_{2(5)}$	(1 2)(3 5)(4 6)(7 8)	b_2^4	$\sigma_{d(3)}$	$\overline{(3)(4)(5)(6)(1\ 8)(2\ 7)}$	$a_1^2 c_2^2$
$C'_{2(3)}$	(1 4)(2 8)(3 5)(6 7)	b_2^4	$\sigma_{d(5)}$	$\overline{(1)(2)(7)(8)(3\ 6)(4\ 5)}$	$a_1^2 c_2^2$
$C_{4(3)}^3$	(1 2 3 4)(5 6 7 8)	b_4^2	$S_{4(3)}$	$\overline{(1\ 8\ 3\ 6)(2\ 5\ 4\ 7)}$	c_4^2
$C_{4(3)}$	(1 4 3 2)(5 8 7 6)	b_4^2	$S_{4(3)}^3$	$\overline{(1\ 6\ 3\ 8)(2\ 7\ 4\ 5)}$	c_4^2
$C_{4(1)}^3$	(1 2 6 5)(3 7 8 4)	b_4^2	$S_{4(1)}$	$\overline{(1\ 8\ 6\ 3)(2\ 4\ 5\ 7)}$	c_4^2
$C_{4(1)}$	(1 5 6 2)(3 4 8 7)	b_4^2	$S_{4(1)}^3$	$\overline{(1\ 3\ 6\ 8)(2\ 7\ 5\ 4)}$	c_4^2
$C_{4(2)}$	(1 5 8 4)(2 6 7 3)	b_4^2	$S_{4(2)}^3$	$\overline{(1\ 3\ 8\ 6)(2\ 4\ 7\ 5)}$	c_4^2
$C_{4(2)}^3$	(1 4 8 5)(2 3 7 6)	b_4^2	$S_{4(2)}$	$\overline{(1\ 6\ 8\ 3)(2\ 5\ 7\ 4)}$	c_4^2

fittingness CI-CF($\mathbf{O}_h, \$_d$) where $\$_d$ is assigned as $a_d, b_d,$ or c_d :

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

For the term *chirality fittingness* which specifies modes of packing orbits (or coset representations) with proligands, see [31, 32]. The same term is used here to specify packing-modes of cycles according to Section 2.3 of [14].

When s_d ($= a_d = b_d = c_d$) is introduced into Eq. 2 as an extreme case, Eq. 2 is degenerated to give the following equation without chirality fittingness:

$$\text{CI}(\mathbf{O}_h, s_d) = \frac{1}{48}s_1^8 + \frac{3}{16}s_2^4 + \frac{1}{6}s_1^2s_3^2 + \frac{1}{8}s_4^4 + \frac{1}{12}s_2^4 + \frac{1}{6}s_2s_6 + \frac{1}{8}s_1^4s_2^2 + \frac{1}{8}s_4^2 \quad (3)$$

which is equivalent to Polyá's cycle index [12, 33].

2.2 Enumeration of Cubane Derivatives as 3D-structural Isomers

2.2.1 With Achiral Proligands Only

As a degenerate case, let us consider an inventory of proligands:

$$\mathbf{L} = \{H, A, B, C, W, X, Y, Z\} \quad (4)$$

where H, A, B, C, W, X, Y, and Z are achiral proligands in isolation. An appropriate set of achiral proligands is selected from the inventory \mathbf{L} so as to be placed on the vertices of $\mathbf{1b}$. Equations 5–7 of in Theorem 1 of [14] are applied to this case to give the following inventory functions:

$$a_d = H^d + A^d + B^d + C^d + W^d + X^d + Y^d + Z^d \quad (5)$$

$$b_d = H^d + A^d + B^d + C^d + W^d + X^d + Y^d + Z^d \quad (6)$$

$$c_d = H^d + A^d + B^d + C^d + W^d + X^d + Y^d + Z^d \quad (7)$$

In order to enumerate cubane derivatives as 3D-structural isomers in this case, these ligand-inventory functions are introduced into the right-hand side of Eq. 2. The expansion of the resulting function gives the following generating function:

$$\begin{aligned} f &= H^8 + H^7A + H^7B + H^7C + H^7W + H^7X + H^7Y + H^7Z \\ &\quad + 3H^6A^2 + 3H^6AB + 3H^6AC + 3H^6AW + 3H^6AX + 3H^6AY + 3H^6AZ + 3H^6B^2 \\ &\quad + 3H^6BC + 3H^6BW + 3H^6BX + 3H^6BY + 3H^6BZ + 3H^6C^2 + 3H^6CW + 3H^6CX \\ &\quad + 3H^6CY + 3H^6CZ + 3H^6W^2 + 3H^6WX + 3H^6WY + 3H^6WZ + 3H^6X^2 + 3H^6XY \\ &\quad + 3H^6XZ + 3H^6Y^2 + 3H^6YZ + 3H^6Z^2 \\ &\quad + 3H^5A^3 + 6H^5A^2B + 6H^5A^2C + 6H^5A^2W + 6H^5A^2X + 6H^5A^2Y + 6H^5A^2Z \\ &\quad + 6H^5AB^2 + 10H^5ABC + 10H^5ABW + 10H^5ABX + 10H^5ABY + 10H^5ABZ \\ &\quad + 6H^5AC^2 + 10H^5ACW + 10H^5ACX + 10H^5ACY + \dots \end{aligned} \quad (8)$$

The coefficient of each term $H^hA^aB^bC^cW^wX^xY^yZ^z$ in the generating function f (Eq. 8) represents the number of cubane derivatives as 3D-structural isomers having h of H, a of A, b

Table 2: Numbers of Cubane Derivatives with Achiral Proligands

pattern	3D	S	A	E	pattern	3D	S	A	E
[8,0,0,0,0,0,0]	1	1	1	0					
[7,1,0,0,0,0,0]	1	1	1	0					
[6,2,0,0,0,0,0]	3	3	3	0	[6,1,1,0,0,0,0]	3	3	3	0
[5,3,0,0,0,0,0]	3	3	3	0	[5,2,1,0,0,0,0]	6	7	5	1
[5,1,1,1,0,0,0]	10	14	6	4					
[4,4,0,0,0,0,0]	6	7	5	1	[4,3,1,0,0,0,0]	10	13	7	3
[4,2,2,0,0,0,0]	16	22	10	6	[4,2,1,1,0,0,0]	22	35	9	13
[4,1,1,1,1,0,0]	38	70	6	32					
[3,3,2,0,0,0,0]	17	24	10	7	[3,3,1,1,0,0,0]	30	48	12	18
[3,2,2,1,0,0,0]	42	70	14	28	[3,2,1,1,1,0,0]	76	140	12	64
[3,1,1,1,1,1,0]	140	280	0	140					
[2,2,2,2,0,0,0]	68	114	22	46	[2,2,2,1,1,0,0]	114	210	18	96
[2,2,1,1,1,1,0]	216	420	12	204	[2,1,1,1,1,1,1]	420	840	0	420
[1,1,1,1,1,1,1]	840	1680	0	840					

These data appear as the coefficients of monomials in respective generating functions: column 3D (Eq. 8), column S (Eq. 15), column A (Eq. 18), and column E (Eq. 21)

of B, c of C, w of W, x of X, y of Y, and z of Z, which can be represented by a substitution pattern $[h, a, b, c, w, x, y, z]$. Note that the term $H^h A^a B^b C^c W^w X^x Y^y Z^z$ is used as being equivalent to molecular formulas. Because the generating function f (Eq. 8) contains these proligands equally, any proligands can be exchanged to give the same coefficient, where, for example, the terms $H^5 A^2 B$, $H^5 B^2 C$, $A^5 B^2 C$, and so on have the same coefficient (6) in f (Eq. 8). Hence, we can presume $h \geq a \geq b \geq c \geq w \geq x \geq y \geq z$ without losing generality. For example, the substitution pattern $[5, 2, 1, 0, 0, 0, 0, 0]$ corresponds to $H^5 A^2 B$, $H^5 B^2 C$, $A^5 B^2 C$, and so on. The coefficients appearing in f (Eq. 8) are collected in a tabular form (column 3D of Table 2).

The data for giving Table 2 were calculated by using the Maple system [34], where a maple file named "cubaneA8-Total.mpl" (extension .mpl), whose source list is shown in Appendix, was used for calculation. After the file was stored in a working directory named "c:/fujita0/", the following commands were input from the display of the Maple system:

```
>restart;
>read "c:/fujita0/cubaneA8-Total.mpl";
```

It is worthwhile here to mention that the data of Table 2 can be alternatively obtained by Pólya's theorem, because we take account of achiral proligand only. From the present point of view, the calculation based on Pólya's theorem is regarded as a degenerate case of the calculation based on the proligand method, where chiral proligands in isolation are not taken into consideration. Thus, Equations 5–7 of in Theorem 1 of [14] give degenerate inventory functions, as found in Eqs. 5–7, which are equal to each other. After we place $s_d = a_d = b_d = c_d$, the resulting s_d is introduced into Eq. 3, which is an expression equivalent to the cycle index due to Pólya's theorem.

2.2.2 With Achiral and Chiral Proligands

As an illustrative case of more general features, let us consider an inventory of proligands:

$$L' = \{H, A, W, X, Y, Z; p, \bar{p}; q, \bar{q}\} \quad (9)$$

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

According to Eqs. 5–7 of in Theorem 1 of [14], we use the following inventory functions:

$$a_d = H^d + A^d + W^d + X^d + Y^d + Z^d \quad (10)$$

$$b_d = H^d + A^d + W^d + X^d + Y^d + Z^d + p^d + \bar{p}^d + q^d + \bar{q}^d \quad (11)$$

$$c_d = H^d + A^d + W^d + X^d + Y^d + Z^d + 2p^{d/2}\bar{p}^{d/2} + 2q^{d/2}\bar{q}^{d/2} \quad (12)$$

It should be noted that the power $d/2$ appearing in Eq. 12 is an integer because the subscript d of c_d is always even in the light of the enantiosphericity of the corresponding cycle.

In order to enumerate cubane derivatives as 3D-structural isomers in this case, these ligand-inventory functions (Eqs. 10–12) are introduced into the right-hand side of Eq. 2. The expansion of the resulting function gives the following generating function:

$$\begin{aligned} g = & H^8 + H^7A + H^7W + H^7X + H^7Y + H^7Z + \frac{1}{2}(H^7p + H^7\bar{p}) \\ & + \frac{1}{2}(H^7q + H^7\bar{q}) + 3H^6A^2 + 3H^6AW + 3H^6AX + 3H^6AY + 3H^6AZ \\ & + \frac{3}{2}(H^6Ap + H^6A\bar{p}) + \frac{3}{2}(H^6Aq + H^6A\bar{q}) + 3H^6W^2 + 3H^6WX \\ & + 3H^6WY + 3H^6WZ + \frac{3}{2}(H^6Wp + H^6W\bar{p}) + \frac{3}{2}(H^6Wq + H^6W\bar{q}) \\ & + 3H^6X^2 + 3H^6XY + 3H^6XZ + \frac{3}{2}(H^6Xp + H^6X\bar{p}) + \frac{3}{2}(H^6Xq + H^6X\bar{q}) \\ & + 3H^6Y^2 + 3H^6YZ + \frac{3}{2}(H^6Yp + H^6Y\bar{p}) + \frac{3}{2}(H^6Yq + H^6Y\bar{q}) \\ & + 3H^6Z^2 + \frac{3}{2}(H^6Zp + H^6Z\bar{p}) + \frac{3}{2}(H^6Zq + H^6Z\bar{q}) \\ & + \frac{3}{2}(H^6p^2 + H^6\bar{p}^2) + 3H^6p\bar{p} + \frac{3}{2}(H^6pq + H^6p\bar{q}) \\ & + \frac{3}{2}(H^6p\bar{q} + H^6\bar{p}q) + \frac{3}{2}(H^6q^2 + H^6\bar{q}^2) + 3H^6q\bar{q} + \dots \end{aligned} \quad (13)$$

The coefficient of each term $H^hA^aW^wX^xY^yZ^z p^h\bar{p}^q q^q\bar{q}^q$ in the generating function g (Eq. 13) represents the number of cubane derivatives as 3D-structural isomers having h of H, a of A, w of W, x of X, y of Y, z of Z, p of p, \bar{p} of \bar{p} , q of q, and \bar{q} of \bar{q} . Such a mode of substitution can be represented by a substitution pattern $[h, a, w, x, y, z; p, \bar{p}, q, \bar{q}]$, where we can presume $h \geq a \geq w \geq x \geq y \geq z$; $p \geq q$, $p \geq \bar{p}$, and $q \geq \bar{q}$ without losing generality. For example, the substitution pattern $[5, 0, 0, 0, 0, 0; 2, 1, 0, 0]$ corresponds to $H^5p^2\bar{p}$, $H^5p\bar{p}^2$, $H^5q^2\bar{q}$, $H^5q\bar{q}^2$, and so on. The coefficients appearing in g (Eq. 13) are collected in a tabular form (column 3D of Tables 3 and 4).

It is to be noted that a coefficient should be duplicated if there is a pair of terms which corresponds to a pair of enantiomers (each substitution pattern with an asterisk). This is because a pair of enantiomers is counted once in 3D-structural-isomer enumeration. For example, the coefficient (1/2) of the term H^7p (or $H^7\bar{p}$) should be duplicated to give 1 (i.e., $2 \times (1/2)$), because there is a pair of terms $\frac{1}{2}(H^7p + H^7\bar{p})$. This treatment is rationalized by considering that H^7p and $H^7\bar{p}$ have the same molecular formula when p and \bar{p} are reduced into their constitutions. Each substitution pattern marked by an asterisk (e.g., $[7,0,0,0,0,0;1,0,0,0]^*$ for H^7p) has the counterpart of opposite chirality sense (e.g., $[7,0,0,0,0,0;0,1,0,0]^*$ for $H^7\bar{p}$) so that the corresponding coefficient should be duplicated to generate the number of cubane derivatives.

The data for giving Tables 3 and 4 were calculated by using the Maple system [34], where a maple file (extension .mpl) was prepared in a similar way to the maple file shown in Appendix.

3 Cubane Derivatives as Steric Isomers

3.1 Cycle Index with Chirality Fittingness of the O Group

According to Def. 3 of [30], the term *steric isomers* is used to refer to a set of inequivalent steric entities which are characterized by the same molecular formula, where each steric entity coincides with itself under proper rotations, while improper rotations (reflections and inversions) are not taken into consideration. This means that a chiral molecule and its enantiomer are counted separately. Then, the number of steric isomers per molecular formula (or equivalent) is referred to the size of such a set of steric isomers.

Equation 2 reported in [14] is calculated to specify the present case of cubane derivatives as steric isomers, where the product of SIs for the point group \mathbf{O} (selected from Table 1) are added and divided by the order of the point group \mathbf{O} ($|\mathbf{O}| = 24$), so as to give the following cycle index with chirality fittingness CI-CF(\mathbf{O}, b_d):

$$\begin{aligned} \text{CI-CF}(\mathbf{O}, b_d) &= \frac{1}{24} \{b_1^8 + 3b_2^4 + 8b_1^2b_3^2 + 6b_2^4 + 6b_4^2\} \\ &= \frac{1}{24}b_1^8 + \frac{3}{8}b_2^4 + \frac{1}{3}b_1^2b_3^2 + \frac{1}{4}b_4^2 \end{aligned} \quad (14)$$

Note that Eq. 14 contains the SI b_d only, so that each achiral derivative, one chiral derivative of each enantiomeric pair, and the other chiral derivative of the enantiomeric pair are counted separately.

3.2 Enumeration of Cubane Derivatives as Steric Isomers

3.2.1 With Achiral Proligands Only

Let us consider an appropriate set of achiral proligands selected from \mathbf{L} (Eq. 4). Such an appropriate set is placed on the eight substitution positions of the skeleton ($\mathbf{1b}$). To enumerate cubane derivatives as steric isomers in this case, the ligand-inventory function b_d (Eq. 6) is introduced into the right-hand side of Eq. 14. The resulting function is expanded to give the following generating function:

$$\begin{aligned} f' &= H^8 + H^7A + H^7B + H^7C + H^7W + H^7X + H^7Y + H^7Z \\ &\quad + 3H^6A^2 + 3H^6AB + 3H^6AC + 3H^6AW + 3H^6AX + 3H^6AY + 3H^6AZ + 3H^6B^2 \end{aligned}$$

Table 3: Numbers of Cubane Derivatives with Proligands Selected from Six Achiral Proligands and Two Enantiomorphic Pairs of Chiral Proligands (Part I)

pattern	3D	S	A	E	pattern	3D	S	A	E
[8,0,0,0,0;0,0,0,0]	1	1	1	0	[7,0,0,0,0;1,0,0,0]*	1/2	1	0	1/2
[7,1,0,0,0;0,0,0,0]	1	1	1	0	[6,0,0,0,0;2,0,0,0]*	3/2	3	0	3/2
[6,2,0,0,0;0,0,0,0]	3	3	3	0	[6,1,0,0,0;1,0,0,0]*	3/2	3	0	3/2
[6,1,1,0,0;0,0,0,0]	3	3	3	0	[6,0,0,0,0;1,0,1,0]*	3/2	3	0	3/2
[6,0,0,0,0;1,1,0,0]	3	3	3	0	[5,0,0,0,0;3,0,0,0]*	3/2	3	0	3/2
[5,3,0,0,0;0,0,0,0]	3	3	3	0	[5,2,0,0,0;1,0,0,0]*	7/2	7	0	7/2
[5,2,1,0,0;0,0,0,0]	6	7	5	1	[5,0,0,0,0;2,1,0,0]*	7/2	7	0	7/2
[5,1,0,0,0;2,0,0,0]*	7/2	7	0	7/2	[5,1,1,1,0,0;0,0,0,0]	10	14	6	4
[5,0,0,0,0;2,0,1,0]*	7/2	7	0	7/2	[5,1,0,0,0;1,1,0,0]	9	14	4	5
[5,1,1,0,0;1,0,0,0]*	7	14	0	7	[5,0,0,0,0;1,1,1,0]*	7	14	0	7
[5,1,0,0,0;1,0,1,0]*	7	14	0	7	[4,0,0,0,0;4,0,0,0]*	7/2	7	0	7/2
[4,4,0,0,0;0,0,0,0]	6	7	5	1	[4,3,0,0,0;1,0,0,0]*	13/2	13	0	13/2
[4,3,1,0,0;0,0,0,0]	10	13	7	3	[4,0,0,0,0;3,1,0,0]*	13/2	13	0	13/2
[4,1,0,0,0;3,0,0,0]*	13/2	13	0	13/2	[4,2,1,1,0,0;0,0,0,0]	22	35	9	13
[4,0,0,0,0;3,0,1,0]*	13/2	13	0	13/2	[4,2,0,0,0;1,1,0,0]	23	35	11	12
[4,2,1,0,0;1,0,0,0]*	35/2	35	0	35/2	[4,1,1,0,0;2,0,0,0]*	35/2	35	0	35/2
[4,2,0,0,0;1,0,1,0]*	35/2	35	0	35/2	[4,1,0,0,0;2,0,1,0]*	35/2	35	0	35/2
[4,1,0,0,0;2,1,0,0]*	35/2	35	0	35/2	[4,1,1,1,0,0;0,0,0,0]	38	70	6	32
[4,0,0,0,0;2,1,1,0]*	35/2	35	0	35/2	[4,1,1,0,0;1,1,0,0]	41	70	12	29
[4,1,1,1,0,0;1,0,0,0]	35	70	0	35	[4,0,0,0,0;1,1,1,1]	40	70	10	30
[4,1,0,0,0;1,1,1,0]	35	70	0	35	[3,3,0,0,0;2,0,0,0]*	12	24	0	12
[3,3,2,0,0;0,0,0,0]	17	24	10	7	[3,0,0,0,0;3,2,0,0]*	12	24	0	12
[3,2,0,0,0;3,0,0,0]*	12	24	0	12	[3,3,1,1,0,0;0,0,0,0]	30	48	12	18
[3,0,0,0,0;3,0,2,0]*	12	24	0	12	[3,3,0,0,0;1,1,0,0]	28	48	8	20
[3,3,1,0,0;1,0,0,0]*	24	48	0	24	[3,1,1,0,0;3,0,0,0]*	24	48	0	24
[3,3,0,0,0;1,0,1,0]	24	48	0	24	[3,1,0,0,0;3,0,1,0]*	24	48	0	24
[3,1,0,0,0;3,1,0,0]*	24	48	0	24	[3,0,0,0,0;3,0,1,1]*	24	48	0	24
[3,0,0,0,0;3,1,1,0]	24	48	0	24	[3,2,2,0,0;1,0,0,0]	35	70	0	35
[3,2,2,1,0,0;0,0,0,0]	42	70	14	28	[3,2,0,0,0;2,0,1,0]*	35	70	0	35
[3,2,0,0,0;2,1,0,0]*	35	70	0	35	[3,0,0,0,0;2,1,2,0]*	35	70	0	35
[3,0,0,0,0;2,2,1,0]*	35	70	0	35	[3,2,1,1,0,0;1,0,0,0]*	70	140	0	70
[3,0,0,0,0;2,2,0,0]	76	140	12	64	[3,2,1,0,0,0;1,0,1,0]*	70	140	0	70
[3,2,1,1,0,0;0,0,0,0]	35	70	0	35	[3,0,0,0,0;2,1,1,1]*	70	140	0	70
[3,2,1,0,0,0;1,1,0,0]	78	140	16	62	[3,1,1,1,0,0;1,0,0,0]	140	280	0	140
[3,2,0,0,0;1,1,1,0]*	70	140	0	70	[3,1,1,1,0,0;1,0,1,0]	140	280	0	140
[3,1,1,1,1,1;0,0,0,0]	140	280	0	140	[3,1,0,0,0;1,1,1,1]	144	280	8	136
[3,1,1,1,0,0;1,1,0,0]	152	280	24	128	[2,2,2,0,0,0;2,0,0,0]	57	114	0	57
[3,1,1,0,0,0;1,1,1,0]*	140	280	0	140	[2,2,0,0,0;2,0,2,0]*	57	114	0	57
[3,1,1,0,0,0;1,1,1,0]	140	280	0	140	[2,2,2,1,1,0;0,0,0,0]	114	210	18	96
[2,2,2,2,0,0;0,0,0,0]	68	114	22	46	[2,2,2,0,0,0;1,1,0,0]	118	210	26	92
[2,2,0,0,0;2,2,0,0]	64	114	14	50	[2,2,1,0,0,0;2,0,0,0]*	105	210	0	105
[2,0,0,0,0;2,2,2,0]*	57	114	0	57	[2,2,0,0,0;2,1,1,0]*	105	210	0	105
[2,2,2,1,0,0;1,0,0,0]*	105	210	0	105	[2,2,0,0,0;2,1,1,0]	105	210	0	105
[2,2,1,0,0,0;2,0,0,0]*	105	210	0	105	[2,1,1,0,0,0;2,0,2,0]*	105	210	0	105
[2,2,1,0,0,0;2,0,1,0]	105	210	0	105	[2,1,0,0,0;2,1,2,0]*	105	210	0	105
[2,1,1,0,0,0;2,2,0,0]	111	210	12	99	[2,0,0,0,0;2,1,2,1]*	105	210	0	105
[2,1,0,0,0;2,2,1,0]	105	210	0	105	[2,2,1,1,0,0;1,0,0,0]	210	420	0	210
[2,0,0,0,0;2,2,1,1]	113	210	16	97	[2,2,1,1,0,0;1,0,1,0]	210	420	0	210
[2,0,0,0,0;2,2,1,1]	113	210	16	97	[2,2,0,0,0;1,1,1,1]	224	420	28	196
[2,2,1,1,1,1;0,0,0,0]	216	420	12	204	[2,1,1,1,0,0;2,1,0,0]*	210	420	0	210
[2,2,1,1,0,0;1,1,0,0]	222	420	24	198	[2,1,1,0,0;2,1,1,0]	210	420	0	210
[2,2,1,0,0,0;1,1,1,0]*	210	420	0	210	[2,1,0,0,0;2,1,1,0]	210	420	0	210
[2,2,1,1,1,0;2,0,0,0]*	210	420	0	210	[2,1,1,0,0;2,1,1,0]	210	420	0	210
[2,1,1,1,0,0;2,0,1,0]	210	420	0	210	[2,1,0,0,0;2,1,1,1]*	210	420	0	210
[2,1,1,0,0,0;2,0,1,1]	210	420	0	210	[2,1,1,1,0,0;1,1,0,0]	432	840	24	408
[2,1,1,1,1,1;1,0,0,0]	420	840	0	420	[2,1,1,1,0,0;1,1,1,0]*	420	840	0	420
[2,1,1,1,1,0;1,0,1,0]	420	840	0	420					
[2,1,1,1,0,0;1,1,1,1]	432	840	24	408					
[2,1,1,1,1,0;2,0,0,0]*	210	420	0	210					
[2,1,1,1,0,0;2,0,1,0]	210	420	0	210					
[2,1,1,0,0,0;2,0,1,1]	210	420	0	210					
[2,1,1,0,0,0;2,0,1,1]	210	420	0	210					
[2,1,1,0,0,0;2,0,1,1]	210	420	0	210					
[2,1,1,1,1,0;1,0,1,0]	420	840	0	420					
[2,1,1,1,1,0;1,0,1,0]	420	840	0	420					
[2,1,1,0,0,0;1,1,1,1]	432	840	24	408					
[1,1,1,1,1,1;1,1,0,0]	840	1680	0	840	[1,1,1,1,1,1;1,0,1,0]*	840	1680	0	840
[1,1,1,1,1,0;1,1,1,0]	840	1680	0	840	[1,1,1,1,0,0;1,1,1,1]	864	1680	48	816

These data appear as the coefficients of monomials in respective generating functions: column 3D (Eq. 13), column S (Eq. 16), column A (Eq. 19), and column E (Eq. 22). Each substitution pattern marked by an asterisk has the counterpart of opposite chirality sense so that the corresponding coefficient should be duplicated to generate the number of cubane derivatives.

Table 4: Numbers of Cubane Derivatives with Proligands Selected from Six Achiral Proligands and Two Enantiomorphic Pairs of Chiral Proligands (Part II)

pattern	3D	S	A	E	pattern	3D	S	A	E
[0,0,0,0,0;8,0,0,0]*	1/2	1	0	1/2	[0,0,0,0,0;7,0,1,0]*	1/2	1	0	1/2
[0,0,0,0,0;7,1,0,0]*	1/2	1	0	1/2	[1,0,0,0,0;7,0,0,0]*	1/2	1	0	1/2
[1,0,0,0,0;7,0,0,0]*	1/2	1	0	1/2	[0,0,0,0,0;6,0,2,0]*	3/2	3	0	3/2
[0,0,0,0,0;6,2,0,0]*	3/2	3	0	3/2	[0,0,0,0,0;6,1,1,0]*	3/2	3	0	3/2
[2,0,0,0,0;6,0,0,0]*	3/2	3	0	3/2	[1,0,0,0,0;6,0,1,0]*	3/2	3	0	3/2
[1,0,0,0,0;6,1,0,0]*	3/2	3	0	3/2	[0,0,0,0,0;5,0,3,0]*	3/2	3	0	3/2
[1,1,0,0,0;6,0,0,0]*	3/2	3	0	3/2	[0,0,0,0,0;5,2,1,0]*	7/2	7	0	7/2
[0,0,0,0,0;5,3,0,0]*	3/2	3	0	3/2	[1,0,0,0,0;5,2,0,0]*	7/2	7	0	7/2
[3,0,0,0,0;5,0,0,0]*	3/2	3	0	3/2	[2,0,0,0,0;5,1,0,0]*	7/2	7	0	7/2
[0,0,0,0,0;5,1,2,0]*	7/2	7	0	7/2	[2,1,0,0,0;5,0,0,0]*	7/2	7	0	7/2
[1,0,0,0,0;5,0,2,0]*	7/2	7	0	7/2	[1,0,0,0,0;5,1,1,0]*	7	14	0	7
[2,0,0,0,0;5,0,1,0]*	7/2	7	0	7/2	[1,1,0,0,0;5,1,0,0]*	7	14	0	7
[0,0,0,0,0;5,1,1,1]*	7	14	0	7	[1,1,1,0,0;5,0,0,0]*	7	14	0	7
[1,0,0,0,0;5,0,1,1]*	7	14	0	7	[0,0,0,0,0;4,0,4,0]*	7/2	7	0	7/2
[1,1,0,0,0;5,0,1,0]*	7	14	0	7	[0,0,0,0,0;4,1,3,0]*	13/2	13	0	13/2
[0,0,0,0,0;4,3,1,0]*	13/2	13	0	13/2	[1,0,0,0,0;4,0,3,0]*	13/2	13	0	13/2
[0,0,0,0,0;4,3,0,0]*	13/2	13	0	13/2	[2,0,0,0,0;4,2,0,0]*	11	22	0	11
[0,0,0,0,0;4,2,2,0]*	11	22	0	11	[2,2,0,0,0;4,0,0,0]*	11	22	0	11
[2,0,0,0,0;4,2,0,0]*	11	22	0	11	[0,0,0,0,0;4,1,2,1]*	35/2	35	0	35/2
[0,0,0,0,0;4,2,1,1]*	35/2	35	0	35/2	[1,0,0,0,0;4,2,0,1]*	35/2	35	0	35/2
[1,0,0,0,0;4,2,1,0]*	35/2	35	0	35/2	[1,1,0,0,0;4,0,2,0]*	35/2	35	0	35/2
[1,1,0,0,0;4,2,0,0]*	35/2	35	0	35/2	[2,1,0,0,0;4,1,0,0]*	35/2	35	0	35/2
[2,0,0,0,0;4,1,1,0]*	35/2	35	0	35/2	[2,1,1,0,0;4,0,0,0]*	35/2	35	0	35/2
[2,1,0,0,0;4,0,1,0]*	35/2	35	0	35/2	[1,1,0,0,0;4,1,1,0]*	35	70	0	35
[1,0,0,0,0;4,1,1,1]*	35	70	0	35	[1,1,1,0,0;4,1,0,0]*	35	70	0	35
[1,1,0,0,0;4,0,1,1]*	35	70	0	35	[1,1,1,1,0;4,0,0,0]*	35	70	0	35
[1,1,1,0,0;4,0,1,0]*	35	70	0	35	[2,0,0,0,0;3,3,0,0]*	15	24	6	9
[0,0,0,0,0;3,3,2,0]*	12	24	0	12	[1,0,0,0,0;3,3,1,0]*	24	48	0	24
[0,0,0,0,0;3,3,1,1]*	30	48	12	18	[0,0,0,0,0;3,2,2,1]*	35	70	0	35
[1,1,0,0,0;3,3,0,0]*	24	48	0	24	[2,0,0,0,0;3,2,1,0]*	35	70	0	35
[1,0,0,0,0;3,2,2,0]*	35	70	0	35	[2,1,0,0,0;3,0,2,0]*	35	70	0	35
[2,1,0,0,0;3,2,0,0]*	35	70	0	35	[1,0,0,0,0;3,2,1,1]*	70	140	0	70
[2,2,1,0,0;3,0,0,0]*	35	70	0	35	[1,1,1,0,0;3,2,0,0]*	70	140	0	70
[1,1,0,0,0;3,2,1,0]*	70	140	0	70	[2,0,0,0,0;3,1,1,1]*	70	140	0	70
[1,1,1,0,0;3,0,2,0]*	70	140	0	70	[2,1,0,0,0;3,0,1,1]*	70	140	0	70
[2,1,0,0,0;3,1,1,0]*	70	140	0	70	[2,1,1,0,0;3,0,1,0]*	70	140	0	70
[2,1,1,0,0;3,1,0,0]*	70	140	0	70	[1,1,1,0,0;3,1,1,0]*	140	280	0	140
[2,1,1,1,0;3,0,0,0]*	70	140	0	70	[1,1,1,1,0;3,1,0,0]*	140	280	0	140
[1,1,0,0,0;3,1,1,1]*	140	280	0	140	[1,1,1,1,0;3,0,0,0]*	140	280	0	140
[1,1,1,0,0;3,0,1,1]*	140	280	0	140	[1,0,0,0,0;2,2,2,1]*	105	210	0	105
[1,1,1,1,0;3,0,1,0]*	140	280	0	140	[1,1,0,0,0;2,2,1,1]*	210	420	0	210
[0,0,0,0,0;2,2,2,2]*	66	114	18	48	[1,1,1,0,0;2,1,2,0]*	210	420	0	210
[1,1,0,0,0;2,2,2,0]*	105	210	0	105	[1,1,1,1,0;2,0,2,0]*	210	420	0	210
[1,1,1,0,0;2,2,1,0]*	210	420	0	210	[1,1,1,1,0;2,1,1,0]*	420	840	0	420
[1,1,1,1,0;2,2,0,0]*	222	420	24	198	[1,1,1,1,1;2,1,0,0]*	420	840	0	420
[1,1,1,0,0;2,1,1,1]*	420	840	0	420	[1,1,1,1,1;2,0,0,0]*	420	840	0	420
[1,1,1,1,0;2,0,1,1]*	420	840	0	420	[1,1,1,1,1;1,1,1,0]*	840	1680	0	840
[1,1,1,1,1;2,0,1,0]*	420	840	0	420	[1,1,1,1,1;1,0,1,0]*	840	1680	0	840
[1,1,1,1,0;1,1,1,1]*	864	1680	48	816					
[1,1,1,1,1;1,1,0,0]*	840	1680	0	840					

See the table footnote of Table 3.

$$\begin{aligned}
 &+ 3H^6BC + 3H^6BW + 3H^6BX + 3H^6BY + 3H^6BZ + 3H^6C^2 + 3H^6CW + 3H^6CX \\
 &+ 3H^6CY + 3H^6CZ + 3H^6W^2 + 3H^6WX + 3H^6WY + 3H^6WZ + 3H^6X^2 + 3H^6XY \\
 &+ 3H^6XZ + 3H^6Y^2 + 3H^6YZ + 3H^6Z^2 \\
 &+ 3H^5A^3 + 7H^5A^2B + 7H^5A^2C + 7H^5A^2W + 7H^5A^2X + 7H^5A^2Y + 7H^5A^2Z \\
 &+ 7H^5AB^2 + 14H^5ABC + 14H^5ABW + 14H^5ABX + 14H^5ABY + 14H^5ABZ \\
 &+ 7H^5AC^2 + 14H^5ACW + 14H^5ACX + 14H^5ACY + \dots
 \end{aligned} \tag{15}$$

The coefficients appearing in f' (Eq. 15) are collected in a tabular form (column S of Table 2), where the substitution patterns are selected in the same way as column 3D.

3.2.2 With Achiral and Chiral Proligands

Let us next consider the case of selecting substituents from the ligand inventory L' (Eq. 9), which contains achiral (H, A, W, X, Y, and Z) and chiral proligands (p, \bar{p} , q, and \bar{q}). To enumerate cubane derivatives as steric isomers in this case, the ligand-inventory function Eq. 11 (among Eqs. 10–12) is introduced into the right-hand side of Eq. 14. Then, the expansion of the resulting function gives the following generating function:

$$\begin{aligned}
 g' = & H^8 + H^7A + H^7W + H^7X + H^7Y + H^7Z + (H^7p + H^7\bar{p}) \\
 & + (H^7q + H^7\bar{q}) + 3H^6A^2 + 3H^6AW + 3H^6AX + 3H^6AY + 3H^6AZ \\
 & + (3H^6Ap + 3H^6A\bar{p}) + (3H^6Aq + 3H^6A\bar{q}) + 3H^6W^2 + 3H^6WX \\
 & + 3H^6WY + 3H^6WZ + (3H^6Wp + 3H^6W\bar{p}) + (3H^6Wq + 3H^6W\bar{q}) \\
 & + 3H^6X^2 + 3H^6XY + 3H^6XZ + (3H^6Xp + 3H^6X\bar{p}) + (3H^6Xq + 3H^6X\bar{q}) \\
 & + 3H^6Y^2 + 3H^6YZ + (3H^6Yp + 3H^6Y\bar{p}) + (3H^6Yq + 3H^6Y\bar{q}) \\
 & + 3H^6Z^2 + 3H^6Zp + 3H^6Z\bar{p} + 3H^6Zq + 3H^6Z\bar{q} \\
 & + (3H^6p^2 + 3H^6\bar{p}^2) + 3H^6p\bar{p} + (3H^6pq + 3H^6\bar{p}q) \\
 & + (3H^6p\bar{q} + 3H^6\bar{p}q) + (3H^6q^2 + 3H^6\bar{q}^2) + 3H^6q\bar{q} + \dots
 \end{aligned} \tag{16}$$

where the coefficient of each term $H^hA^aW^wX^xY^yZ^z p^p\bar{p}^{\bar{p}}q^q\bar{q}^{\bar{q}}$ represents the number of cubane derivatives as steric isomers having h of H, a of A, w of W, x of X, y of Y, z of Z, p of p , \bar{p} of \bar{p} , q of q , and \bar{q} of \bar{q} .

The coefficients appearing in g' (Eq. 16) are collected in a tabular form (column S in Tables 3 and 4). It should be noted that each coefficient collected for a substitution pattern with an asterisk is concerned with one member of an enantiomeric pair. Thus, each substitution pattern marked by an asterisk (e.g., [7,0,0,0,0,0;1,0,0,0]* for H^7p) has the counterpart (enantiomer) of opposite chirality sense (e.g., [7,0,0,0,0,0;0,1,0,0]* for $H^7\bar{p}$). The two enantiomers are counted separately as steric isomers, as shown in Tables 3 and 4 (the column S), which have been obtained by using Eq. 14.

4 Achiral Cubane Derivatives

4.1 Cycle Index with Chirality Fittingness for Counting Achiral Cubane Derivatives

The CI-CF($\mathbf{O}_h, \mathcal{S}_d$) (Eq. 2) for counting cubane derivatives as 3D-structural isomers is concerned with the number of achiral derivatives plus the number of enantiomeric pairs, while the

CI-CF(\mathbf{O}, b_d) (Eq. 14) for counting cubane derivatives as steric isomers is concerned with the number of achiral derivatives plus the number of chiral derivatives (i.e., two times of the number of enantiomeric pairs). As a result, the CI-CF^(a)($\mathbf{O}_h, \$_d$) for obtaining the number of achiral derivatives is evaluated to be 2CI-CF($\mathbf{O}_h, \$_d$) – CI-CF(\mathbf{O}, b_d) on a similar line to Eq. 31 of [35], so as to give the following equation:

$$\begin{aligned} \text{CI-CF}^{(a)}(\mathbf{O}_h, \$_d) &= 2\text{CI-CF}(\mathbf{O}_h, \$_d) - \text{CI-CF}(\mathbf{O}, b_d) \\ &= \frac{1}{6}c_2^4 + \frac{1}{3}c_2c_6 + \frac{1}{4}a_1^4c_2^2 + \frac{1}{4}c_4^2 \end{aligned} \quad (17)$$

As found by comparing between Eq. 2 and Eq. 17, only the terms for improper rotations appearing in Eq. 2 are adopted and multiplied by two to give Eq. 17. In other words, Eq. 17 contains no b_d . This feature holds true generally.

4.2 Enumeration of Achiral Cubane Derivatives

4.2.1 With Achiral Proligands Only

The numbers of achiral cubane derivatives under adopting the ligand inventory \mathbf{L} (Eq. 4) are calculated by introducing the ligand-inventory functions (Eqs. 5 and 7 among Eqs. 5–7) into the right-hand side of Eq. 17 on a similar line to Theorem 5 of [35]. The resulting function is expanded to give the following generating function:

$$\begin{aligned} f^{(a)} &= 2f - f' \\ &= \text{H}^8 + \text{H}^7\text{A} + \text{H}^7\text{B} + \text{H}^7\text{C} + \text{H}^7\text{W} + \text{H}^7\text{X} + \text{H}^7\text{Y} + \text{H}^7\text{Z} + 3\text{H}^6\text{A}^2 + 3\text{H}^6\text{AB} \\ &\quad + 3\text{H}^6\text{AC} + 3\text{H}^6\text{AW} + 3\text{H}^6\text{AX} + 3\text{H}^6\text{AY} + 3\text{H}^6\text{AZ} + 3\text{H}^6\text{B}^2 + 3\text{H}^6\text{BC} + 3\text{H}^6\text{BW} \\ &\quad + 3\text{H}^6\text{BX} + 3\text{H}^6\text{BY} + 3\text{H}^6\text{BZ} + 3\text{H}^6\text{C}^2 + 3\text{H}^6\text{CW} + 3\text{H}^6\text{CX} + 3\text{H}^6\text{CY} \\ &\quad + 3\text{H}^6\text{CZ} + 3\text{H}^6\text{W}^2 + 3\text{H}^6\text{WX} + 3\text{H}^6\text{WY} + 3\text{H}^6\text{WZ} + 3\text{H}^6\text{X}^2 + 3\text{H}^6\text{XY} \\ &\quad + 3\text{H}^6\text{XZ} + 3\text{H}^6\text{Y}^2 + 3\text{H}^6\text{YZ} + 3\text{H}^6\text{Z}^2 \\ &\quad + 3\text{H}^5\text{A}^3 + 5\text{H}^5\text{A}^2\text{B} + 5\text{H}^5\text{A}^2\text{C} + 5\text{H}^5\text{A}^2\text{W} + 5\text{H}^5\text{A}^2\text{X} + 5\text{H}^5\text{A}^2\text{Y} + \dots \end{aligned} \quad (18)$$

This result can be alternatively obtained by calculating two times of f (Eq. 8) minus f' (Eq. 18). The coefficients appearing in $f^{(a)}$ (Eq. 18) are collected in a tabular form (column A of Table 2), where the substitution patterns are selected in the same way as column 3D of Table 2.

Obviously, each value appearing in column A of Table 2 can be obtained by considering column 3D and column S.

4.2.2 With Achiral and Chiral Proligands

As an example of enumerating achiral cubane derivatives by taking account of achiral and chiral proligands, we adopt the ligand inventory \mathbf{L}' (Eq. 9), which contains achiral (H, A, W, X, Y, and Z) and chiral proligands (p , \bar{p} , q , and \bar{q}). In this case, the ligand-inventory functions shown in Eqs. 10 and 12 (among Eqs. 10–12) are introduced into the right-hand side of Eq. 17. The expansion of the resulting function gives the following generating function:

$$\begin{aligned} g^{(a)} &= 2g - g' \\ &= \text{H}^8 + \text{H}^7\text{A} + \text{H}^7\text{W} + \text{H}^7\text{X} + \text{H}^7\text{Y} + \text{H}^7\text{Z} + 3\text{H}^6\text{A}^2 + 3\text{H}^6\text{AW} + 3\text{H}^6\text{AX} \end{aligned}$$

$$\begin{aligned}
 &+ 3H^6AY + 3H^6AZ + 3H^6W^2 + 3H^6WX + 3H^6WY + 3H^6WZ \\
 &+ 3H^6X^2 + 3H^6XY + 3H^6XZ + 3H^6Y^2 + 3H^6YZ + 3H^6Z^2 \\
 &+ 3H^6\bar{p}\bar{p} + 3H^6\bar{q}\bar{q} + 3H^5A^3 + 5H^5A^2W + 5H^5A^2X + 5H^5A^2Y \\
 &+ 5H^5A^2Z + 5H^5AW^2 + 6H^5AWX + 6H^5AWY + 6H^5AWZ + 5H^5AX^2 \\
 &+ 6H^5AXY + 6H^5AXZ + 5H^5AY^2 + 6H^5AYZ + 5H^5AZ^2 \\
 &+ 4H^5A\bar{p}\bar{p} + 4H^5A\bar{q}\bar{q} + 3H^5W^3 + 5H^5W^2X + 5H^5W^2Y + 5H^5W^2Z + \dots \quad (19)
 \end{aligned}$$

where the coefficient of each term $H^hA^aW^wX^xY^yZ^z\bar{p}^p\bar{q}^q$ represents the number of achiral cubane derivatives having h of H, a of A, w of W, x of X, y of Y, z of Z, p of \bar{p} , q of \bar{q} , and \bar{q} of \bar{q} .

This result can be alternatively obtained by calculating two times of g (Eq. 13) minus g' (Eq. 16). The coefficients appearing in $g^{(a)}$ (Eq. 19) are collected in a tabular form (column A of Tables 3 and 4).

5 Enantiomeric Pairs of Cubane Derivatives

5.1 Cycle Index with Chirality Fittingness for Counting Enantiomeric Pairs of Cubane Derivatives

The relationships described in Subsection 4.1 show that the CI-CF^(e)($\mathbf{O}_h, \$_d$) for obtaining the number of enantiomeric pairs can be evaluated to be CI-CF(\mathbf{O}, b_d) – CI-CF($\mathbf{O}_h, \$_d$) on a similar line to Eq. 27 of [35]. Thereby, we obtain the following equation:

$$\begin{aligned}
 \text{CI-CF}^{(e)}(\mathbf{O}_h, \$_d) &= \text{CI-CF}(\mathbf{O}, b_d) - \text{CI-CF}(\mathbf{O}_h, \$_d) \\
 &= \frac{1}{48}b_1^8 + \frac{3}{16}b_2^4 + \frac{1}{6}b_1^2b_3^2 + \frac{1}{8}b_4^2 - \frac{1}{12}c_2^4 - \frac{1}{6}c_2c_6 - \frac{1}{8}a_1^4c_2^2 - \frac{1}{8}c_2^4 \quad (20)
 \end{aligned}$$

As found by comparing between Eq. 2 and Eq. 20, the plus signs of the terms for improper rotations appearing in Eq. 2 are all changed into minus signs in Eq. 20. As found easily, this feature holds true generally.

5.2 Enumeration of Enantiomeric Pairs of Cubane Derivatives

5.2.1 With Achiral Proligands Only

To calculating the number of enantiomeric pairs of cubane derivatives under adopting the ligand inventory \mathbf{L} (Eq. 4), the ligand-inventory functions represented by Eqs. 5–7 are introduced into the right-hand side of Eq. 20 on a similar line to Theorem 4 of [35]. The resulting function is expanded to give the following generating function:

$$\begin{aligned}
 f^{(e)} &= f' - f \\
 &= H^5A^2B + H^5A^2C + H^5A^2W + H^5A^2X + H^5A^2Y + H^5A^2Z + H^5AB^2 + 4H^5ABC \\
 &\quad + 4H^5ABW + 4H^5ABX + 4H^5ABY + 4H^5ABZ + H^5AC^2 + 4H^5ACW + 4H^5ACX \\
 &\quad + 4H^5ACY + 4H^5ACZ + H^5AW^2 + 4H^5AWX + 4H^5AWY + 4H^5AWZ \\
 &\quad + H^5AX^2 + 4H^5AXY + 4H^5AXZ + H^5AY^2 + 4H^5AYZ + H^5AZ^2 \\
 &\quad + H^5B^2C + H^5B^2W + H^5B^2X + H^5B^2Y + H^5B^2Z + H^5BC^2
 \end{aligned}$$

$$\begin{aligned}
 &+ 4H^5BCW + 4H^5BCX + 4H^5BCY + 4H^5BCZ + H^5BW^2 + 4H^5BWX \\
 &+ 4H^5BWY + 4H^5BWZ + H^5BX^2 + 4H^5BXY + 4H^5BXZ + H^5BY^2 + \dots \quad (21)
 \end{aligned}$$

This generating function can be alternatively obtained by calculating f' (Eq. 15) minus f (Eq. 8). The coefficients appearing in $f^{(e)}$ (Eq. 21) are collected in a tabular form (column E of Table 2), where the substitution patterns are selected in the same way as the other columns of Table 2.

Obviously, each value appearing in column E of Table 2 is obtained by subtracting the corresponding value in column 3D from the corresponding value in column S.

5.2.2 With Achiral and Chiral Proligands

To take account of achiral and chiral proligands in the enumeration of enantiomeric pairs of cubane derivatives, we adopt the ligand inventory L' (Eq. 9), which contains achiral (H, A, W, X, Y, and Z) and chiral proligands (p, \bar{p} , q, and \bar{q}). In this case, the ligand-inventory functions shown in Eqs. 10–12 are introduced into the right-hand side of Eq. 20. The expansion of the resulting function gives the following generating function:

$$\begin{aligned}
 g^{(e)} &= g' - g \\
 &= \frac{1}{2}(H^7p + H^7\bar{p}) + \frac{1}{2}(H^7q + H^7\bar{q}) + \frac{3}{2}(H^6Ap + H^6A\bar{p}) \\
 &\quad + \frac{3}{2}(H^6Aq + H^6A\bar{q}) + \frac{3}{2}(H^6Wp + H^6W\bar{p}) + \frac{3}{2}(H^6Wq + H^6W\bar{q}) \\
 &\quad + \frac{3}{2}(H^6Xp + H^6X\bar{p}) + \frac{3}{2}(H^6Xq + H^6X\bar{q}) + \frac{3}{2}(H^6Yp + H^6Y\bar{p}) \\
 &\quad + \frac{3}{2}(H^6Yq + H^6Y\bar{q}) + \frac{3}{2}(H^6Zp + H^6Z\bar{p}) + \frac{3}{2}(H^6Zq + H^6Z\bar{q}) \\
 &\quad + \frac{3}{2}(H^6p^2 + H^6\bar{p}^2) + \frac{3}{2}(H^6pq + H^6\bar{p}\bar{q}) + \frac{3}{2}(H^6p\bar{q} + H^6\bar{p}q) \\
 &\quad + \frac{3}{2}(H^6q^2 + H^6\bar{q}^2) + H^5A^2W + H^5A^2X + H^5A^2Y + H^5A^2Z \\
 &\quad + \frac{7}{2}(H^5A^2p + H^5A^2\bar{p}) + \frac{7}{2}(H^5A^2q + H^5A^2\bar{q}) + H^5AW^2 \\
 &\quad + 4H^5AWX + 4H^5AWY + 4H^5AWZ + 7(H^5AWp + H^5AW\bar{p}) + \dots \quad (22)
 \end{aligned}$$

where the coefficient of each term $H^hA^aW^wX^xY^yZ^z p^p\bar{p}^{\bar{p}} q^q\bar{q}^{\bar{q}}$ represents the number of cubane derivatives as 3D-structural isomers having h of H, a of A, w of W, x of X, y of Y, z of Z, p of p, \bar{p} of \bar{p} , q of q, and \bar{q} of \bar{q} .

This result can be alternatively obtained by calculating g' (Eq. 16) minus g (Eq. 13). The coefficients appearing in $g^{(e)}$ (Eq. 22) are collected in a tabular form (column E of Tables 3 and 4). Each substitution pattern marked by an asterisk (e.g., [7,0,0,0,0,0;1,0,0,0]* for H^7p) has the counterpart of opposite chirality sense (e.g., [7,0,0,0,0,0;0,1,0,0]* for $H^7\bar{p}$) so that the same comments described for the coefficients appearing in the generating function g (Eq. 13) hold true for this case in which each pair of enantiomers is also counted once.

6 Illustration of Enumerated Cubane Derivatives

6.1 Cubane Derivatives with Achiral Proligands Only

Figure 2 shows cubane derivatives with the formula H^5A^2B , which correspond to the substitution pattern [5,2,1,0,0,0,0]. In accord with the [5,2,1,0,0,0,0]-row of Table 2 (or equivalently the [5,2,1,0,0,0;0,0,0,0]-row of Table 3), there exist six 3D-structural isomers (the 3D column), which are categorized into five achiral isomers (the A column) and one enantiomeric pair (the E column). Because one enantiomeric pair contains two enantiomers, their exist seven steric isomers ($7 = 5 + 1 \times 2$), as collected in the S column of the row at issue. In Figure 2, the five achiral isomers are illustrated to be **2–6** and one enantiomeric pair is illustrated to be a pair of **7a** and **7b**.

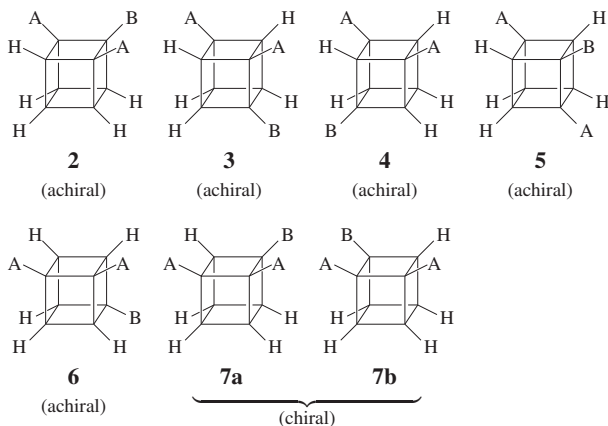


Figure 2: Cubane derivatives with H^5A^2B ([5,2,1,0,0,0,0])

The [4,3,1,0,0,0,0]-row of Table 2 (or equivalently the [4,3,1,0,0,0;0,0,0,0]-row of Table 3) indicates that there exist ten 3D-structural isomers of H^4A^3B (the 3D column), which are categorized into seven achiral isomers (the A column) and three enantiomeric pairs (the E column). The number of steric isomers is calculated to be 13 ($= 7 + 2 \times 3$), which appears in the S column at issue. These cubane derivatives are illustrated in Figure 3, where the seven achiral isomers (**8**, **9**, **10**, **12**, **15**, **16**, and **17**) and the three enantiomeric pairs (**11a/11b**, **13a/13b**, and **14a/14b**) are depicted.

6.2 Cubane Derivatives with Achiral and Chiral Proligands

Incorporation of chiral proligands p and/or \bar{p} exhibits complicated effects, as illustrated in Figure 4 and 5. The value $3/2$ in the [6,0,0,0,0,0;2,0,0,0]-row (the 3D column and the E column) of Table 3 implies the same value $3/2$ in the [6,0,0,0,0,0;0,2,0,0]-row, although the latter is omitted. This means that this value corresponds to the term $\frac{3}{2}(H^6p^2 + H^6\bar{p}^2)$, which represents three ($2 \times \frac{3}{2}$) pairs of enantiomers (i.e., **18a/18b**, **19a/19b**, and **20a/20b** for the pair $H^6p^2/H^6\bar{p}^2$),

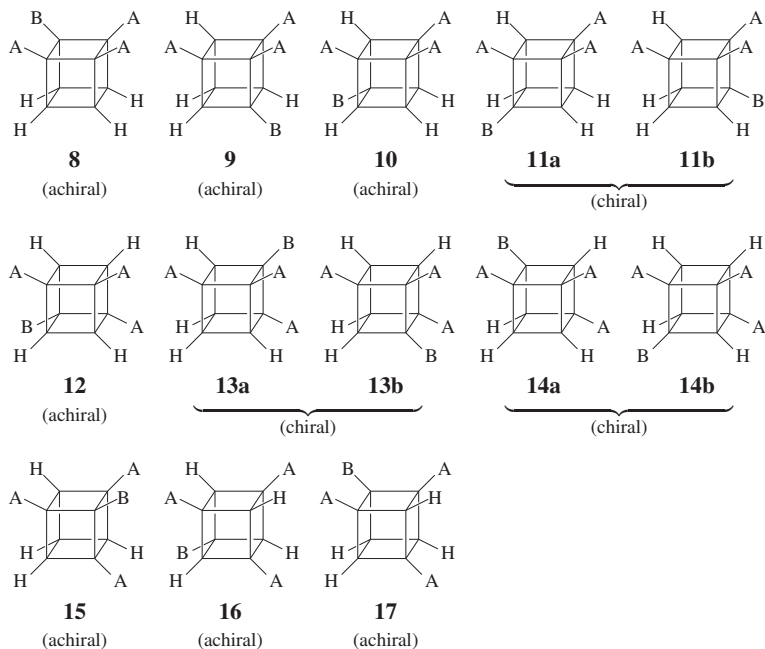


Figure 3: Cubane derivatives with H^4A^3B ([4,3,1,0,0,0,0])

as illustrated in Figure 4. Note that H^6p^2 and $H^6\bar{p}^2$ have the same molecular formula when p and \bar{p} are reduced into their constitutions. The value 3 in the S column at issue corresponds to $3(H^6p^2 + H^6\bar{p}^2)$ and should be duplicated to give 6, which corresponds six derivatives (**18a**, **18b**, **19a**, **19b**, **20a**, and **20b**) regarded as steric isomers.

The value 3 in the [6,0,0,0,0,0;1,1,0,0]-row (the 3D column and the A column) of Table 3 means that there are three achiral derivatives with $H^6p\bar{p}$ (**21**, **22**, and **23**), which are depicted in Figure 5. These cases are akin to such *meso* cases as $p-\bar{p}$ (e.g., *meso*-tartaric acid) or to such pseudoasymmetric cases as $CH(OH)p\bar{p}$ (e.g., 2,3,4-trihydroxyglutaric acids).

It should be noted that the cubane derivatives shown in Figure 4 and the counterparts shown in Figure 5 (i.e., the set of **18a/18b** vs. **21**; the set of **19a/19b** vs. **22**; as well as the set of **20a/20b** vs. **23**) are stereoisomeric, because each of the sets has the same constitution (or graph) when p and \bar{p} are reduced into their constitutions (graphs).

7 Conclusions

To demonstrate the versatility of the proligand method developed by us [14–16], cubane derivatives with chiral and achiral proligands are counted as 3D structural isomers and as steric isomers. The results are further applied to count achiral derivatives as well as enantiomeric pairs of chiral derivatives. By taking account of the sphericities of cycles, the proligand method is

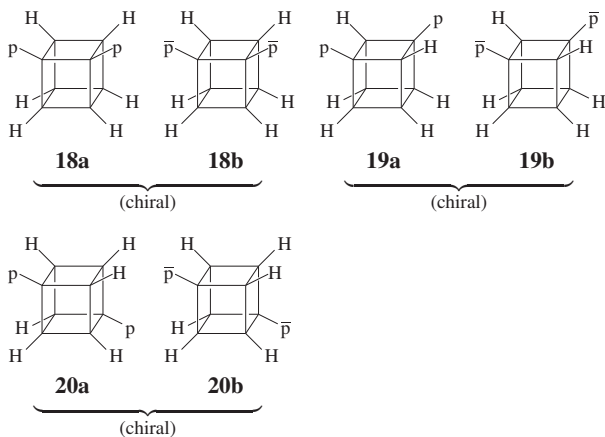


Figure 4: Cubane derivatives with H^6p^2 or $H^6\bar{p}^2$ ($[6,0,0,0,0,0;2,0,0,0]$ or $[6,0,0,0,0,0;0,2,0,0]$), where p and \bar{p} represents a pair of enantiomeric proligands.

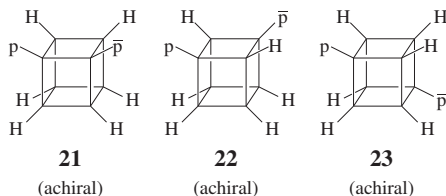


Figure 5: Cubane derivatives with $H^6p\bar{p}$ ($[6,0,0,0,0,0;1,1,0,0]$), where p and \bar{p} represents a pair of enantiomeric proligands.

capable of counting cubane derivatives with chiral and achiral proligands, where the chirality of each proligand is judged in isolation. On the other hand, Pólya's theorem lacks such sphericities of cycles, so that it is capable of counting cubane derivatives with achiral proligands only, but incapable of counting cubane derivatives with chiral and achiral proligands.

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Appendix

Maple Program for Generating the Data of Table 2

```
#cubaneA8-Total.mpl
#restart;
#read "c:/fujita0/cubaneA8-Total.mpl";
#with H^k A^l B^m C^n W^kk X^ll Y^mm Z^nn

CICF := (1/48)*b1^8 + (1/16)*b2^4 + (1/8)*b2^4
```

```

+ (1/16)*c2^4 + (1/8)*a1^4*c2^2 + (1/48)*c2^4
+ (1/6)*b1^2*b3^2 + (1/8)*b4^2 + (1/8)*c4^2 + (1/6)*c2*c6;
CICFo := (1/24)*b1^8 + (1/8)*b2^4 + (1/4)*b2^4
+ (1/3)*b1^2*b3^2 + (1/4)*b4^2;

```

```

a1 := H + A + B + C + W + X + Y + Z;
a2 := H^2 + A^2 + B^2 + C^2 + W^2 + X^2 + Y^2 + Z^2;
a3 := H^3 + A^3 + B^3 + C^3 + W^3 + X^3 + Y^3 + Z^3;
a4 := H^4 + A^4 + B^4 + C^4 + W^4 + X^4 + Y^4 + Z^4;
a6 := H^6 + A^6 + B^6 + C^6 + W^6 + X^6 + Y^6 + Z^6;
b1 := H + A + B + C + W + X + Y + Z;
b2 := H^2 + A^2 + B^2 + C^2 + W^2 + X^2 + Y^2 + Z^2;
b3 := H^3 + A^3 + B^3 + C^3 + W^3 + X^3 + Y^3 + Z^3;
b4 := H^4 + A^4 + B^4 + C^4 + W^4 + X^4 + Y^4 + Z^4;
b6 := H^6 + A^6 + B^6 + C^6 + W^6 + X^6 + Y^6 + Z^6;
c2 := H^2 + A^2 + B^2 + C^2 + W^2 + X^2 + Y^2 + Z^2;
c4 := H^4 + A^4 + B^4 + C^4 + W^4 + X^4 + Y^4 + Z^4;
c6 := H^6 + A^6 + B^6 + C^6 + W^6 + X^6 + Y^6 + Z^6;

```

```

# Maple procedure for calculating the coefficient of
# the term H^k A^l B^m C^n W^kk X^ll Y^mm Z^nn

```

```

cubaneHABCWXYZ := proc(k::integer,
l::integer, m::integer, n::integer, kk::integer, ll::integer,
mm::integer, nn::integer)
local N1g, N2g, N3g, N4g, N5g, N6g, N7g, N8g,
SN1g, SN2g, SN3g, SN4g, SN5g, SN6g, SN7g, SN8g, AN8g, CN8g;
if (k=0) then N1g := expand(coeff(H*CICF, H));
SN1g := expand(coeff(H*CICFo, H));
else N1g := expand(coeff(CICF, H^k));
SN1g := expand(coeff(CICFo, H^k));
end if;
if (l=0) then N2g := expand(coeff(A*N1g, A));
SN2g := expand(coeff(A*SN1g, A));
else N2g := expand(coeff(N1g, A^l));
SN2g := expand(coeff(SN1g, A^l));
end if;
if (m=0) then N3g := expand(coeff(B*N2g, B));
SN3g := expand(coeff(B*SN2g, B));
else N3g := expand(coeff(N2g, B^m));
SN3g := expand(coeff(SN2g, B^m));
end if;
if (n=0) then N4g := expand(coeff(C*N3g, C));
SN4g := expand(coeff(C*SN3g, C));
else N4g := expand(coeff(N3g, C^n));
SN4g := expand(coeff(SN3g, C^n));
end if;
if (kk=0) then N5g := expand(coeff(W*N4g, W));
SN5g := expand(coeff(W*SN4g, W));
else N5g := expand(coeff(N4g, W^kk));
SN5g := expand(coeff(SN4g, W^kk));
end if;
if (ll=0) then N6g := expand(coeff(X*N5g, X));
SN6g := expand(coeff(X*SN5g, X));
else N6g := expand(coeff(N5g, X^ll));
SN6g := expand(coeff(SN5g, X^ll));
end if;
if (mm=0) then N7g := expand(coeff(Y*N6g, Y));
SN7g := expand(coeff(Y*SN6g, Y));
else N7g := expand(coeff(N6g, Y^mm));
SN7g := expand(coeff(SN6g, Y^mm));
end if;
end proc;

```

```
end if;
if (nn=0) then N8g := expand(coeff(Z*N7g,Z));
SN8g := expand(coeff(Z*SN7g,Z));
else N8g := expand(coeff(N7g,Z^nn));
SN8g := expand(coeff(SN7g,Z^nn));
end if;

AN8g := 2*N8g - SN8g; CN8g := SN8g - N8g;

printf("[%d,%d,%d,%d,%d,%d,%d,%d] & ",
k, l, m, n, kk, ll, mm, nn);
printf("%a & %a & %a & %a YYYY %n", N8g, SN8g, AN8g, CN8g);
end proc;

"Print H8";
cubaneHABCWXYZ(8,0,0,0,0,0,0,0);
"Print H7";
cubaneHABCWXYZ(7,1,0,0,0,0,0,0);
"Print H6";
cubaneHABCWXYZ(6,2,0,0,0,0,0,0);
cubaneHABCWXYZ(6,1,1,0,0,0,0,0);
"Print H5";
cubaneHABCWXYZ(5,3,0,0,0,0,0,0);
cubaneHABCWXYZ(5,2,1,0,0,0,0,0);
cubaneHABCWXYZ(5,1,1,1,0,0,0,0);
"Print H4";
cubaneHABCWXYZ(4,4,0,0,0,0,0,0);
cubaneHABCWXYZ(4,3,1,0,0,0,0,0);
cubaneHABCWXYZ(4,2,2,0,0,0,0,0);
cubaneHABCWXYZ(4,2,1,1,0,0,0,0);
cubaneHABCWXYZ(4,1,1,1,1,0,0,0);
"Print H3";
cubaneHABCWXYZ(3,3,2,0,0,0,0,0);
cubaneHABCWXYZ(3,3,1,1,0,0,0,0);
cubaneHABCWXYZ(3,2,2,1,0,0,0,0);
cubaneHABCWXYZ(3,2,1,1,1,0,0,0);
cubaneHABCWXYZ(3,1,1,1,1,1,0,0);
"Print H2";
cubaneHABCWXYZ(2,2,2,2,0,0,0,0);
cubaneHABCWXYZ(2,2,2,1,1,0,0,0);
cubaneHABCWXYZ(2,2,1,1,1,1,0,0);
cubaneHABCWXYZ(2,1,1,1,1,1,1,0);
"Print H1";
cubaneHABCWXYZ(1,1,1,1,1,1,1,1);
```