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Symmetry Adapted Enumeration of Substituted Cubane Derivatives and Heteroanalogues by the Denumerants of the Octahedral Group. II.

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Abstract

Ten entries vectors of permutational isomers numbers N_{g_i} calculated with respect to distinct symmetry operations g_i of O_h group and the degrees of homo or heteropolysubstitution are derived for substituted cubanes and transformed into Sylvester's denumerants of type $N_{g_i} = \sum_{G_j} a_{G_j} w_{G_j,g_i}$. Such associated partition equations decomposing these numbers as sum of symmetry adapted isomers numbers $a_{G_1},...,a_{G_j},...,a_{G_k}$ scaled by the weights w_{G_j,g_i} of the subgroups G_j of O_h are used for systematic enumeration of substituted cubane derivatives and cubane heteroanalogues of given symmetries.

1 Introduction

During the last 3 decades Fujita has introduced the USCI-method [1-7] for symmetry adapted enumeration of chemical compounds in addition to Pólya's classical isomers inventories based on cycle indices.[8-12] Despite these enumeration methods stereoisomers distribution among a sequence of subgroups (SSG_G) $G_1, G_2, ... G_i ..., G_j$ of a parent group G remains a pending partition problem of stereochemistry which requires mathematical solutions. We recall that a partition of an integer number N called denumerant of N has been introduced in combinatorics by Sylvester [13]. In chemistry stereoisomers result from homogeneous and heterogeneous placements (arrangements) in distinct ways of substituents among different positions permuted by a set of symmetry operations of a point group acting on a parent molecular skeleton. Homogeneous arrangements of ligands are placements in distinct ways of substituents of the same kind among a given set of positions. Heterogeneous arrangements of ligands are placements in distinct ways of substituents of different kinds among a given set of positions. Regarding these characteristics of arrangements of substituents, one can classify cubane derivatives (MX) among 4 groups:

1-Homogeneous arrangements of qX substituents of the same kind among 8 substitution sites of cubane permuted by distinct symmetry operation $g_i \in O_h$ yield permutomers of homosubstituted cubanes derivatives $C_8H_{8-q}X_q$.

2-Homogeneous arrangements operated in accord with the obligatory minimum valency (OMV) restriction (OMV=3) are processes of putting in distinct ways qX trivalent heteroatoms of the same kind among 8 tertiary carbon atoms positions permuted by distinct symmetry operations $g_i \in O_h$ give rise to cubane homo hetero-analogues $(CH)_{8-q} X_q$.

3-Heterogeneous arrangements of q_0H and $q_1X,...,q_iY,...,q_kZ$ substituents of different kinds among 8 tertiary carbon atoms positions permuted by distinct symmetry operations $g_i \in O_h$ yield heterosubstituted cubane derivatives $C_8H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$.

4-Heterogeneous arrangements operated in accord with the obligatory minimum valency restriction (OMV=3) are processes of putting in distinct ways q_0H and $q_1X,...,q_iY,...,q_kZ$ trivalent heteroatoms of different kinds among 8 tertiary carbon atoms positions permuted by distinct symmetry operations $g_i \in O_h$ give rise to cubane hetero hetero-analogues $(CH)_{q_0} X_{q_1}...Y_{q_i}...Z_{q_k}$.

In this study integer sequences of permutational isomers numbers $N_{g_i,q}$ of substituted cubane derivatives are derived from the O_h group action. Then, Sylvester's denumerants of type $N_{g_i,q} = \sum_{G_j} a_{G_j} w_{G_j,g_i}$ are constructed to partition these numbers as sum of symmetry adapted isomers numbers $a_{G_j,q}$ $a_{G_1},...,a_{G_i},...,a_{G_j}$ scaled by w_{G_j,g_i} the weights of the subgroups G_j *of* O_h calculated with respect to g_i the symmetry operations of G_j. This model is applied for a systematic enumeration of homo and hetero-polysubstituted cubane derivatives, cubane homo hetero-analogues and cubane hetero hetero-analogues of given symmetries.

2 Permutations of carbon and hydrogen atoms of cubane

Let us represent the structure of cubane by a tridimensional graph given in fig.1 part I where black and white vertices symbolizing carbon and hydrogen atoms indicated by numerical and alphabetical labels form two embedded orbits $H_8 = (1,2,3,4,1',2',3',4')$ and $C_8 = (a,b,c,d,a',b',c',d')$ respectively. The connections of black and white vertices are C-H bonds and the edges interconnecting black vertices form a cubic cluster of 12 C-C bonds giving rise to a cage shaped hydrocarbon of O_h symmetry defined in eq.1:

$$O_h = E, 8C_3, 6C_2', 6C_4, \ 3C_4^2 = C_2, i, \ 6S_4, 8S_6, 3\sigma_h, 6\sigma_d \qquad (1)$$

The O_h group action on cubane consisting to apply distinct symmetry operations $g_i \in O_h$ to the orbits H_8 and C_8 gives rise to the following permutations representations:

$$P^{O_h}\Delta_H = \backslash P^E\Delta_H, P^{C_2}\Delta_H, P^{C_2'}\Delta_H, P^{C_3}\Delta_H, P^{C_4}\Delta_H, P^i\Delta_H, P^{S_4}\Delta_H, P^{S_6}\Delta_H, P^{\sigma_h}\Delta_H, P^{\sigma_d}\Delta_H \qquad (2)$$

$$P^{O_h}\Delta_C = P^E\Delta_C, P^{C_2}\Delta_C, P^{C_2'}\Delta_C, P^{C_3}\Delta_C, P^{C_4}\Delta_C, P^i\Delta_C, P^{S_4}\Delta_C, P^{S_6}\Delta_C, P^{\sigma_h}\Delta_C, P^{\sigma_d}\Delta_C \qquad (3)$$

$P^{O_h}H_8$ and $P^{O_h}C_8$ having their right-hand side terms $P^{(g_i)}H_8 \cong P^{(g_i)}C_8$ are 2 sets of congruent permutations given in cycle structure notation as follows:

$$P^{O_h}\Delta_H = P^{O_h}\Delta_C = \left[1^8\right], 8\left[1^2 3^2\right], 6\left[2^4\right], 6\left[4^2\right], 3\left[2^4\right], \left[2^4\right], 6\left[4^2\right], 8\left[2^1 6^1\right], 3\left[2^4\right], 6\left[1^4 2^2\right] \qquad (4)$$

3 Determination of permutational isomers numbers for poly substituted cubane derivatives and cubane heteroanalogues

Let N_{g_i} denote the number of permutomers i.e. the number of arrangements of achiral substituents of the same kind or of different kinds among 8 substitution sites of cubane permuted by a distinct symmetry operation $g_i \in O_h$. For 10 conjugacy classes of symmetry operations of O_h group one obtains a set of integer numbers $N_{g_i} = N_E, N_{C_2}, N_{C_2'}, N_{C_3}, N_{C_4}, N_i, N_{S_4}, N_{S_6}, N_{\sigma_h}, N_{\sigma_d}$ which are derived as follows:

For homopolysubstituted cubane derivatives $C_8H_{8-q}X_q$ and cubane homo hetero-analogues $(CH)_{8-q}X_q$ having a degree of substitution q:

$$1^8 \rightarrow N_E = \binom{8}{q} \tag{5}$$

$$2^4 \rightarrow N_{C_2,q} = N_{C_2'} = N_i = N_{\sigma_h} = \binom{4}{\frac{q}{2}} \tag{6}$$

$$4^2 \rightarrow N_{C_4} = N_{S_4} = \binom{2}{\frac{q}{4}} \tag{7}$$

$$1^2 3^2 \rightarrow N_{C_3,q} = \sum_{\beta=0}^{2} \binom{2}{\beta} \binom{2}{\frac{q-\beta}{3}} \tag{8}$$

$$1^4 2^2 \rightarrow N_{\sigma_d,q} = \sum_{\alpha=0}^{4} \binom{4}{\alpha} \binom{2}{\frac{q-\alpha}{2}} \tag{9}$$

$$2^1 6^1 \rightarrow N_{S_6,q} = \sum_{\lambda=0}^{1} \binom{1}{\lambda} \binom{1}{\frac{q-2\lambda}{6}} \tag{10}$$

For heteropolysubstituted cubane derivatives ($C_8H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$) and cubane hetero hetero analogues $(CH)_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$:

$$1^8 \rightarrow N_E = \binom{8}{q_0,...,q_i,...q_k} \tag{11}$$

$$2^4 \rightarrow N_{C_2} = N_{C_2'} = N_i = N_{\sigma_h} = \binom{4}{\frac{q_0}{2},...,\frac{q_i}{2},...,\frac{q_k}{2}} \tag{12}$$

$$4^2 \rightarrow N_{C_4} = N_{S_4} = \binom{2}{\frac{q_0}{4},...,\frac{q_i}{4},...,\frac{q_k}{4}} \tag{13}$$

$$1^2 3^2 \rightarrow N_{C_3} = \sum_{\lambda_1} \binom{2}{p_0,...,p_i,...,p_k} \binom{2}{q_0',...,q_i',...,q_k'} \tag{14}$$

with the restrictions $\sum_{i=0}^{k} p_i = 2 \Leftrightarrow \sum_{i=0}^{k} q_i' = 2$ and $q_i' = \frac{q_i - p_i}{3}$ (15)

$$1^4 2^2 \rightarrow N_{\sigma_d} = \sum_{\lambda_2} \binom{4}{p_0',...,p_i',...,p_k'} \binom{2}{q_0'',...,q_i'',...,q_k''}: \tag{16}$$

with the restrictions $\sum_{i=0}^{k} p'_i = 4 \Leftrightarrow \sum_{i=0}^{k} q''_i = 2 \text{ and } q''_i = \frac{q_i - p'_i}{2}$ (17)

$$2^1 6^1 \to N_{S_6} = \sum_{\lambda_3} \binom{1}{p''_0, ..., p''_i, ..., p''_k} \binom{1}{q'''_0, ..., q'''_i, ..., q'''_k} \quad (18)$$

with the restrictions $\sum_{i=0}^{k} p''_i = 1 \Leftrightarrow \sum_{i=0}^{k} q'''_i = 1 \text{ and } q'''_i = \frac{q_i - 2p''_i}{6}$ (19)

This integer sequence generates a permutomers count vector (PCV) for MX=$C_8H_{8-q}X_q$, $(CH)_{8-q}X_q$, $C_8H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ or $(CH)_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ denoted:

$$PCV(MX) = \left(N_E, N_{C_2}, N_{C'_2}, N_{C_3}, N_{C_4}, N_{i}, N_{S_4}, N_{S_6}, N_{\sigma_h}, N_{\sigma_d}\right)_{MX} \quad (20)$$

4 The Sylvester's denumerants of the octahedral symmetry

The combinations of different symmetry operations $g_i \in O_h$ given in the right-hand side of eq.1 generate a sequence of subgroups for O_h (SSG_{O_h}) listed in table 1 and summarized in eq.21.

Table 1. Sequence of subgroups of the octahedral point group.

$C_1=E$	$C_{2v}=E, C_2, 2\sigma_v$	$D_{2d}=E, C_2=C_4^2, 2C'_2, 2S_4, 2\sigma_d$
$C_2=E,C_2$	$C'_{2v}=E, C_2, 2\sigma_d$	$D'_{2d}=E, C_2=C_4^2, 2C''_2, 2S_4, 2\sigma_v$
$C'_2=E,C'_2$	$C''_{2v}=E, C'_2, \sigma_v, \sigma_d$	$D_{2h}=E, 3C_2=C_4^2, i, 3\sigma_v$
$C_s=E,\sigma_v$	$C_{2h}=E, C_2, \sigma_v, i$	$D'_{2h}=E, C_2=C_4^2, 2C'_2, \sigma_v, i, 2\sigma_d$
$C'_s=E,\sigma_d$	$C'_{2h}=E, C'_2, \sigma_d, i$	$T=E, 3C_2, 4C_3^1, 4C_3^2$
$C_i=E,i$	$D_3=E, 3C'_2, 2C_3$	$D_{3d}=E, 3C'_2, 2C_3, 3\sigma_d, i, 2S_6$
$C_3=E, 2C_3$	$C_{3v}=E, 2C_3, 3\sigma_d$	$D_{4h}=E, C_2, 2C'_2, 2C''_2, 2C_4, i, 2S_4, \sigma_h, 2\sigma_v, 2\sigma_d$
$C_4=E, C_4^2=C_2, 2C_4$	$C_{3i}=E, 2C_3, i, 2S_6$	$O=E, 3C_2, 6C'_2, 8C_3, 6C_4$
$S_4=E, C_4^2=C_2, 2S_4$	$D_4=E, C_2=C_4^2, 2C'_2, 2C''_2, 2C_4$	$T_h=E, 4C_3, 4C_3^2, 3C_2, i, 4S_6, 4S_6^5, 3\sigma_h$
$D_2=E, C_4^2=3C_2$	$C_{4v}=E, C_2=C_4^2, 2C_4, 2\sigma_v, 2\sigma_d$	$T_d=E, 8C_3, 3C_4^2=C_2, 6S_4, 6\sigma_d$
$D'_2=E, C_4^2=C_2, 2C'_2$	$C_{4h}=E, C_2=C_4^2, 2C_4, i, 2S_4, \sigma_h$	$O_h=E, 8C_3, 6C'_2, 6C_4, 3C_4^2=C_2, i, 6S_4, 8S_6, 3\sigma_h, 6\sigma_d$

$$SSG_{O_h} = \begin{pmatrix} C_1, C_2, C'_2, C_s, C'_s, C_i, C_3, C_4, S_4, D_2, D'_2, C_{2v}, C'_{2v}, C''_{2v}, C_{2h}, C'_{2h}, D_3, \\ C_{3v}, C_{3i}, D_4, C_{4v}, C_{4h}, D_{2d}, D'_{2d}, D_{2h}, D'_{2h}, T, D_{3d}, D_{4h}, O, T_h, T_d, O_h \end{pmatrix} \quad (21)$$

Let us consider $\mu_{g_i \in G_j}$ and $\mu_{g_i \in O_h}$ as the respective multiplicities of a symmetry operation $g_i \in G_j$ and $g_i \in O_h$ given in table 1. We define the weight w_{G_j, g_i} of a subgroup

$G_j \in SSG_{O_h}$ calculated with respect to a symmetry operation $g_i \in G_j$ as the quotient of the ratios $\frac{\mu_{g_i \in G_j}}{|G_j|}$ and $\frac{\mu_{g_i \in O_h}}{|O_h|}$ given in eq.14 where $|O_h|$ and $|G_j|$ are the orders of these groups.

$$w_{G_j,g_i} = \begin{cases} \dfrac{\mu_{g_i \in G_j}}{\mu_{g_i \in O_h}} \times \dfrac{|O_h|}{|G_j|} \text{ for } g_i \in G_j, g_i \in O_h \\ 0 \quad for\ g_i \notin G_j \end{cases} \tag{22}$$

For 10 distinct conjugacy classes of symmetry operations $g_i \in O_h$ and 33 subgroups G_j of O_h given in table I one obtains 330 distinct w_{G_j,g_i} values which are the elements of the matrix of the weights of subgroups for O_h denoted :

$$W_{O_h} = \left[w_{G_j,g_i} \right] \text{ where } G_j \in SSG_{O_h}, g_i \in G_j \text{ and } g_i \in O_h \tag{23}$$

and the entries w_{G_j,g_i} are equivalent to the marks of coset representations (O_h/G_j) of Fujita.[14]

If N_{g_i} permutomers of a cubane derivative (MX) are distributed among the subgroups $G_j \in SSG_{O_h}$, this partition has 33 indeterminate symmetry adapted isomers numbers a_{G_j} which form an itemized-isomers count vector *IICV* for MX denoted:

$$IICV(MX) = \begin{pmatrix} a_{C_1}, a_{C_2}, a_{C_2'}, a_{C_s}, a_{C_s'}, a_{C_i}, a_{C_3}, a_{C_4}, a_{S_4}, a_{D_2}, a_{D_2'}, a_{C_{2v}}, a_{C_{2v}'}, a_{C_{2v}''}, a_{C_{2h}}, a_{C_{2h}}, \\ a_{D_3}, a_{C_{3v}}, a_{C_{3i}}, a_{D_4}, a_{C_{4v}}, a_{C_{4h}}, a_{D_{2d}}, a_{D_{2d}'}, a_{D_{2h}}, a_{D_{2h}'}, a_T, a_{D_{3d}}, a_{D_{4h}}, a_O, a_{T_h}, a_{T_d}, a_{O_h} \end{pmatrix}_{MX} \tag{24}$$

The relation linking $IICV[MX]$ and $PCV[MX]$ is the dot product: [15-16]

$$IICV[MX] \times W_{O_h} = PCV[MX] \tag{25}$$

explicitely denoted :

$$\overbrace{\begin{pmatrix} a_{C_1}, a_{C_2}, a_{C'_2}, a_{C_s}, a_{C'_s}, a_{C_i}, a_{C_3}, a_{C_4}, a_{S_4}, a_{D_2}, a_{D'_2}, a_{C_{2v}}, a_{C'_{2v}}, a_{C''_{2v}}, a_{C_{2h}}, a_{C_{2h}}, \\ a_{D_3}, a_{C_{3v}}, a_{C_{3i}}, a_{D_4}, a_{C_{4v}}, a_{C_{4h}}, a_{D_{2d}}, a_{D'_{2d}}, a_{D_{2h}}, a_{D'_{2h}}, a_T, a_{D_{3d}}, a_{D_{4h}}, a_O, a_{T_h}, a_{T_d}, a_{O_h} \end{pmatrix}}^{\text{IICV[MX]}}$$

$$\times$$

$$W_{Oh}$$

SSG_{O_h}	E	$3C_2$	$6C'_2$	$8C_3$	$6C_4$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$
C_1	48	0	0	0	0	0	0	0	0	0
C_2	24	8	0	0	0	0	0	0	0	0
C'_2	24	0	4	0	0	0	0	0	0	0
C_s	24	0	0	0	0	0	0	0	8	0
C'_s	24	0	0	0	0	0	0	0	0	4
C_i	24	0	0	0	0	24	0	0	0	0
C_3	16	0	0	4	0	0	0	0	0	0
C_4	12	4	0	0	4	0	0	0	0	0
S_4	12	4	0	0	0	0	4	0	0	0
D_2	12	12	0	0	0	0	0	0	0	0
D'_2	12	4	4	0	0	0	0	0	0	0
C_{2v}	12	4	0	0	0	0	0	0	8	0
C'_{2v}	12	4	0	0	0	0	0	0	0	4
C''_{2v}	12	0	2	0	0	0	0	0	4	2
C_{2h}	12	4	0	0	0	12	0	0	4	0
C'_{2h}	12	0	2	0	0	12	0	0	0	2
D_3	8	0	4	2	0	0	0	0	0	0
C_{3v}	8	0	0	2	0	0	0	0	0	4
C_{3i}	8	0	0	2	0	8	0	2	0	0
D_4	6	6	2	0	2	0	0	0	0	0
C_{4v}	6	2	0	0	2	0	0	0	4	2
C_{4h}	6	2	0	0	2	6	2	0	2	0
D_{2d}	6	6	0	0	0	0	2	0	0	2
D'_{2d}	6	2	2	0	0	0	2	0	4	0
D_{2h}	6	6	0	0	0	6	0	0	6	0
D'_{2h}	6	2	2	0	0	6	0	0	2	2
T	4	4	0	4	0	0	0	0	0	0
D_{3d}	4	0	2	1	0	4	0	1	0	2
D_{4h}	3	3	1	0	1	3	1	0	3	1
O	2	2	2	2	2	0	0	0	0	0
T_h	2	2	0	2	0	2	0	2	2	0
T_d	2	2	0	2	0	0	2	0	0	2
O_h	1	1	1	1	1	1	1	1	1	1

(25')

$$=$$

$$\overbrace{\left(N_{E,q}, N_{C_2,q}, N_{C'_2,q}, N_{C_3,q}, N_{C_4,q}, N_{i,q}, N_{S_4,q}, N_{S_6,q}, N_{\sigma_h,q}, N_{\sigma_d,q}\right)}^{PCV[MX]}$$

The expansion of eq.25’ gives rise to 10 associated partition equations 26-45 called Sylvester’s denumerants[13] of permutomers numbers $N_{g_i,MX}$ for the derivative MX. For homosubstituted cubane derivatives $C_8H_{8-q}X_q$ and cubane homo hetero-analogues $(CH)_{8-q}X_q$:

$$N_E = \begin{pmatrix} 48a_{C_1} + 24a_{C_2} + 24a_{C'_2} + 24a_{C_s} + 24a_{C'_s} + 24a_{C_i} + 16a_{C_3} + 12a_{C_4} + 12a_{S_4} + 12a_{D_2} + 12a_{D'_2} \\ +12a_{C_{2v}} + 12a_{C'_{2v}} + 12a_{C''_{2v}} + 12a_{C_{2h}} + 12a_{C'_{2h}} + 8a_{D_3} + 8a_{C_{3v}} + 8a_{C_{3i}} + 6a_{D_4} + 6a_{C_{4v}} + 6a_{C_{4h}} \\ +6a_{D_{2d}} + 6a_{D'_{2d}} + 6a_{D_{2h}} + 6a_{D'_{2h}} + 4a_T + 4a_{D_{3d}} + 3a_{D_{4h}} + 2a_O + 2a_{T_h} + 2a_{T_d} + a_{O_h} \end{pmatrix} = \binom{8}{q} \quad (26)$$

$$N_{C_2} = \begin{pmatrix} 8a_{C_2} + 4a_{C_4} + 4a_{S_4} + 12a_{D_2} + 4a_{D'_2} + 4a_{C_{2v}} + 4a_{C'_{2v}} + 4a_{C_{2h}} + 6a_{D_4} + 2a_{C_{4v}} \\ +2a_{C_{4h}} + 6a_{D_{2d}} + 2a_{D'_{2d}} + 6a_{D_{2h}} + 2a_{D'_{2h}} + 4a_T + 3a_{D_{4h}} + 2a_O + 2a_{T_h} + 2a_{T_d} + a_{O_h} \end{pmatrix} = \binom{4}{\frac{q}{2}} \quad (27)$$

$$N_{C'_2} = 4a_{C'_2} + 4a_{D'_2} + 2a_{C''_{2v}} + 2a_{C'_{2h}} + 4a_{D_3} + 2a_{D_4} + 2a_{D'_{2d}} + 2a_{D'_{2h}} + 2a_{D_{3d}} + a_{D_{4h}} + 2a_O + a_{O_h} = \binom{4}{\frac{q}{2}} \quad (28)$$

$$N_{\sigma_h} = 8a_{C_s} + 8a_{C_{2v}} + 4a_{C''_{2v}} + 4a_{C_{2h}} + 4a_{C_{4v}} + 2a_{C_{4h}} + 4a_{D'_{2d}} + 6a_{D_{2h}} + 2a_{D'_{2h}} + 3a_{D_{4h}} + 2a_{T_h} + a_{O_h} = \binom{4}{\frac{q}{2}} \quad (29)$$

$$N_{\sigma_d} = 4a_{C'_s} + 4a_{C'_{2v}} + 2a_{C''_{2v}} + 2a_{C'_{2h}} + 4a_{C_{3v}} + 2a_{C_{4v}} + 2a_{D_{2d}} + 2a_{D'_{2h}} + 2a_{D_{3d}} + a_{D_{4h}} + 2a_{T_d} + a_{O_h} = \sum_{\alpha=0}^{4} \binom{4}{\alpha} \binom{2}{\frac{q-\alpha}{2}} \quad (30)$$

$$N_i = 24a_{C_i} + 12a_{C_{2h}} + 12a_{C'_{2h}} + 8a_{C_{3i}} + 6a_{C_{4h}} + 6a_{D_{2h}} + 6a_{D'_{2h}} + 4a_{D_{3d}} + 3a_{D_{4h}} + 2a_{T_h} + a_{O_h} = \binom{4}{\frac{q}{2}} \quad (31)$$

$$N_{C_3} = 4a_{C_3} + 2a_{D_3} + 2a_{C_{3v}} + 2a_{C_{3i}} + 4a_T + a_{D_{3d}} + 2a_O + 2a_{T_h} + 2a_{T_d} + a_{O_h} = \sum_{\beta=0}^{2} \binom{2}{\beta} \binom{2}{\frac{q-\beta}{3}} \quad (32)$$

$$N_{C_4} = 4a_{C_4} + 2a_{D_4} + 2a_{C_{4v}} + 2a_{C_{4h}} + a_{D_{4h}} + 2a_O + a_{O_h} = \binom{2}{\frac{q}{4}} \quad (33)$$

$$N_{S_4,q} = 4a_{S_4} + 2a_{C_{4h}} + 2a_{D_{2d}} + 2a_{D'_{2d}} + a_{D_{4h}} + 2a_{T_d} + a_{O_h} = N_{S_4,q} = \binom{2}{\frac{q}{4}} \quad (34)$$

$$N_{S_6} = 2a_{C_{3i}} + a_{D_{3d}} + 2a_{T_h} + a_{O_h} = \sum_{\lambda=0}^{1} \binom{1}{\lambda} \binom{1}{\frac{q-2\lambda}{6}} \quad (35)$$

The integer values N_{gi} and a_{G_j} satisfy the conditions $N_{gi,q} = N_{gi,8-q}$ and $a_{G_j,q} = a_{G_j,8-q}$ due to the complementarity of the degrees of homosubstitution q and $8-q$.

For heterosubstituted cubane derivatives $C_8H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ and cubane hetero hetero-analogues $(CH)_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$:

$$N_E = \begin{pmatrix} 48a_{C_1} + 24a_{C_2} + 24a_{C'_2} + 24a_{C_s} + 24a_{C'_s} + 24a_{C_i} + 16a_{C_3} + 12a_{C_4} + 12a_{S_4} + 12a_{D_2} + 12a_{D'_2} \\ +12a_{C_{2v}} + 12a_{C'_{2v}} + 12a_{C''_{2v}} + 12a_{C_{2h}} + 12a_{C'_{2h}} + 8a_{D_3} + 8a_{C_{3v}} + 8a_{C_{3i}} + 6a_{D_4} + 6a_{C_{4v}} + 6a_{C_{4h}} \\ +6a_{D_{2d}} + 6a_{D'_{2d}} + 6a_{D_{2h}} + 6a_{D'_{2h}} + 4a_T + 4a_{D_{3d}} + 3a_{D_{4h}} + 2a_O + 2a_{T_h} + 2a_{T_d} + a_{O_h} \end{pmatrix} = \begin{pmatrix} 8 \\ q_0, ..., q_i, ...q_k \end{pmatrix} \tag{36}$$

$$N_{C_2} = \begin{pmatrix} 8a_{C_2} + 4a_{C_4} + 4a_{S_4} + 12a_{D_2} + 4a_{D'_2} + 4a_{C_{2v}} + 4a_{C'_{2v}} + 4a_{C_{2h}} + 6a_{D_4} + 2a_{C_{4v}} \\ +2a_{C_{4h}} + 6a_{D_{2d}} + 2a_{D'_{2d}} + 6a_{D_{2h}} + 2a_{D'_{2h}} + 4a_T + 3a_{D_{4h}} + 2a_O + 2a_{T_h} + 2a_{T_d} + a_{O_h} \end{pmatrix} = \begin{pmatrix} 4 \\ \frac{q_0}{2}, ..., \frac{q_i}{2}, ... \frac{q_k}{2} \end{pmatrix} \tag{37}$$

$$N_{C'_2} = 4a_{C'_2} + 4a_{D'_2} + 2a_{C''_{2v}} + 2a_{C'_{2h}} + 4a_{D_3} + 2a_{D_4} + 2a_{D'_{2d}} + 2a_{D'_{2h}} + 2a_{D_{3d}} + a_{D_{4h}} + 2a_O + a_{O_h} = \begin{pmatrix} 4 \\ \frac{q_0}{2}, ..., \frac{q_i}{2}, ... \frac{q_k}{2} \end{pmatrix} \tag{38}$$

$$N_{\sigma_h} = 8a_{C_s} + 8a_{C_{2v}} + 4a_{C''_{2v}} + 4a_{C_{2h}} + 4a_{C_{4v}} + 2a_{C_{4h}} + 4a_{D'_{2d}} + 6a_{D_{2h}} + 2a_{D'_{2h}} + 3a_{D_{4h}} + 2a_{T_h} + a_{O_h} = \begin{pmatrix} 4 \\ \frac{q_0}{2}, ..., \frac{q_i}{2}, ... \frac{q_k}{2} \end{pmatrix} \tag{39}$$

$$N_{\sigma_d} = 4a_{C'_s} + 4a_{C'_{2v}} + 2a_{C''_{2v}} + 2a_{C'_{2h}} + 4a_{C_{3v}} + 2a_{C_{4v}} + 2a_{D_{2d}} + 2a_{D'_{2h}} + 2a_{D_{3d}} + a_{D_{4h}} + 2a_{T_d} + a_{O_h} = \sum_{\lambda_2} \begin{pmatrix} 4 \\ p'_0, ..., p'_i, ..., p'_k \end{pmatrix} \begin{pmatrix} 2 \\ q''_0, ..., q''_i, ..., q''_k \end{pmatrix} \tag{40}$$

$$N_i = 24a_{C_i} + 12a_{C_{2h}} + 12a_{C'_{2h}} + 8a_{C_{3i}} + 6a_{C_{4h}} + 6a_{D_{2h}} + 6a_{D'_{2h}} + 4a_{D_{3d}} + 3a_{D_{4h}} + 2a_{T_h} + a_{O_h} = \begin{pmatrix} 4 \\ \frac{q_0}{2}, ..., \frac{q_i}{2}, ... \frac{q_k}{2} \end{pmatrix} \tag{41}$$

$$N_{C_3} = 4a_{C_3} + 2a_{D_3} + 2a_{C_{3v}} + 2a_{C_{3i}} + 4a_T + a_{D_{3d}} + 2a_O + 2a_{T_h} + 2a_{T_d} + a_{O_h} = \sum_{\lambda_1} \begin{pmatrix} 2 \\ p_0, ..., p_i, ..., p_k \end{pmatrix} \begin{pmatrix} 2 \\ q'_0, ..., q'_i, ..., q'_k \end{pmatrix} \tag{42}$$

$$N_{C_4} = 4a_{C_4} + 2a_{D_4} + 2a_{C_{4v}} + 2a_{C_{4h}} + a_{D_{4h}} + 2a_O + a_{O_h} = \begin{pmatrix} 2 \\ \frac{q_0}{4}, ..., \frac{q_i}{4}, ... \frac{q_k}{4} \end{pmatrix} \tag{43}$$

$$N_{S_4} = 4a_{S_4} + 2a_{C_{4h}} + 2a_{D_{2d}} + 2a_{D'_{2d}} + a_{D_{4h}} + 2a_{T_d} + a_{O_h} = N_{S_4,q} = \begin{pmatrix} 2 \\ \frac{q_0}{4}, ..., \frac{q_i}{4}, ... \frac{q_k}{4} \end{pmatrix} \tag{44}$$

$$N_{S_6} = 2a_{C_{3i}} + a_{D_{3d}} + 2a_{T_h} + a_{O_h} = \sum_{\lambda_3} \begin{pmatrix} 1 \\ p''_0, ..., p''_i, ..., p''_k \end{pmatrix} \begin{pmatrix} 1 \\ q'''_0, ..., q'''_i, ..., q'''_k \end{pmatrix} \tag{45}$$

The selection rules for forbidden and allowed G_j symmetries are applied to find numerical values of the indeterminates $a_{G_j,MX} \geq 0$.

1- If $N_{g_i,MX} = 0$, the numbers $a_{G_j,MX}$ in such equation are nil $a_{G_j,MX} = 0$. Such nil values in the *IICV*(MX) indicate G_j symmetries (in subscript) forbidden to the molecular system MX.

2-If $N_{g_i,MX} > 0$ positive integers $a_{G_j,MX} > 0$ indicate the number of stereoisomers assigned to the symmetries G_j (in subscript) occurring for a molecular system MX.

For the sake of comparison, the $a_{G_j,MX}$ values of this pattern inventory satisfy eq.46 where C_{ho} and C_{he} are the coefficients of Polya's generating functions of types $f\left(x^q,MX\right)=\sum_{q=0}^{8}C_{ho}x^q$

and $f\left(x^{q_1},...,y^{q_i},...,z^{q_k};MX\right)=\sum_{q_1,...,q_i,...,q_k} \mathrm{C_{he}}x^{q_1}...y^{q_i}...z^{q_k}$ for homo and hetero-polysubstituted cubanes (MX) respectively:

$$\overbrace{\sum_{G_j} a_{G_j,MX}}^{\text{Denumerant}} = \overbrace{A_{c,MX}+A_{ac,MX}}^{\text{Bipartite enumeration}} = \begin{cases} C_{ho} \\ C_{he} \end{cases} \tag{46}$$

Note that for O_h group acting on a molecular skeleton MX the partition of the numbers $A_{ac,MX}$ of chiral and $A_{c,MX}$ of achiral cubane derivatives MX calculated from eqs.47-49 for bipartite enumeration reported in part I of this study are respectively expressed in this part II as sum total of $a_{G_j^c}$ the numbers of MX stereoisomers having chiral G_j^c-symmetries eq.48 and sum total of $a_{G_j^{ac}}$ the numbers of MX stereoisomers having achiral G_j^{ac}-symmetries eq.50:

$$A_{c,MX}=\frac{1}{48}\left(N_E+3N_{C_2}+6N_{C_2'}+8N_{C_3}+6N_{C_4}\right)-\left(N_i+6N_{S_4}+8N_{S_6}+3N_{\sigma_h}+6N_{\sigma_d}\right) \tag{47}$$

$$A_{c,MX}=\sum_{G_j^c} a_{G_j^c,MX}=\begin{pmatrix} a_{C_1}+a_{C_2}+a_{C_2'}+a_{C_3}+a_{C_4}+a_{D_2} \\ +a_{D_2'}+8a_{D_3}+a_{D_4}+a_T+2a_O \end{pmatrix} \tag{48}$$

$$A_{ac,MX}=\frac{1}{24}\left[N_i+6N_{S_4}+8N_{S_6}+3N_{\sigma_h}+6N_{\sigma_d}\right] \tag{49}$$

$$A_{ac,MX}=\sum_{G_j^{ac}} a_{G_j^{ac},MX}=\begin{pmatrix} a_{C_s}+a_{C_s'}+a_{C_i}+a_{S_4}+a_{C_{2v}}+a_{C_{2v}'}+a_{C_{2v}''}+a_{C_{2h}}+a_{C_{2h}'}+a_{C_{3v}}+a_{C_{3i}} \\ +a_{C_{4v}}+a_{C_{4h}}+a_{D_{2d}}+a_{D_{2d}'}+a_{D_{2h}}+a_{D_{2h}'}+a_{D_{3d}}+a_{D_{4h}}+a_{T_h}+a_{T_d}+a_{O_h} \end{pmatrix} \tag{50}$$

5 Applications to itemized enumeration of substituted cubane derivatives and cubane heteroanalogues

Example 1: Let us apply the Sylvester denumerants of O_h symmetry to itemized enumeration of homosubstituted cubane derivatives $C_8H_{8-q}X_q$ and cubane homo hetero-analogues

$(CH)_{8\text{-}q}X_q$ where $0\leq q\leq 8$. By applying eqs.11-19 and 26-35 with the selection rules one derives:

For $q=0,$

$$N_{E,0}=\binom{8}{0}=1,\; N_{C_2}=N_{C_2'}=N_i=N_{\sigma_h}=\binom{4}{0}=1$$

$$N_{C_3,0}=\binom{2}{0}\binom{2}{0}=1,\; N_{C_4}=N_{S_4}=\binom{2}{0}=1,\; N_{S_6}=\binom{1}{0}\binom{1}{0}=1\;\; N_{\sigma_d}=\binom{4}{0}\binom{2}{0}=1$$

$$N_E=N_{C_2}=N_{C_2'}=N_i=N_{C_3}=N_{C_4}=N_{\sigma_h}=N_{S_4}=N_{S_6}=N_{\sigma_d}=a_{O_h}=1$$

$$PCV(C_8H_8)=(1,1,1,1,1,1,1,1,1,1)$$

$$IICV(C_8H_8)=(0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1)$$

This trivial result predicts the occurrence of one cubane skeleton of O_h symmetry. The other subgroups of O_h are forbidden.

For q=1,7, $N_{C_2}=N_{C_2'}=N_{C_4}=N_i=N_{\sigma_h}=N_{S_4}=N_{S_6}=0$

$$N_E=8a_{C_{3v}}=\binom{8}{1}=8;\;\; N_{\sigma_d}=4a_{C_{3v}}=\binom{4}{1}\binom{2}{0}=4;\; N_{C_3}=2a_{C_{3v}}=\binom{2}{1}\binom{2}{0}=2;\;\; a_{C_{3v}}=1$$

$$PCV(C_8H_7X)=(8,0,0,2,0,0,0,0,0,4)$$

$$IICV(C_8H_7X)=(0,0,0,0,0,\; 0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)$$

For $q=2,\;\; ,N_{C_4,2}=0, N_{S_4,2}=0,$

$$N_E=12a_{C_{2v}}+12a_{C_{2v}'}+12a_{C_{2v}''}+4a_{D_{3d}}=\binom{8}{2}=28,\; N_{C_2,2}=4a_{C_{2v}}+4a_{C_{2v}'}=\binom{4}{1}=4,\; N_{C_2',2}=2a_{C_{2v}'}+2a_{D_{3d}}=\binom{4}{1}=4$$

$$N_{C_3}=a_{D_{3d}}+2a_{C_{3v}}=\binom{2}{2}\binom{2}{0}=1,\; N_{i,2}=4a_{D_{3d}}=\binom{4}{1}=4,\; N_{\sigma_h,2}=4a_{C_{2v}''}=\binom{4}{1}=4$$

$$N_{S_6}=a_{D_{3d}}=\binom{1}{1}\binom{1}{0}=1$$

$$PCV(C_8H_6X_2)=(28,4,4,1,0,4,0,1,4,8)$$

$a_{D_{3d}}=a_{C_{2v}'}=a_{C_{2v}''}=1$ the other symmetries are forbidden.

$$IICV(C_8H_6X_2)=(0,0,0,0,0,\; 0,0,0,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0)$$

For $q=3,\ N_{C_2}=N_{C_2'}=N_{C_4}=N_{S_4}=N_{\boldsymbol{i}}=N_{S_6}=N_{\sigma_{\boldsymbol{h}}}=0$

$$\left.\begin{aligned} &N_{E,2}=24a_{C_s'}+8a_{C_{3v}}=\binom{8}{2}=56\ ,\ N_{C_3,2}=2a_{C_{3v}}=\binom{2}{0}\binom{2}{1}=2\\ &N_{\sigma_{\boldsymbol{d}},3}=4a_{C_{3v}}+4a_{C_s'}=\binom{4}{1}\binom{2}{1}+\binom{4}{3}\binom{2}{0}=12 \end{aligned}\right\} a_{C_s'}=2\quad a_{C_{3v}}=1;$$

$$PCV\left(C_8H_5X_3\right)=\left(56,0,0,2,0,0,0,0,0,12\right)$$

$$IICV\left(C_8H_5X_3\right)=\left(0,0,0,0,2,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0\right)$$

For $q=4,\ N_{S_6}=0\Rightarrow a_{S_6}=0$

$$\boldsymbol{N}_E=24a_{C_2'}+24a_{C_s'}+8a_{C_{3v}}+6a_{C_{4v}}+6a_{D_{2h}'}+2a_{T_d}=\binom{8}{4}=70$$

$$\boldsymbol{N}_{C_2}=2a_{C_{4v}}+2a_{D_{2h}'}+2a_{T_d}=\binom{4}{2}=6,\ \boldsymbol{N}_{C_2',4}=4a_{C_2'}+2a_{D_{2h}'}=\binom{4}{2}=6$$

$$\boldsymbol{N}_{C_3}=2a_{C_{3v}}+2a_{T_d}=\binom{2}{1}\binom{2}{1}=4,\ \ \boldsymbol{N}_{C_4,4}=2a_{C_{4v}}=\binom{2}{1}=2$$

$$\boldsymbol{N}_i=6a_{D_{2h}'}=\binom{4}{2}=6,\quad \boldsymbol{N}_{\boldsymbol{S}_4,4}=2a_{T_d}=\binom{2}{1}\binom{2}{0}=2,\ \boldsymbol{N}_{\sigma_h,4}=4a_{C_{4v}}+a_{D_{2h}'}=\binom{4}{2}=6$$

$$\boldsymbol{N}_{\sigma_d}=4a_{C_s'}+4a_{C_{3v}}+2a_{C_{4v}}+2a_{D_{2h}'}+2a_{T_d}=\binom{4}{0}\binom{2}{2}+\binom{4}{2}\binom{2}{1}+\binom{4}{4}\binom{2}{0}=14,$$

$a_{C_2'}=a_{C_s'}=a_{C_{3v}}=a_{C_{4v}}=a_{D_{2h}'}=a_{T_d}=1$ the other symmetries are forbidden

$$PCV\left(C_8H_4X_4\right)=\left(70,6,6,4,2,6,2,0,6,14\right)$$

$$IICV\left(C_8H_4X_4\right)=\left(0,0,1,0,1,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,1,0,0,0,0,1,0,0,0,0,0,1,0\right)$$

Integer numbers $N_{gi,q}$ and $a_{G_j,q}$ permuting their degrees of substitution *q* and *8-q* satisfy the conditions:

$N_{gi,q}=N_{gi,8\text{-}q}$ and $a_{G_j,q}=a_{G_j,8\text{-}q}$ for the series $C_8H_{8\text{-}q}X_q$ and $C_8H_qX_{8\text{-}q}$ (51)

These equalities are used to compute the components of $IICV(C_8H_{8\text{-}q}X_q)$ and $PCV(C_8H_{8\text{-}q}X_q)$ in the range $0\le q\le 8$. The collection of PCVs and IICVs calculated in this range generates the permutomers count matrix $PCM(C_8H_{8\text{-}q}X_q)$ and the itemized isomers count matrix $IICM(C_8H_{8\text{-}q}X_q)$ which satisfy the generalized dot product:

$$IICM\left[MX\right]_{q=0}^{q=8} \times W_{O_h} = PCM\left[MX\right]_{q=0}^{q=8} \qquad (52)$$

explicitely written in eq.52 which summarizes the results of the symmetry adapted enumeration of homosubstituted cubanes $C_8H_{8\text{-}q}X_q$ and cubane homo hetero-analogues $(CH)_{8\text{-}q}X_q$.

$IICM(C_8H_{8\text{-}q}X_q)$

n,n-q	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
0,8	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	1
1,7	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
2,6	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
3,5	0	0	0	2	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
4,4	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	1	0	0	0	0	0	0	1	0

×

W_{O_h}

SSG_{O_h}	E	$3C_2$	$6C'_2$	$8C_3$	$6C_4$	*i*	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$
C_1	48	0	0	0	0	0	0	0	0	0
C_2	24	8	0	0	0	0	0	0	0	0
C'_2	24	0	4	0	0	0	0	0	0	0
C_s	24	0	0	0	0	0	0	0	8	0
C'_s	24	0	0	0	0	0	0	0	0	4
C_i	24	0	0	0	0	24	0	0	0	0
C_3	16	0	0	4	0	0	0	0	0	0
C_4	12	4	0	0	4	0	0	0	0	0
S_4	12	4	0	0	0	0	4	0	0	0
D_2	12	12	0	0	0	0	0	0	0	0
D'_2	12	4	4	0	0	0	0	0	0	0
C_{2v}	12	4	0	0	0	0	0	0	8	0
C'_{2v}	12	4	0	0	0	0	0	0	0	4
C''_{2v}	12	0	2	0	0	0	0	0	4	2
C_{2h}	12	4	0	0	0	12	0	0	4	0
C'_{2h}	12	0	2	0	0	12	0	0	0	2
D_3	8	0	4	2	0	0	0	0	0	0
C_{3v}	8	0	0	2	0	0	0	0	0	4
C_{3i}	8	0	0	2	0	8	0	2	0	0
D_4	6	6	2	0	2	0	0	0	0	0
C_{4v}	6	2	0	0	2	0	0	0	4	2
C_{4h}	6	2	0	0	2	6	2	0	2	0
D_{2d}	6	6	0	0	0	0	2	0	0	2
D'_{2d}	6	2	2	0	0	0	2	0	4	0
D_{2h}	6	6	0	0	0	6	0	0	6	0
D'_{2h}	6	2	2	0	0	6	0	0	2	2
T	4	4	0	4	0	0	0	0	0	0
D_{3d}	4	0	2	1	0	4	0	1	0	2
D_{4h}	3	3	1	0	1	3	1	0	3	1
O	2	2	2	2	2	0	0	0	0	0
T_h	2	2	0	2	0	2	0	2	2	0
T_d	2	2	0	2	0	0	2	0	0	2
O_h	1	1	1	1	1	1	1	1	1	1

(52)

=

$PCM(C_8H_{8\text{-}q}X_q)$

$q, n-q$	N_E	N_{C_2}	$N_{C_2'}$	N_{C_3}	N_{C_4}	N_i	N_{S_4}	N_{S_6}	N_{σ_h}	N_{σ_d}
0,8	1	1	1	1	1	1	1	1	1	1
1,7	8	0	0	2	0	0	0	0	0	4
2,6	28	4	4	1	0	4	0	1	4	8
3,5	56	0	0	2	0	0	0	0	0	12
4,4	70	6	6	4	2	6	2	0	6	14

N_{gi} and a_{G_j} values reported in the PCM and the ICM predict: one C_{3v}- stereoisomer for mono- and hepta-substituted cubane derivatives C_8H_7X, C_8HX_7; $D_{3d}+C_{2v}'+C_{2v}''$-stereoisomers for di- and hexa-substituted cubane derivatives; $C_8H_6X_2$, $C_8H_2X_6$; $C_{3v}+2C_s'-$ stereoisomers for $C_8H_5X_3, C_8H_3X_5$ then $C_2'+C_s'+C_{3v}+C_{4v}+D_{2h}'+T_d-$isomers for tetra-homosubstituted cubane derivatives $C_8H_4X_4$. Similar enumerations are found in the series of cubane homo hetero-analogues $(CH)_{8-q}X_q$. These results summarized in table 2 and illustrated in fig.1 are in agreement with the data $C_{ho} = A_c + A_{ac}$ (eq.46) obtained in part I.

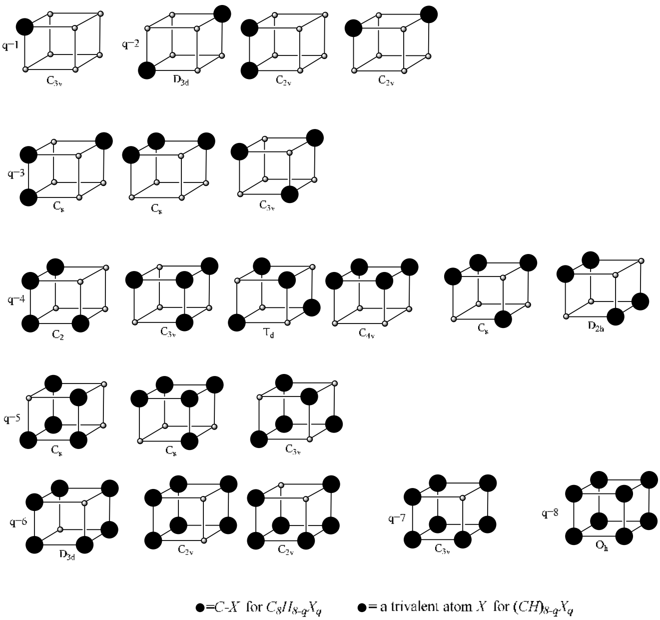

Figure 1. Graphs of 21 possible homosubstituted cubane derivatives $C_8H_{8-q}X_q$ and cubane homo hetero-analogues $(CH)_{8-q}X_q$.

Table 2. Numbers of stereoisomers and symmetries predicted for homosubstituted cubane derivatives ($C_8H_{8-q}X_q$) and cubane homo hetero-analogues ($C_8H_{8-q}X_q$).

q		$(CH)_{8-q}X_q$	A_c	A_{ac}	C_{ho}	*Occurring Symmetries*
0	C_8H_8	$(CH)_8$	0	1	1	O_h
1	C_8H_7X	$(CH)_7X$	0	1	1	C_{3V}
2	$C_8H_6X_2$	$(CH)_6X_2$	0	3	3	$D_{3d}+2C_{2v}$
3	$C_8H_5X_3$	$(CH)_5X_3$	0	3	3	$2C_s+C_{3v}$
4	$C_8H_4X_4$	$(CH)_4X_4$	1	5	6	$C_2+C_s+C_{3v}+C_{4v}+D_{2h}+T_d$
5	$C_8H_3X_5$	$(CH)_3X_5$	0	3	3	$2C_s+C_{3v}$
6	$C_8H_2X_6$	$(CH)_2X_6$	0	3	3	$D_{3d}+2C_{2v}$
7	C_8HX_7	$(CH)X_7$	0	1	1	C_{3V}
8	C_8X_8	X_8	0	1	1	O_h

Example 2: Denumerants of O_h group for symmetry adapted enumeration of di, tri, tetra,penta,hexa and hepta hetero-polysubstituted cubane derivatives and their corresponding hetero hetero-analogues given in table 3.

Table 3. Molecular formula of di, tri, tetra, penta, hexa and hepta hetero-polysubstituted cubane derivatives $C_8H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ and cubane hetero hetero-analogues $(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$

*k	$C_8H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}/(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$	k	$C_8H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}/(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$
2	C_8H_6XY /$(CH)_6XY$	4	$C_8H_2X_2W_2YZ$/$(CH)_2X_2W_2YZ$
	$C_8H_5X_2Y$/ $CH)_5X_2Y$		C_8H_4XWYZ /$(CH)_4XWYZ$
	$C_8H_4X_2Y_2$/ $(CH)_4X_2Y_2$		$C_8H_3X_2WYZ$ / $(CH)_3X_2WYZ$
3	$C_8H_3X_2Y_2Z$/ $(CH)_3X_2Y_2Z$	5	$C_8H_2X_2UWYZ$ /$(CH)_2X_2UWYZ$
	C_8H_5XYZ/ $CH)_5XYZ$	6	$C_8H_2XPUWYZ$/ $(CH)_2XPUWYZ$
		7	$C_8HXSPUWYZ$ / $(CH)XSPUWYZ$

**k=number of achiral substituents of different kinds.*

To solve this problem for each compound aforementioned we use the appropriate values $q_0,\dots q_i,\dots,q_k$ and compatible pairs of integer sequences $(\beta_0,\dots,\beta_i,\dots,\beta_k)\leftrightarrow(q'_0,\dots,q'_i,\dots,q'_k)$, $(\alpha_0,\dots,\alpha_i,\dots,\alpha_k)\leftrightarrow(q''_0,\dots,q''_i,\dots,q''_k)$ and

$(\lambda_0,\dots,\lambda_i,\dots,\lambda_k)\leftrightarrow(q'''_0,\dots,q'''_i,\dots,q'''_k)$

given in table 3 of part I.

For C_8H_6XY , $(q_0,q_1,q_2)=(6,1,1)$, $k=2$, we derive from eqs.15-24 the N_{gi} distinct arrangements of achiral substituents X and Y as follows:

$$\left.\begin{array}{l} N_E = 48a_{C_1} + 24a_{C'_s} + 8a_{C_{3v}} = \binom{8}{6,1,1} = 56 \\ N_{C_3} = 2a_{C_{3v}} = \binom{2}{0,1,1}\binom{2}{2,0,0} = 2 \\ N_{\sigma_d} = 4a_{C'_s} + 4a_{C_{3v}} = \binom{4}{2,1,1}\binom{2}{2,0,0} = 12 \end{array}\right\} \Rightarrow a_{C_1} = 0,\ a_{C'_s} = 2,\ a_{C_{3v}} = 1,$$

$N_{C_2} = N_{C'_2} = N_{C_4} = N_i = N_{S_4} = N_{S_6} = N_{\sigma_h} = 0$ and their a_{G_j} values are nil.

In accordance with the selection rules the symmetries forbidden to C_8H_6XY are:

$$G_j = \left(\begin{array}{l} C_1, C_2, C'_2, C_s, C_i, C_3, C_4, S_4, D_2, D'_2, C_{2v}, C'_{2v}, C''_{2v}, C_{2h}, C'_{2h}, D_3, \\ C_{3i}, D_4, C_{4v}, C_{4h}, D_{2d}, D'_{2d}, D_{2h}, D'_{2h}, T, D_{3d}, D_{4h}, O, T_h, T_d, O_h \end{array}\right)$$

while $G_j = (C'_s, C_{3v})$ are allowed symmetries

$$PCV(C_8H_6XY) = (56,0,0,2,0,0,0,0,0,12)$$

$$IICV(C_8H_6XY) = (0,0,0,0,2,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)$$

For $C_8H_5X_2Y, (q_0,q_1,q_2) = (5,2,1)$, $k=2$,

$$N_E = 48a_{C_1} + 24a_{C'_s} = \binom{8}{5,2,1} = 168$$

$$N_{C_2} = N_{C'_2} = N_{C_3} = N_{C_4} = N_i = N_{S_4} = N_{S_6} = N_{\sigma_h} = 0$$

$$N_{\sigma_d} = 4a_{C'_s} = \binom{4}{1,2,1}\binom{2}{2,0,0} + \binom{4}{3,0,1}\binom{2}{1,1,0} = 20$$

$$PCV(C_8H_5X_2Y) = (168,0,0,0,0,0,0,0,0,20)$$

$a_{C_1} = 1,\ a_{C'_s} = 5$. Hence C_1 and C'_s are allowed the other symmetries are forbidden.

$$IICV(C_8H_5X_2Y) = (1,0,0,0,5,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)$$

For $C_8H_4X_2Y_2, (q_0,q_1,q_2) = (4,2,2)$, $k=2$,

$$N_E = 48a_{C_1} + 24a_{C'_2} + 24a_{C_s} + 24a_{C'_s} + 12a_{C'_{2v}} + 12a_{C''_{2v}} + 12a_{C'_{2h}} = \binom{8}{5,2,1} = 420$$

$$N_{C_2} = 4a_{C'_{2v}} = \binom{4}{2,1,1} = 12$$

$$N_{C'_2} = 4a_{C'_2} + 2a_{C''_{2v}} + 2a_{C_{2h}} = \binom{4}{2,1,1} = 12$$

$$N_i = 12a_{C'_{2h}} = \binom{4}{2,1,1} = 12$$

$$N_{\sigma_h} = 8a_{C_s} + 4a_{C''_{2v}} = \binom{4}{2,1,1} = 12$$

$$N_{\sigma_d} = 4a_{C'_s} + 4a_{C'_{2v}} + 2a_{C''_{2v}} + 2a_{C'_{2h}} = \left.\begin{matrix} \binom{4}{4,0,0}\binom{2}{0,1,1} + \binom{4}{2,2,0}\binom{2}{1,0,1} \\ \binom{4}{2,0,2}\binom{2}{1,1,0} + \binom{4}{0,2,2}\binom{2}{2,0,0} \end{matrix}\right\} = 32$$

$$N_{C_3} = N_{C_4} = N_{S_4} = N_{S_6} = 0$$

$$PCV\left(C_8H_4X_2Y_2\right) = \left(420, 12, 12, 0, 0, 12, 0, 0, 12, 32\right)$$

$a_{C_1} = 4,\ a_{C_2} = 2, a_{C_s} = 1,\ a_{C'_s} = 4,\ a_{C'_{2v}} = 3,\ a_{C''_{2v}} = 1, a_{C'_{2h}} = 1,$ the other symmetries are forbidden.

$$IICV\left(C_8H_4X_2Y_2\right) = \left(4,0,2,1,4,0,0,0,0,0,0,0,3,1,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0\right)$$

For C_8H_5XYZ , $(q_0, q_1, q_2, q_3) = 5,1,1,1$, $k=3$, the pairs of 4-tuples $\left(p_0, p_1, p_2, p_3 \leftrightarrow q'_0, q'_1, q'_2, q'_3\right)$ and $\left(p''_0, p''_1, p''_2, p''_3, \leftrightarrow q'''_0, q'''_1, q'''_2, q'''_3\right)$ are incompatible with the restrictions (7) and (11) and we compute from eq.9:

$p'_0, p'_1, p'_2, p'_3 = (1,1,1,1)$, $\quad q''_0, q''_1, q''_2, q''_3 = (2,0,0,0)$ then,

$$N_E = 48a_{C_1} + 24a_{C'_s} = \binom{8}{5,1,1,1} = 336\,,$$

$$N_{C_2} = N_{C'_2} = N_{C_3} = N_{C_4} = N_i = N_{S_4} = N_{S_6} = N_{\sigma_h} = 0$$

$$N_{\sigma_d} = 4a_{C'_s} = \binom{4}{1,1,1,1}\binom{2}{2,0,0,0} = 24$$

$$PCV\left(C_8H_5XYZ\right) = \left(336, 0, 0, 0, 0, 0, 0, 0, 0, 24\right)$$

$a_{C_1} = 4,\ a_{C'_s} = 6$. Hence C'_s and C_1-symmetries are allowed for C_8H_5XYZ the others are forbidden.

$$IICV\left(C_8H_5XYZ\right) = \left(4,0,0,0,6,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0\right)$$

For $C_8H_4XWYZ / (CH)_4XWYZ, k=4$, $q_0, q_1, q_2, q_3, q_4 = 4,1,1,1,1$, compatible pairs of integer sequences $(\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4) \leftrightarrow (q''_0, q''_1, q''_2, q''_3, q''_4) = (0,1,1,1,1) \leftrightarrow (2,0,0,0,0)$ then we compute:

$$N_E = 48a_{C_1} + 24a_{C'_s} = \binom{8}{4,1,1,1,1} = 1680$$

$$N_{\sigma_d} = 4a_{C'_s} = \binom{4}{0,1,1,1,1}\binom{2}{2,0,0,0,0} = 24$$

$$N_{C_2} = N_{C'_2} = N_{C_3} = N_{C_4} = N_i = N_{\sigma_h} = N_{S_4} = N_{S_6} = 0$$

$a_{C_1} = 32$, $a_{C'_s} = 6$ for allowed symmetries the others are forbidden.

$$PCV(C_8H_4XYWZ) = (1680, 0, 0, 0, 0, 0, 0, 0, 0, 24)$$

$$IICV(C_8H_4XYWZ) = (32, 0, 0, 0, 6, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

For $C_8H_3X_2WYZ$ and $(CH)_3X_2WYZ$, $k=4$, $q_0, q_1, q_2, q_3, q_4 = 3,2,1,1,1$, compatible pairs of integer sequences $(\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4) \leftrightarrow (q''_0, q''_1, q''_2, q''_3, q''_4) = (1,0,1,1,1) \leftrightarrow (1,1,0,0,0)$; then we compute:

$$N_E = 48a_{C_1} + 24a_{C'_s} = \binom{8}{3,2,1,1,1} = 3360$$

$$N_{\sigma_d} = 4a_{C'_s} = \binom{4}{1,0,1,1,1}\binom{2}{1,1,0,0,0} = 48$$

$$N_{C_2} = N_{C'_2} = N_{C_3} = N_{C_4} = N_i = N_{\sigma_h} = N_{S_4} = N_{S_6} = 0$$

$a_{C_1} = 64$, $a_{C'_s} = 12$ for allowed symmetries the others are forbidden.

$$PCV(C_8H_3X_2YWZ) = (3360, 0, 0, 0, 0, 0, 0, 0, 0, 48)$$

$$IICV(C_8H_3X_2YWZ) = (64, 0, 0, 0, 12, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

For $C_8H_2X_2W_2YZ$ and $(CH)_2X_2W_2YZ$, $k=4$, $q_0, q_1, q_2, q_3, q_4 = 2,2,2,1,1$, compatible pairs of integer sequences are $(\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4) \leftrightarrow$

$(q''_0, q''_1, q''_2, q''_3, q''_4) = (2,0,0,1,1) \leftrightarrow (0,1,1,0,0)$,

$(0,0,2,1,1) \leftrightarrow (1,1,0,0,0)$, $(0,2,0,1,1) \leftrightarrow (1,0,1,0,0)$ then we compute:

$$N_E = 48a_{C_1} + 24a_{C_s'} = \binom{8}{2,2,2,1,1} = 5040$$

$$N_{\sigma_d} = 4a_{C_s'} = \left[\binom{4}{2,0,0,1,1}\binom{2}{0,1,1,0,0} + \binom{4}{0,2,0,1,1}\binom{2}{1,0,1,0,0} + \binom{4}{0,0,2,1,1}\binom{2}{1,1,0,0,0}\right] = 72$$

$$N_{C_2} = N_{C_2'} = N_{C_3} = N_{C_4} = N_i = N_{\sigma_h} = N_{S_4} = N_{S_6} = 0$$

$a_{C_1} = 96,\ a_{C_s'} = 18$ for allowed symmetries the others are forbidden.

$$PCV(C_8H_2X_2W_2YZ) = (5040, 0, 0, 0, 0, 0, 0, 0, 0, 72)$$

$$IICV(C_8H_2X_2W_2YZ) = (96, 0, 0, 0, 18, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

For $C_8H_2X_2UWYZ/(CH)_2X_2UWYZ$, $k=5, q_0, q_1, q_2, q_3, q_4, q_5 = 2,2,1,1,1,1$ there is no compatible pairs of integer sequences $(\beta_0,...,\beta_i,...,\beta_k) \leftrightarrow (q_0',...,q_i',...,q_k')$, $(\alpha_0,...,\alpha_i,...,\alpha_k) \leftrightarrow (q_0'',...,q_i'',...,q_k'')$ and $(\lambda_0,...,\lambda_i,...,\lambda_k) \leftrightarrow (q_0''',...,q_i''',...,q_k''')$ then we compute

$$N_E = 48a_{C_1} = \binom{8}{2,2,1,1,1,1} = 10080$$

$$N_{C_2} = N_{C_2'} = N_{C_3} = N_{C_4} = N_i = N_{\sigma_h} = N_{S_4} = N_{S_6} = N_{\sigma_d} = 0$$

$a_{C_1} = 210$ only C_1 is the allowed symmetry the others are forbidden.

$$PCV(C_8H_2X_2UWYZ) = (10080, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

$$IICV(C_8H_2X_2UWYZ) = (210, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

For $C_8H_2XPUWYZ/(CH)_2XPUWYZ$, $k=6, q_0, q_1, q_2, q_3, q_4, q_5, q_6 = 2,1,1,1,1,1,1$ there is no compatible pairs of integer sequences $(\beta_0,...,\beta_i,...,\beta_k) \leftrightarrow (q_0',...,q_i',...,q_k')$, $(\alpha_0,...,\alpha_i,...,\alpha_k) \leftrightarrow (q_0'',...,q_i'',...,q_k'')$ and $(\lambda_0,...,\lambda_i,...,\lambda_k)$ $(q_0''',...,q_i''',...,q_k''')$ then we compute:

$$N_E = 48a_{C_1} = \binom{8}{2,1,1,1,1,1,1} = 20160$$

$$N_{C_2} = N_{C_2'} = N_{C_3} = N_{C_4} = N_i = N_{\sigma_h} = N_{S_4} = N_{S_6} = N_{\sigma_d} = 0$$

$a_{C_1} = 420$ only C_1 is the allowed symmetry the others are forbidden.

$$PCV\left(C_8H_2XPUWYZ\right) = \left(20160, 0, 0, 0, 0, 0, 0, 0, 0, 0\right)$$

$$IICV\left(C_8H_2XPUWYZ\right) = \left(420, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0\right)$$

For $C_8HXSPUWYZ / (CH)XSPUWYZ, k=7, q_0, q_1, q_2, q_3, q_4, q_5, q_6, q_7 = 1,1,1,1,1,1,1,1$ there is no compatible pairs of integer sequences $(\beta_0,...,\beta_i,...,\beta_k) \leftrightarrow (q'_0,...,q'_i,...,q'_k)$, $(\alpha_0,...,\alpha_i,...,\alpha_k) \leftrightarrow (q''_0,...,q''_i,...,q''_k)$ and $(\lambda_0,...,\lambda_i,...,\lambda_k) \leftrightarrow (q'''_0,...,q'''_i,...,q'''_k)$ then we compute :

$$N_E = 48a_{C_1} = \binom{8}{1,1,1,1,1,1,1,1} = 40320$$

$$N_{C_2} = N_{C'_2} = N_{C_3} = N_{C_4} = N_i = N_{\sigma_h} = N_{S_4} = N_{S_6} = N_{\sigma_d} = 0$$

$a_{C_1} = 840$ only C_1 is the allowed symmetry the others are forbidden.

$$PCV\left(C_8HXSPUWYZ\right) = \left(40320, 0, 0, 0, 0, 0, 0, 0, 0, 0\right)$$

$$IICV\left(C_8HXSPUWYZ\right) = \left(840, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0\right)$$

These calculations agree with the entries of the generalized dot product given in eq.52. The sum of occurring symmetries obtained from the denumerants method and summarized in column 7 of table 3 matches up with the isomers numbers $C_{he} = A_c + A_{ac}$ predicted in part I of this study. Some molecular graphs are given in fig.2 for illustration.

Table 4. Numbers of stereoisomers and symmetries predicted for some heteropolysubstituted cubane derivatives $C_8H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ and cubane hetero hetero-analogues $(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$.

$q_0,...,q_i,...,q_7$	$C_8H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$	$(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$	A_c	A_{ac}	C_{he}	*Occurring Symmetries*
6,1,1	C_8H_6XY	$(CH)_6XY$	*0*	*3*	*3*	$C_{3v} + 2C'_s$
5,2,1	$C_8H_5X_2Y$	$(CH)_5X_2Y$	*1*	*5*	*6*	$C_1 + 5C'_s$
5,1,1,1	C_8H_5XYZ	$(CH)_5XYZ$	*4*	*6*	*10*	$4C_1 + 6C'_s$
4,2,2	$C_8H_4X_2Y_2$	$(CH)_4X_2Y_2$	*6*	*10*	*16*	$4C_1 + 2C'_2 + 4C'_s + C_s + 3C'_{2v} + C''_{2v} + C_{2h}$
3,2,2,1	$C_8H_3X_2Y_2Z$	$(CH)_3X_2Y_2Z$	*28*	*14*	*42*	$28C_1 + 14C'_s$
4,1,1,1,1	C_8H_4XWYZ	$(CH)_4XWYZ$	*32*	*6*	*38*	$32C_1 + 6C'_s$
3,2,1,1,1	$C_8H_3X_2WYZ$	$(CH)_3X_2WYZ$	*64*	*12*	*76*	$64C_1 + 12C'_s$
2,2,2,1,1	$C_8H_2X_2W_2YZ$	$(CH)_2X_2W_2YZ$	*96*	*18*	*114*	$96C_1 + 18C'_s$
2,2,1,1,1,1	$C_8H_2X_2UWYZ$	$(CH)_2X_2UWYZ$	*210*	*0*	*210*	$210C_1$
2,1,1,1,1,1,1	$C_8H_2XPUWYZ$	$(CH)_2XPUWYZ$	*420*	*0*	*420*	$420C_1$
1,1,1,1,1,1,1,1	$C_8HXSPUWYZ$	$(CH)XSPUWYZ$	*840*	*0*	*840*	$840C_1$

$IICM(C_8Hq_0Xq_1...Yq_i...Zq_k)$

$C_8Hq_0Xq_1...Yq_i...Zq_k$	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
C_8H_6XY	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
$C_8H_5X_2Y$	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
$C_8H_4X_2Y_2$	4	0	2	1	4	0	0	0	0	0	0	0	3	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C_8H_5XYZ	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
C_8H_4XWYZ	32	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$C_8H_3X_2WYZ$	64	0	0	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$C_8H_2X_2W_2YZ$	96	0	0	0	18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$C_8H_2X_2UWYZ$	210	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
$C_8H_2XPUWYZ$	420	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
$C_8HXSPUWYZ$	840	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

×

SSG_{O_h}	E	$3C_2$	$6C'_2$	$8C_3$	$6C_4$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$
C_1	48	0	0	0	0	0	0	0	0	0
C_2	24	8	0	0	0	0	0	0	0	0
C'_2	24	0	4	0	0	0	0	0	0	0
C_s	24	0	0	0	0	0	0	0	8	0
C'_s	24	0	0	0	0	0	0	0	0	4
C_i	24	0	0	0	0	24	0	0	0	0
C_3	16	0	0	4	0	0	0	0	0	0
C_4	12	4	0	0	4	0	0	0	0	0
S_4	12	4	0	0	0	0	4	0	0	0
D_2	12	12	0	0	0	0	0	0	0	0
D'_2	12	4	4	0	0	0	0	0	0	0
C_{2v}	12	4	0	0	0	0	0	0	8	0
C'_{2v}	12	4	0	0	0	0	0	0	0	4
C''_{2v}	12	0	2	0	0	0	0	0	4	2
C_{2h}	12	4	0	0	0	12	0	0	4	0
C'_{2h}	12	0	2	0	0	12	0	0	0	2
D_3	8	0	4	2	0	0	0	0	0	0
C_{3v}	8	0	0	2	0	0	0	0	0	4
C_{3i}	8	0	0	2	0	8	0	2	0	0
D_4	6	6	2	0	2	0	0	0	0	0
C_{4v}	6	2	0	0	2	0	0	0	4	2
C_{4h}	6	2	0	0	2	6	2	0	2	0
D_{2d}	6	6	0	0	0	0	2	0	0	2
D'_{2d}	6	2	2	0	0	0	2	0	4	0
D_{2h}	6	6	0	0	0	6	0	0	6	0
D'_{2h}	6	2	2	0	0	6	0	0	2	2
T	4	4	0	4	0	0	0	0	0	0
D_{3d}	4	0	2	1	0	4	0	1	0	2
D_{4h}	3	3	1	0	1	3	1	0	3	1
O	2	2	2	2	2	0	0	0	0	0
T_h	2	2	0	2	0	2	0	2	2	0
T_d	2	2	0	2	0	0	2	0	0	2
O_h	1	1	1	1	1	1	1	1	1	1

(52)

=

$PCM(C_8Hq_0Xq_1...Yq_i...Zq_k)$

$C_8Hq_0Xq_1...Yq_i...Zq_k$										
C_8H_6XY	56	0	0	2	0	0	0	0	0	12
$C_8H_5X_2Y$	168	0	0	0	0	0	0	0	0	20
$C_8H_4X_2Y_2$	420	12	12	0	0	12	0	0	12	32
C_8H_5XYZ	336	0	0	2	0	0	0	0	0	24
C_8H_4XWYZ	1680	0	0	0	0	0	0	0	0	24
$C_8H_3X_2WYZ$	3360	0	0	0	0	0	0	0	0	48
$C_8H_2X_2W_2YZ$	5040	0	0	0	0	0	0	0	0	72
$C_8H_2X_2UWYZ$	10080	0	0	0	0	0	0	0	0	0
$C_8H_2XPUWYZ$	20160	0	0	0	0	0	0	0	0	0
$C_8HXSPUWYZ$	40320	0	0	0	0	0	0	0	0	0

Eq.52 summarizes N_{gi} and a_{G_j} values computed and collected to form the permutomers count matrix $PCM(C_8H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k})$ and the itemized isomers count matrix $IICM(C_8H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k})$ for heteropolysubstituted cubane derivatives $C_8H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ and their heteroanalogues considered in this study. These results predict: $2C_s' + C_{3v}$-stereoisomers for C_8H_6XY ; $C_1 + 5C_s'$ –stereoisomers for $C_8H_5X_2Y$; $4C_1 + 2C_2'$-chiral and $C_s + 4C_s' + 3C_{2v}'$
$+C_{2v}'' + C_{2h}'$-achiral stereoisomers for $C_8H_4X_2Y_2$ then $4C_1 + 6C_s'$-isomers for C_8H_5XYZ , $32C_1 + 6C_s'$-isomers for C_8H_4XYWZ , $64C_1 + 12C_s'$-isomers for $C_8H_3X_2YWZ$, $96C_1 + 18C_s'$ -isomers for $C_8H_2X_2W_2YZ$, $210, 420, 840 - C_1$-isomers for $C_8H_2X_2UWYZ$, $C_8H_2XPUWYZ$ and $C_8HXSPUWYZ$ respectively. Similar results are found for their corresponding cubane hetero-hetero-analogues series $(CH)_6XY$, $(CH)_5X_2Y$, $(CH)_4X_2Y_2$, $(CH)_5XYZ$, $(CH)_4XYWZ$, $(CH)_3X_2YWZ$,
$(CH)_2X_2W_2YZ$, $(CH)_2X_2UWYZ$, $(CH)_2XPUWYZ$ and $(CH)XSPUWYZ$.

6 Conclusion

A six-steps algorithm including: (1)-the determination of permutations induced by 10 conjugacy classes of symmetry operations of O_h group acting on cubane skeleton; (2)-the transformation of these permutations into generic formulae for deriving ten permutational isomers numbers $N_E, N_{C_2}, N_{C_2'}, N_{C_3}, N_{C_4}, N_i, N_{S_4}, N_{S_6}, N_{\sigma_h}, N_{\sigma_d}$ characterizing series of substituted cubane derivatives; (3)-the determination of 33 non-redundant subgroups of O_h; (4)-the determination of $W_{O_h} = [w_{G_j,g_i}]$ a matrix of 33x10 elements w_{G_j,g_i} called matrix of the weights of the subgroups G_j of O_h calculated with respect to their symmetry operations $g_i \in G_j$;(5)-the construction of ten Sylvester's denumerants of type $N_{g_i} = \sum_{G_j} a_{G_j} w_{G_j,g_i}$ equating these integer numbers as sum of symmetry adapted isomers numbers a_{G_j} scaled by the weights w_{G_j,g_i} of 33 subgroups of $O_{h,}$; (6) -The resolution of this mathematical model of 10 associated partition equations generates row vectors with 33 entries $a_{G_j} \geq 0$ enumerating substituted cubane derivatives or cubane heteroanalogues of given symmetries. The results provide a systematic decomposition of A_c and A_{ac} obtained in part I as sum of $a^{c}_{G_j}$ chiral and $a^{ac}_{G_j}$ achiral symmetry adapted isomers numbers. Such pattern inventories can be used for stereochemical analyses and molecular design.

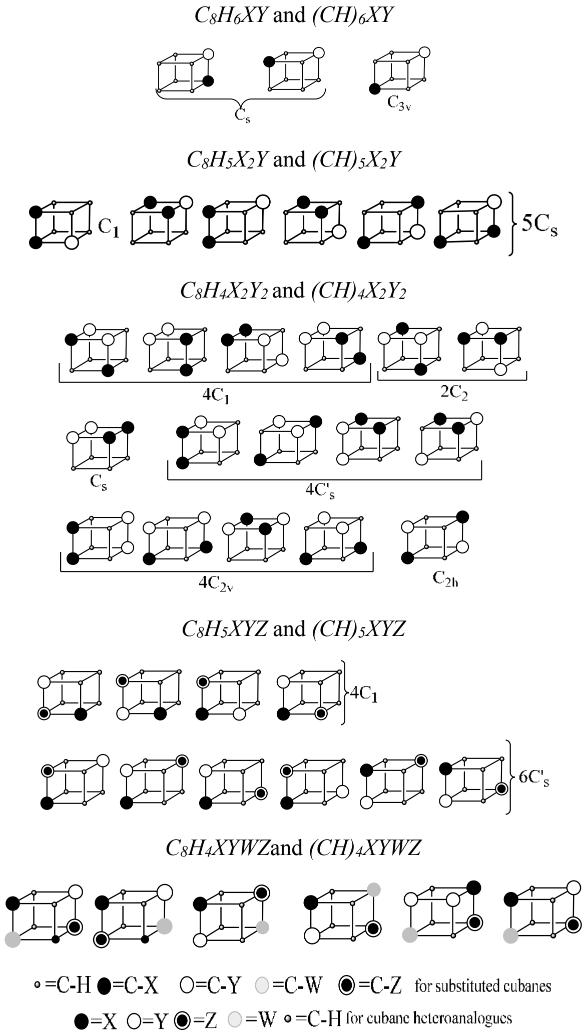

Figure 2. Graphs of di, tri and tetra-heterosubstituted cubane derivatives of types *C_8H_6XY, $C_8H_5X_2Y$, C_8H_5XYZ, $C_8H_4X_2Y_2$, C_8H_4XYWZ* and their corresponding cubane di, tri, and tetra-hetero hetero-analogues *$(CH)_6XY$, $(CH)_5X_2Y$, $(CH)_5XYZ$, $(CH)_4X_2Y_2$, $(CH)_4XYWZ$*.

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