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The Denumerants of Icosahedral Group for Symmetry Itemized Enumeration of Coisomeric Dodecahedrane Derivatives and Heteroanalogues. II.

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Abstract

Integer sequences of permutational isomers numbers (N_{g_ℓ}) issued from placements in distinct ways of achiral substituents among substitution sites of a parent dodecahedrane skeleton are derived under the I_h group action. The construction of eight associated Sylvester's denumerants of type $N_{g_\ell} = \sum_{G_j} a_{G_j} w_{G_j,g_\ell}$ decomposing these numbers as sum of symmetry adapted isomers numbers ($a_{G_1},\dots,a_{G_i},\dots,a_{G_j}$) scaled by the weights w_{G_j,g_ℓ} of the subgroups G_j *of* I_h is used as a novel method for symmetry itemized enumeration of coisomeric substituted DDH derivatives and DDH heteroanalogues.

1 Introduction

The enumeration of dodecahedrane (DDH) skeletons under the I_h group action reported by Fujita are based on Unit Subduced Cycle Indices (USCI) and Restricted Partial Cycle Index (RPCI) methods [1,7] which require like Polya's classical isomers inventories [8,12] the transformation of cycle indices into generating functions expanded with high power series. The application of such complex mathematical procedures to the enumeration of 3D- structures is a dunting problem for chemists. To simplify its solution and in continuation of part I presenting the algorithm for bipartite enumeration of chiral and achiral isomers of DDH derivatives and DDH heteroanalogues we propose in this paper the formulation of Sylvester's denumerants[13,14] of the I_h group and their applications to symmetry itemized enumeration of these compounds. Such an accessible mathematical approach is needed for subsequent stereochemical studies and molecular design of these series of topologically spherical molecules.

2 Classification of coisomeric DDH substituted derivatives and DDH heteroanalogues

Let us consider homogeneous arrangements of substituents among 20 positions of the spherical orbit of DDH as placements in distinct ways of objects of the same kind among a given set of positions and heterogeneous arrangements of substituents as placements in distinct ways of objects of different kinds among a given set of positions. With regard to these characteristics of arrangements of achiral substituents one can divide into 4 groups DDH substituted derivatives and their heteroanalogues as follows:

1- Homosubstituted DDH derivatives $C_{20}H_{20-q}X_q$ are issued from homogeneous arrangements of qX substituents of the same kind among 20 substitution sites of DDH submitted to permutations induced by distinct symmetry operations of I_h.

2- DDH homo hetero-analogues $(CH)_{20-q}X_q$ are issued from homogeneous arrangements putting, in accord with the obligatory minimum valency (OMV) restriction (OMV=3), qX trivalent heteroatoms of the same kind among 20 CH groups permuted by distinct symmetry operations of I_h.

3- Heterosubstituted DDH derivatives $C_{20}H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ are issued from heterogeneous arrangements of q_0H and $q_1X,...,q_iY,...,q_kZ$ substituents of different kinds among 20 tertiary carbon atoms positions permuted by distinct symmetry operations of I_h.

4- DDH hetero hetero-analogues $(CH)_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ are obtained from heterogeneous arrangements putting in accord with the obligatory minimum valency restriction (OMV=3) q_0H and $q_1X,...,q_iY,...,q_kZ$ trivalent heteroatoms of different kinds among 20CH groups permuted by distinct symmetry operations of I_h.

3 Mathematical formulation of symmetry itemized enumeration from the denumerants of I_h group

3.1 Permutations of carbon and hydrogen atoms of DDH under the I_h group action

Let us represent the structure of DDH by a tridimensional hydrogen depleted graph given in fig.1 part I where 20 equivalent black vertices of degree 3 symbolizing 20 carbon atoms indicated by alphabetical labels form a spherical orbit denoted $\boldsymbol{C}_{20} = (a,b,c,d,e,f,g,h,i,j,a',b',c',d',e',f',g',h',i',j')$. The 20 hydrogen atoms (not indicated in the graph) attached to this set of carbon atoms are located on an external spherical orbit H_{20}. This special geometrical feature connecting 20H to 20 interconnected C atoms form a cluster of 20CH groups giving rise to a cage shaped hydrocarbon of I_h symmetry defined by equation 1.

$$I_h = E, 20C_3, 15C_2, 24C_5, i, 20S_6, 24S_{10}, 15\sigma \tag{1}$$

The I_h group action on DDH skeleton consisting to apply 8 distinct classes of symmetry operations $g_\ell \in I_h$ to the spherical orbits $\boldsymbol{H}_{20}$ and $\boldsymbol{C}_{20}$ generate the permutations representations $P^{I_h}\boldsymbol{H}_{20}$ and $P^{I_h}\boldsymbol{C}_{20}$ given in eqs.2-3 :

$$P^{I_h}\boldsymbol{H}_{20} = P^{E}\boldsymbol{H}_{20}, P^{C_2}\boldsymbol{H}_{20}, P^{C_3}\boldsymbol{H}_{20}, P^{C_5}\boldsymbol{H}_{20}, P^{i}\boldsymbol{H}_{20}, P^{S_6}\boldsymbol{H}_{20}, P^{S_{10}}\boldsymbol{H}_{20}, P^{\sigma}\boldsymbol{H}_{20} \tag{2}$$

$$P^{I_h}\boldsymbol{C}_{20} = P^{E}\boldsymbol{C}_{20}, P^{C_2}\boldsymbol{C}_{20}, P^{C_3}\boldsymbol{C}_{20}, P^{C_5}\boldsymbol{C}_{20}, P^{i}\boldsymbol{C}_{20}, P^{S_6}\boldsymbol{C}_{20}, P^{S_{10}}\boldsymbol{C}_{20}, P^{\sigma}\boldsymbol{C}_{20} \tag{3}$$

The right-hand side terms of Eqs. 2 and 3 are distinct types of permutations induced by 8 conjugacy classes of symmetry operations of I_h group. These permutations are written in cycle structure notation as follows:

$$\begin{aligned} &P^{E}\boldsymbol{H}_{20} = 1^{20},\ P^{C_2}\boldsymbol{H}_{20} = 2^{10},\ P^{C_3}\boldsymbol{H}_{20} = 1^2 3^6,\ P^{C_5}\boldsymbol{H}_{20} = 5^4, \\ &P^{i}\boldsymbol{H}_{20} = 2^{10},\ P^{S_6}\boldsymbol{H}_{20} = 2^1 6^3,\ P^{S_{10}}\boldsymbol{H}_{20} = 10^2,\ P^{\sigma}\boldsymbol{H}_{20} = 1^4 2^8 \end{aligned} \tag{4}$$

$$\begin{aligned} &P^{E}\boldsymbol{C}_{20} = 1^{20},\ P^{C_2}\boldsymbol{C}_{20} = 2^{10},\ P^{C_3}\boldsymbol{C}_{20} = 1^2 3^6,\ P^{C_5}\boldsymbol{C}_{20} = 5^4, \\ &P^{i}\boldsymbol{C}_{20} = 2^{10},\ P^{S_6}\boldsymbol{C}_{20} = 2^1 6^3,\ P^{S_{10}}\boldsymbol{C}_{20} = 10^2,\ P^{\sigma}\boldsymbol{C}_{20} = 1^4 2^8 \end{aligned} \tag{5}$$

One may notice that the right-hand side terms of types $P^{g_i}\boldsymbol{C}_{20} \cong P^{g_i}\boldsymbol{H}_{20}$ in eqs.4-5 are equivalent. Therefore $P^{I_h}\boldsymbol{C}_{20}$ and $P^{I_h}\boldsymbol{H}_{20}$ are two sets of congruent permutations written in cycle structure notation as follows:

$$P^{I_h}\boldsymbol{H}_{20} = P^{I_h}\boldsymbol{C}_{20} = \left[1^{20}\right], 20\left[1^2 2^6\right], 15\left[2^{10}\right], 24\left[5^4\right], \left[2^{10}\right], \left[2^1 6^3\right], 24\left[10^2\right], 15\left[1^4 2^8\right] \quad (6)$$

3.2 Determination of permutational isomers numbers for homo-or hetero-polysubstituted DDH derivatives and DDH heteroanalogues.

Let N_{g_ℓ} denote the number of permutomers i.e., the number of arrangements of achiral substituents of the same kind or different kinds among 20 substitution sites of DDH submitted to 8 distinct classes of permutations defined in eq.6. For 8 distinct conjugacy classes of symmetry operations $g_\ell \in I_h$ one obtains an 8 entries row vector of permutomer numbers $\left[N_{g_\ell}\right] = N_E, N_{C_2}, N_{C_3}, N_{C_5}, N_i, N_{S_6}, N_{S_{10}}, N_\sigma$ which are derived in accordance with the placements of achiral substituents of the same kind or different kinds.

Rule 1 : Permutational isomers numbers for homopolysubstituted DDH derivatives $C_{20}H_{20\text{-}q}X_q$ and DDH homo hetero-analogues $(CH)_{20\text{-}q}X_q$ or number of distinct ways of putting q substituents of the same kind among 20 positions submitted to permutation permutations of classes $\ell^{\frac{20}{\ell}}$, $1^2 6^3$, $2^1 6^3$ and $1^4 2^8$ are derived from binomial theorem as follows :

$$1^{20} \rightarrow N_E = \binom{20}{q}, \ \ell = 1 \quad (7)$$

$$2^{10} \rightarrow N_{C_2} = N_i = \binom{10}{\frac{q}{2}}, \ \ell = 2 \quad (8)$$

$$5^4 \rightarrow N_{C_5} = \binom{4}{\frac{q}{5}}, \ \ell = 5 \quad (9)$$

$$10^2 \rightarrow N_{S_{10}} = \binom{2}{\frac{q}{10}}, \ \ell = 10 \quad (10)$$

$$1^4.2^8 \rightarrow N_\sigma = \sum_{\alpha=0}^{4} T(4,\alpha)\, T\left(8, \frac{q-\alpha}{2}\right) = \sum_{\alpha'=0}^{4} \binom{4}{\alpha'} \binom{8}{\frac{q-\alpha'}{2}} \# \quad (11)$$

$$2^1.6^3 \rightarrow N_{S_6} = \sum_{\alpha''=0,1} \binom{1}{\alpha''} \binom{3}{\frac{q-2\alpha''}{6}} \quad (12)$$

$$1^2.3^6 \rightarrow N_{C_3} = \sum_{\alpha=0}^{2} \binom{2}{\alpha} \binom{6}{\frac{q\text{-}\alpha}{3}} \quad (13)$$

Rule 2 : Permutational isomers numbers for heteropolysubstituted DDH derivatives $C_{20}H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ and DDH hetero hetero-analogues $(CH)_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ or numbers of distinct ways of putting q_0H and $q_1X,...,q_iY,...,q_kZ$ achiral substituents of different kinds among 20 positions submitted to permutations of classes $\ell^{\frac{20}{\ell}}$, $1^2 3^6$, $2^1 6^3$ and $1^4 2^8$ are derived from multinomial theorem as follows:

$$1^{20} \rightarrow N_E = \binom{20}{q_0,,,q_i,,,q_k}, \ \ell = 1 \quad (14)$$

$$2^{10} \rightarrow N_{C_2} = N_i = \binom{10}{\frac{q_0}{2},,,\frac{q_i}{2},,,\frac{q_k}{2}}, \quad \ell = 2 \quad (15)$$

$$5^4 \rightarrow N_{C_5} = \binom{4}{\frac{q_0}{5},,,\frac{q_i}{5},,,\frac{q_k}{5}}, \quad \ell = 5 \quad (16)$$

$$10^2 \rightarrow N_{S_{10}} = \binom{2}{\frac{q_0}{10},,,\frac{q_i}{10},,,\frac{q_k}{10},}, \ \ell = 10 \quad (17)$$

$$1^2.3^6 \rightarrow N_{C_3} = \sum_{\lambda} \binom{2}{p'_0,...,p'_i,...,p'_k} \binom{6}{q'_0,...,q'_i,...,q'_k} \quad (18)$$

with the restrictions $\sum_{i=0}^{k} p'_i = 2, \quad \sum_{i=0}^{k} q'_i = 6, \quad q'_i = \frac{q_i - p'_i}{3}$ (19)

$$2^1 6^3 \rightarrow N_{S_6} = \sum_{\lambda} \binom{1}{p'''_0,..., p'''_i,..., p'''_k} \binom{3}{q'''_0,,...,q'''_i,,...,,q'''_k} \quad (20)$$

with the restrictions $\sum_{i=0}^{k} p_i''' = 1, \quad \sum_{i=0}^{k} q_i''' = 3, \quad q_i''' = \frac{q_i - 2p_i'}{6}$ (21)

$$1^4 2^8 \rightarrow N_\sigma = \sum_\lambda \binom{4}{p_0'',\ldots,p_i'',\ldots,p_k''} \binom{8}{q_0'',\ldots,q_i'',\ldots,q_k''} \quad (22)$$

with the restrictions $\sum_{i=0}^{k} p_i'' = 4, \quad \sum_{i=0}^{k} q_i'' = 8, \quad q_i'' = \frac{q_i - p_i''}{3}$ (23)

The N_{g_ℓ} calculated from eqs.7-13 and 14-22 are collected to form the permutomers count vector for MX denoted *:*

$$PCV(MX) = \left(N_E, N_{C_2}, N_{C_3}, N_{C_5}, N_i, N_{S_6}, N_{S_{10}}, N_\sigma\right) \quad (24)$$

where MX= $C_{20}H_{20-q}X_q, (CH)_{20-q}X_q, C_{20}H_{q_0}X_{q_1}\ldots Y_{q_i}\ldots Z_{q_k}$ or $(CH)_{q_0}X_{q_1}\ldots Y_{q_i}\ldots Z_{q_k}$

3.3 The Sylvester's denumerants of the icosahedral group

The combinations of different symmetry operations $g_\ell \in I_h$ given in the right-hand side of eq.1 generate a sequence of subgroups for I_h (SSG_{I_h}) listed in table 1 and summarized in eq.25.

Table 1. Sequence of subgroups of the icosahedral point group I_h.

$C_1 = E$	$C_{2h} = E, C_2, \sigma_v, i$	$C_{5i} = E,\ 4C_5, i, 4S_{10}$
$C_2 = E, C_2$	$C_5 = E, 4C_5$	$T = E, 3C_2, 4C_3^1, 4C_3^2$
$C_s = E, \sigma_v$	$D_3 = E, 3C_2', 2C_3$	$D_{3d} = E, 3C_2', 2C_3, 3\sigma_d, i, 2S_6$
$C_i = E, i$	$C_{3v} = E, 2C_3, 3\sigma_d$	$D_{5d} = E, 5C_2', 4C_5, 5\sigma, i, 4S_{10}$
$C_3 = E, 2C_3$	$C_{3i} = E,\ 2C_3, i, 2S_6$	$T_h = E, 4C_3, 4C_3^2, 3C_2,\ i, 4S_6, 4S_6^5, 3\sigma_h$
$D_2 = E, 3C_2$	$D_{2h} = E, 3C_2, i, 3\sigma_v$	$I = E, 20C_3, 24C_5, 15C_2$
$C_{2v} = E, C_2, 2\sigma_v$	$D_5 = E, 5C_2', 4C_5$	$I_h = E, 20C_3, 24C_5, 15C_2, i, 20S_6, 24S_{10}, 15\sigma$
	$C_{5v} = E, 4C_5, 5\sigma_v$	

$$SSG_{I_h} = \left(C_1, C_2, C_s, C_i, C_3, D_2, C_{2v}, C_{2h}, C_5, D_3, C_{3v}, C_{3i}, D_{2h}, D_5, C_{5v}, C_{5i}, T, D_{3d}, D_{5d}, T_h, I, I_h\right) \quad (25)$$

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

calculated with respect to a symmetry operation $g_\ell \in G_j$ as the quotient of the ratios $\frac{\mu_{g_\ell \in G_j}}{|G_j|}$ and $\frac{\mu_{g_\ell \in I_h}}{|I_h|}$ where $|I_h|$ and $|G_j|$ are the orders of these groups.

$$w_{G_j,g_\ell} = \begin{cases} \frac{\mu_{g_\ell \in G_j}}{\mu_{g_\ell \in I_h}} \times \frac{|I_h|}{|G_j|} & \text{for } g_\ell \in G_j, g_\ell \in I_h, G_j \in SSG_{I_h} \\ 0 \quad for\ g_\ell \notin G_j \end{cases} \tag{26}$$

For 8 distinct conjugacy classes of symmetry operations $g_\ell \in I_h$ and 22 subgroups $G_j \in SSG_{I_h}$ given in table 1 one obtains 176 distinct values w_{G_j,g_ℓ} which are the elements of the matrix of the weights of subgroups for I_h denoted :

$$W_{I_h} = [w_{G_j,g_\ell}] \qquad \text{where} \quad G_j \in SSG_{I_h}, \quad g_\ell \in G_j \text{ and } g_\ell \in I_h \tag{27}$$

The 22 x 8 numerical values of the entries w_{G_j,g_ℓ} of the matrix W_{I_h} given in eq.27' are equivalent to the marks of coset representations of Fujita.[15]

If N_{g_ℓ} permutomers of a DDH derivative (MX) are distributed among the subgroups $G_j \in SSG_{I_h}$ such a partition has 22 indeterminates symmetry adapted isomers numbers a_{G_j} which form an itemized isomer count vector *IICV* for MX denoted:

$$IICV(MX) = \begin{pmatrix} a_{C_1}, a_{C_2}, a_{C_s}, a_{C_i}, a_{C_3}, a_{D_2}, a_{C_{2v}}, a_{C_{2h}}, a_{C_5}, a_{D_3}, a_{C_{3v}}, \\ a_{C_{3i}}, a_{D_{2h}}, a_{D_5}, a_{C_{5v}}, a_{C_{5i}}, a_T, a_{D_{3d}}, a_{D_{5d}}, a_{T_h}, a_I, a_{I_h} \end{pmatrix} \tag{28}$$

The relation between $IICV[MX]$ and $PCV[MX]$ is the dot product: [16-18]

$$IICV[MX] \times W_{I_h} = PCV[MX] \tag{29}$$

explicitly denoted:

$$\overbrace{\left(a_{C_1},a_{C_2},a_{C_s},a_{C_i},a_{C_3},a_{D_2},a_{C_{2v}},a_{C_{2h}},a_{C_5},a_{D_3},a_{C_{3v}},a_{C_{3i}},a_{D_{2h}},a_{D_5},a_{C_{5v}},a_{C_{5i}},a_T,a_{D_{3d}},a_{D_{5d}},a_{T_h},a_I,a_{I_h}\right)}^{IICV[\text{MX}]}$$

$$\times$$

$W_{I_h} =$ (29')

SSG-I_h	E	$15C_2$	$20C_3$	$24C_5$	i	$20S_6$	$24S_{10}$	15σ
C_1	120	0	0	0	0	0	0	0
C_2	60	4	0	0	0	0	0	0
C_s	60	0	0	0	0	0	0	4
C_i	60	0	0	0	60	0	0	0
C_3	40	0	4	0	0	0	0	0
D_2	30	6	0	0	0	0	0	0
C_{2v}	30	2	0	0	0	0	0	4
C_{2h}	30	2	0	0	30	0	0	2
C_5	24	0	0	4	0	0	0	0
D_3	20	4	2	0	0	0	0	0
C_{3v}	20	0	2	0	0	0	0	4
C_{3i}	20	0	2	0	20	2	0	0
D_{2h}	15	3	0	0	15	0	0	3
D_5	12	4	0	2	0	0	0	0
C_{5v}	12	0	0	2	0	0	0	4
C_{5i}	12	0	0	2	12	0	2	0
T	10	2	4	0	0	0	0	0
D_{3d}	10	2	1	0	10	1	0	2
D_{5d}	6	2	0	1	6	0	1	2
T_h	5	1	2	0	5	2	0	1
I	2	2	2	2	0	0	0	0
I_h	1	1	1	1	1	1	1	1

$$=$$

$$\overbrace{\left(N_E,N_{C_2},N_{C_3},N_{C_5},N_i,N_{S_6},N_{S_{10}},N_\sigma\right)}^{PCV[MX]}$$

We replace the N_{g_ℓ} of *PCV*(MX) by their equivalent algebraic expressions given in eqs.7-13 and 14-23. The expansion of eq.29' gives rise to 8 associated partition equations 30-37 and 38-45 called Sylvester's denumerants of permutomers numbers N_{g_ℓ} for I_h-based derivative MX.

For coisomeric series of homopolysubstituted DDH derivatives $C_{20}H_{20\text{-}q}X_q$ and DDH homo hetero-analogues $(CH)_{20\text{-}q}\,X_q$:

$$N_E = \begin{pmatrix} 120a_{C_1} + 60a_{C_2} + 60a_{C_s} + 60a_{C_i} + 40a_{C_3} + 30a_{D_2} + 30a_{C_{2v}} + 30a_{C_{2h}} + 24a_{C_5} + 20a_{D_3} + 20a_{C_{3v}} \\ +20a_{C_{3i}} + 15a_{D_{2h}} + 12a_{D_5} + 12a_{C_{5v}} + 12a_{C_{5i}} + 10a_T + 10a_{D_{3d}} + 6a_{D_{5d}} + 5a_{T_h} + 2a_I + a_{I_h} \end{pmatrix} = \binom{20}{q} \qquad (30)$$

$$N_{C_2} = \begin{pmatrix} 4a_{C_2} + 6a_{D_2} + 2a_{C_{2v}} + 2a_{C_{2h}} + 4a_{D_3} + 3a_{D_{2h}} + 4a_{D_5} + \\ 2a_T + 2a_{D_{3d}} + 2a_{D_{5d}} + a_{T_h} + 2a_I + a_{I_h} \end{pmatrix} = \binom{10}{\frac{q}{2}} \qquad (31)$$

$$N_{C_3} = 4a_{C_3} + +2a_{D_3} + 2a_{C_{3v}} + 2a_{C_{3i}} + 4a_T + a_{D_{3d}} + 2a_{T_h} + 2a_I + a_{I_h} = \sum_{\alpha=0}^{2} \binom{2}{\alpha} \binom{6}{\frac{q\text{-}\alpha}{3}} \qquad (32)$$

$$N_{C_5} = 4a_{C_5} + 2a_{D_5} + 2a_{C_{5v}} + 2a_{C_{5i}} + a_{D_{5d}} + 2a_I + a_{I_h} = \binom{4}{\frac{q}{5}} \qquad (33)$$

$$N_i = 60a_{C_i} + 30a_{C_{2h}} + 20a_{C_{3i}} + 15a_{D_{2h}} + 12a_{C_{5i}} + 10a_{D_{3d}} + 6a_{D_{5d}} + 5a_{T_h} + a_{I_h} = \binom{10}{\frac{q}{2}} \qquad (34)$$

$$N_{S_6} = 2a_{C_{3i}} + a_{D_{3d}} + 2a_{T_h} + a_{I_h} = \sum_{\alpha''=0,1} \binom{1}{\alpha''} \binom{3}{\frac{q-2\alpha''}{6}} \qquad (35)$$

$$N_{S_{10}} = 2a_{C_{5i}} + a_{D_{5d}} + a_{I_h} = \binom{2}{\frac{q}{10}} \qquad (36)$$

$$N_\sigma = 4a_{C_s} + 4a_{C_{2v}} + 2a_{C_{2h}} + 4a_{C_{3v}} + 3a_{D_{2h}} + 4a_{C_{5v}} + 2a_{D_{3d}} + 2a_{D_{5d}} + a_{T_h} + a_{I_h} = \sum_{\alpha'=0}^{4} \binom{4}{\alpha'} \binom{8}{\frac{q\text{-}\alpha'}{2}} \qquad (37)$$

For coisomeric series of heteropolysubstituted DDH derivatives $C_{20}H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ and DDH hetero hetero-analogues $(CH)_{q_0}\,X_{q_1}...Y_{q_i}...Z_{q_k}$:

$$N_E = \begin{pmatrix} 120a_{C_1} + 60a_{C_2} + 60a_{C_s} + 60a_{C_i} + 40a_{C_3} + 30a_{D_2} + 30a_{C_{2v}} + 30a_{C_{2h}} + 24a_{C_5} + 20a_{D_3} + 20a_{C_{3v}} \\ +20a_{C_{3i}} + 15a_{D_{2h}} + 12a_{D_5} + 12a_{C_{5v}} + 12a_{C_{5i}} + 10a_T + 10a_{D_{3d}} + 6a_{D_{5d}} + 5a_{T_h} + 2a_I + a_{I_h} \end{pmatrix} = \binom{20}{q_0,...,q_i,...q_k} \qquad (38)$$

$$N_{C_2} = \begin{pmatrix} 4a_{C_2} + 6a_{D_2} + 2a_{C_{2v}} + 2a_{C_{2h}} + 4a_{D_3} + 3a_{D_{2h}} + 4a_{D_5} + \\ 2a_T + 2a_{D_{3d}} + 2a_{D_{5d}} + a_{T_h} + 2a_I + a_{I_h} \end{pmatrix} = \binom{10}{\frac{q_0}{2},...,\frac{q_i}{2},...\frac{q_k}{2}} \qquad (39)$$

$$N_{C_3} = 4a_{C_3} + +2a_{D_3} + 2a_{C_{3v}} + 2a_{C_{3i}} + 4a_T + a_{D_{3d}} + 2a_{T_h} + 2a_{I_h} + a_{I_h} = \sum_{\lambda} \binom{2}{p'_0,...,p'_i,...,p'_k} \binom{6}{q'_0,...,q'_i,...,q'_k} \qquad (40)$$

$$N_{C_5} = 4a_{C_5} + 2a_{D_5} + 2a_{C_{5v}} + 2a_{C_{5i}} + a_{D_{5d}} + 2a_I + a_{I_h} = \binom{4}{\frac{q_0}{5},...,\frac{q_i}{5},...\frac{q_k}{5}} \qquad (41)$$

$$N_i = 60a_{C_i} + 30a_{C_{2h}} + 20a_{C_{3i}} + 15a_{D_{2h}} + 12a_{C_{5i}} + 10a_{D_{3d}} + 6a_{D_{5d}} + 5a_{T_h} + a_{I_h} = \binom{10}{\frac{q_0}{2},\ldots,\frac{q_i}{2},\ldots\frac{q_k}{2}} \quad (42)$$

$$N_{S_6} = 2a_{C_{3i}} + a_{D_{3d}} + 2a_{T_h} + a_{I_h} = \sum_{\lambda}\binom{1}{p_0''',\ldots,p_i''',\ldots,p_k'''}\binom{3}{q_0''',\ldots,q_i''',\ldots,q_k'''} \quad (43)$$

$$N_{S_{10}} = 2a_{C_{5i}} + a_{D_{5d}} + a_{I_h} = \binom{2}{\frac{q_0}{10},\ldots,\frac{q_i}{10},\ldots,\frac{q_k}{10}} \quad (44)$$

$$N_{\sigma} = 4a_{C_s} + 4a_{C_{2v}} + 2a_{C_{2h}} + 4a_{C_{3v}} + 3a_{D_{2h}} + 4a_{C_{5v}} + 2a_{D_{3d}} + 2a_{D_{5d}} + a_{T_h} + a_{I_h} = \sum_{\lambda}\binom{4}{p_0'',\ldots,p_i'',\ldots,p_k''}\binom{8}{q_0'',\ldots,q_i'',\ldots,q_k''} \quad (45)$$

The integer values N_{g_ℓ} and a_{G_j} satisfy the following conditions : (a)-for permuting degrees of homopolysubstitution *q, 20-q* in the molecular formulas $C_{20}H_{20-q}X_q$ and $C_{20}H_qX_{20-q}$:

$$N_{g_\ell,q} = N_{g_\ell,20-q} \text{ and } a_{G_j,q} = a_{G_j,20-q} \quad (46)$$

(b)-for permuting partial degrees of heteropolysubstitution $(q_0,q_1,\ldots,q_i,\ldots,q_k)$ and $(q_i,q_1,\ldots,q_k,\ldots,q_0)$ in the molecular formulas $C_{20}H_{q_0}X_{q_1}\ldots Y_{q_i}\ldots Z_{q_k}$ and $(CH)_{q_0}X_{q_1}\ldots Y_{q_i}\ldots Z_{q_k}$:

$$N_{g_\ell}(q_0,q_1,\ldots,q_i,\ldots,q_k) = N_{g_\ell}(q_i,q_1,\ldots,q_0,q_k) \text{ and } a_{G_j}(q_0,q_1,\ldots,q_i,\ldots,q_k) = a_{G_j}(q_i,q_1,\ldots,q_0,q_k) \quad (47)$$

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

1- For $N_{g_\ell,MX} = \sum_{G_j} a_{G_j,MX} w_{G_j,g_\ell} = 0$ where $w_{G_j,g_\ell} > 0$, the symmetry itemized isomers numbers $a_{G_j,MX}$ in such equations are nil $a_{G_j,MX} = 0$. These nil values are reported in the *IICV*(MX) to indicate G_j symmetries (in the subscripts) forbidden to the molecular system MX.

2- For $N_{g_\ell,MX} = \sum_{G_j} a_{G_j,MX} w_{G_j,g_\ell} > 0$ where $w_{G_j,g_\ell} > 0$ all positive integers $a_{G_j,MX} > 0$ indicate the numbers of stereoisomers assigned to distinct symmetries G_j (written in the subscripts) which are allowed to the molecular system MX. For the sake of comparison the numbers $A_{c,MX}$ and $A_{ac,MX}$ found from bipartite enumeration (part I of this study) and the set of symmetry itemized isomers numbers $a_{G_j,MX}$ found from this pattern inventory satisfy eq.48-50.

$$A_{c,MX} = \sum_{G_j^c} a_{G_{j,MX}^c} = \left(a_{C_1} + a_{C_2} + a_{C_3} + a_{C_5} + a_{D_2} + a_{D_3} + a_{D_5} + a_T + a_I\right) \quad (48)$$

$$A_{ac,MX} = \sum_{G_j^{ac}} a_{G_j^{ac},MX} = \left(a_{C_s} + a_{C_i} + a_{C_{2v}} + a_{C_{2h}} + a_{C_{3v}} + a_{C_{3i}} + a_{D_{2h}} + a_{C_{5v}} + a_{C_{5i}} + a_{D_{3d}} + a_{D_{5d}} + a_{T_h} + a_{I_h}\right) \quad (49)$$

where $a_{G_j^c} \geq 0$ and $a_{G_j^{ac}} \geq 0$are respectively the numbers of chiral symmetries G_j^c and achiral symmetries G_j^{ac}allowed to a DDH derivative MX. Diastereoisomers numbers $A_{dia,MX}$ for I_h-based molecules MX are obtained from eq.50 and their values match up with Polya's coefficients derived from cycle indices.

$$A_{dia,MX} = A_{c,MX} + A_{ac,MX} = \sum_{G_j^{ac}} a_{G_j^{ac},MX} + \sum_{G_j^{ac}} a_{G_j^{ac},MX} \quad (50)$$

4 Applications to symmetry itemized enumeration of substituted DDH derivatives and DDH heteroanalogues

Example 1: Symmetry itemized enumeration of homosubstituted DDH derivatives $C_{20}H_{20-q}X_q$ and DDH homo hetero-analogues $(CH)_{20-q}X_q$ where $0 \leq q \leq 20$. By applying the Sylvester denumerants given in eqs.30-37 and the selection rules to these series characterized by the complementarity of the degrees of substitution q and $20-q$, one derives the following results:

For $q=0$, $20-q = 20$

$$N_E = \binom{20}{0} = 1,\ N_{C_2} = N_i = \binom{10}{0} = 1,\ N_{C_3} = \binom{2}{0}\binom{6}{0} = 1,\ N_{C_5} = \binom{4}{0},$$

$$N_{S_6} = \binom{1}{0}\binom{3}{0} = 1,\ N_{S_{10}} = \binom{2}{0} = 1\ \ N_{\sigma_d} = \binom{4}{0}\binom{8}{0} = 1$$

$$N_E = N_{C_2} = N_i = N_{C_3} = N_{C_5} = N_{S_6} = N_{S_{106}} = N_\sigma = a_{I_h} = 1$$

$$PCV\left(C_{20}H_{20}\right) = \left(1,1,1,1,1,1,1,1\right)$$

$$IICV\left(C_{20}H_{20}\right) = \left(0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1\right)$$

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

For $q=1$, $20-q =19$

$$N_E = 20a_{C_{3v}} = \binom{20}{1} = 20;\ \ N_\sigma = 4a_{C_{3v}} = \binom{4}{1}\binom{8}{0} = 4$$

$N_{C_3} = 2a_{C_{3v}} = \binom{2}{1}\binom{3}{0} = 2;\ a_{C_{3v}} = 1$ the other symmetries are forbidden.

$N_{C_2} = N_{C_5} = N_i = N_{S_6} = N_{S_{10}} = 0$

$PCV\left(C_{20}H_{19}X\right) = \left(20, 0, 2, 0, 0, 0, 0, 4\right)$

$IICV\left(C_{20}H_{19}X\right) = \left(0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0\right)$

For q=2, 20-q =18

$N_E = 60a_{C_2} + 60a_{C_s} + 30a_{C_{2v}} + 10a_{D_{3d}} = \binom{20}{2} = 190,$

$N_{C_2} = 4a_{C_{2v}} + 2a_{C_{2v}} + 2a_{D_{3d}} = \binom{10}{1} = 10,\ N_{C_3} = \binom{2}{2}\binom{6}{0} = a_{D_{3d}} = 1,$

$N_\sigma = 4a_{C_s} + 4a_{C_{2v}} + 2a_{D_{3d}} = \binom{4}{0}\binom{8}{1} + \binom{4}{2}\binom{8}{0} = 14,\ N_{C_5} = N_{S_6} = N_{S_{10}} = 0$

$N_i = 10a_{D_{3d}} = \binom{10}{1} = 10$

$a_{C_2} = 1,\ a_{C_s} = 1,\ \ a_{C_{2v}} = 2, a_{D_{3d}} = 1$ the other symmetries are forbidden.

$PCV\left(C_{20}H_{18}X_2\right) = \left(190, 10, 1, 0, 10, 0, 0, 14\right)$

$IICV\left(C_{20}H_{18}X_2\right) = \left(0,1,1,0,0,0,2,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0\right)$

For q=3, 20-q=17

$N_E = 120a_{C_1} + 60a_{C_s} + 40a_{C_3} + 20a_{C_{3v}} = \binom{20}{3} = 1140$

$N_{C_3} = 4a_{C_3} + 2a_{C_{3v}} = \binom{2}{0}\binom{6}{1} = 6,$

$N_\sigma = 4a_{C_s} + 4a_{C_{3v}} = \binom{4}{1}\binom{8}{1} + \binom{4}{3}\binom{8}{0} = 36,$

$N_{C_2} = N_{C_i} = N_{C_5} = N_{S_6} = N_{S_{10}} = 0$

$a_{C_1} = 5,\ a_{C_s} = 8,\ a_{C_3} = 1,\ \ a_{C_{3v}} = 1$ the other symmetries are forbidden.

$PCV\left(C_{20}H_{17}X_3\right) = \left(1140, 0, 6, 0, 0, 0, 0, 36\right)$

$IICV\left(C_{20}H_{17}X_3\right) = \left(5,0,8,0,1,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0\right)$

For q=4, 20-q =16

$$N_E = 120a_{C_1} + 60a_{C_2} + 60a_{C_s} + 40a_{C_3} + 30a_{C_{2v}} + 30a_{C_{2h}} + 20a_{C_{3v}} + 15a_{D_{2h}} + 10a_T = \binom{20}{4} = 4845$$

$$N_{C_2} = 4a_{C_2} + 2a_{C_{2v}} + 2a_{C_{2h}} + 3a_{D_{2h}} + 2a_T = \binom{10}{2} = 45,$$

$$N_{C_3} = 4a_{C_3} + 2a_{C_{3v}} + 4a_T = \binom{2}{1}\binom{6}{1} = 12$$

$$N_i = 30a_{C_{2h}} + 15a_{D_{2h}} = \binom{10}{2} = 45,$$

$$N_{S_6} = N_{S_{10}} = N_{C_5} = 0$$

$$N_\sigma = 4a_{C_s} + 4a_{C_{2v}} + 2a_{C_{2h}} + 4a_{C_{3v}} + 3a_{D_{2h}} = \binom{4}{0}\binom{8}{2} + \binom{4}{2}\binom{8}{1} + \binom{4}{4}\binom{8}{0} = 232$$

$a_{C_1} = 28,\ a_{C_2} = 8,\ a_{C_3} = 1,\ a_{C_s} = 13,\ a_{C_{2v}} = 3,\ a_{C_{2h}} = 1,\ a_{C_{3v}} = 2, a_{D_{2h}} = 1,\ a_T = 1$

the other symmetries are forbidden

$PCV(C_{20}H_{16}X_4) = (4845, 45, 12, 0, 45, 0, 0, 77)$

$IICV(C_{20}H_{16}X_4) = (28,8,13,0,1,0,3,1,0,0,2,0,1,0,0,0,1,0,0,0,0,0)$

For $q=5,\ 20-q=15$

$$N_{C_2} = N_{C_i} = N_{C_5} = N_{S_6} = N_{S_{10}} = 0$$

$a_{C_1} = 112,\ a_{C_s} = 33,\ a_{C_3} = 1,\ \ a_{C_{3v}} = 1, a_{C_{5v}} = 2$ the others symmetries are forbidden.

$PCV(C_{20}H_{15}X_5) = (15504,\ 0,\ 6,\ 4,\ 0,\ 0,\ 0,\ 144)$

$ICV(C_{20}H_{15}X_5) = (112,0,33,0,1,0,0,0,0,0,1,0,0,0,2,0,0,0,0,0,0,0)$

For $q=6,\ 20-q=$ 14

$$N_E = 120a_{C_1} + 60a_{C_2} + 60a_{C_s} + 40a_{C_3} + 30a_{C_{2v}} + 30a_{C_{2h}} + 20a_{D_3} + 20a_{C_{3v}} + 20a_{C_{3i}} + 10a_{D_{3d}} = \binom{20}{6} = 38760$$

$$N_{C_2} = 4a_{C_2} + 2a_{C_{2v}} + 2a_{C_{2h}} + 4a_{D_3} + 2a_{D_{3d}} + 2a_T = \binom{10}{3} = 120$$

$$N_{C_3} = 4a_{C_3} + 2a_{D_3} + 2a_{C_{3v}} + 2a_{C_{3i}} + a_{D_{3d}} = \binom{2}{0}\binom{6}{2} = 15$$

$$N_i = 60a_{C_i} + 30a_{C_{2h}} + 20a_{C_{3i}} + 10a_{D_{3d}} = \binom{10}{2} = 120$$

$$N_{S_6} = 2a_{C_{3i}} + a_{D_{3d}} = \binom{1}{0}\binom{3}{1} = 3$$

$$N_{C_5} = N_{S_{10}} = 0$$

$$N_\sigma = 4a_{C_s} + 4a_{C_{2v}} + 2a_{C_{2h}} + 4a_{C_{3v}} + 2a_{D_{3d}} = \binom{4}{0}\binom{8}{3} + \binom{4}{2}\binom{8}{2} + \binom{4}{4}\binom{8}{1} = 232$$

$a_{C_1} = 284$, $a_{C_2} = 23$, $a_{C_3} = 2$, $a_{D_3} = 1$, $a_{C_s} = 47$, $a_{C_{2v}} = 8$, $a_{C_{2h}} = 3$, $a_{C_{3v}} = 1$, $a_{C_{3i}} = 1$, $a_{D_{3d}} = 1$

the other symmetries are forbidden

$$PCV\left(C_{20}H_{14}X_6\right) = \left(38760,\ 120,\ 15,\ 0,\ 120,\ 3,\ 0,\ 232\right)$$

$$IICV\left(C_{20}H_{14}X_6\right) = \left(284, 23, 47, 0, 2, 0, 8, 3, 0, 1, 1, 1, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0\right)$$

For $q=7,\ 20\text{-}q=13$

$$N_E = 120a_{C_1} + 60a_{C_s} + 40a_{C_3} + 30a_{D_2} + 20a_{C_{3v}} = \binom{20}{7} = 77520$$

$$N_{C_3} = 4a_{C_3} + 2a_{C_{3v}} = \binom{2}{1}\binom{6}{2} = 30$$

$$N_\sigma = 4a_{C_s} + 4a_{C_{3v}} = \binom{4}{1}\binom{8}{3} + \binom{4}{3}\binom{8}{2} = 336$$

$$N_{C_2} = N_i = N_{C_5} = N_{S_6} = N_{S_{10}} = 0$$

$a_{C_3} = 6$ $a_{C_{3v}} = 3$ $a_{C_s} = 81$ the others symmetries are forbidden.

$$PCV\left(C_{20}H_{13}X_7\right) = \left(77520,\ 0,\ 30,\ 0,\ 0,\ 0,\ 0,\ 336\right)$$

$$IICV\left(C_{20}H_{13}X_7\right) = \left(603, 0, 81, 0, 6, 0, 0, 0, 0, 0, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0\right)$$

For $q=8,\ 20\text{-}q=12$

$$N_E = 120a_{C_1} + 60a_{C_2} + 60a_{C_s} + 60a_{C_i} + 40a_{C_3} + 30a_{D_2} + 30a_{C_{2v}} + 30a_{C_{2h}}$$
$$+20a_{D_3} + 20a_{C_{3v}} + 15a_{D_{2h}} + 10a_{D_{3d}} + 10_{T_h} = \binom{20}{8} = 125970$$

$$N_{C_2} = 4a_{C_2} + 6a_{D_2} + 2a_{C_{2v}} + 2a_{C_{2h}} + 4a_{D_3} + 3a_{D_{2h}} + 4a_{D_5} + 2a_T + 2a_{D_{3d}} + 2a_{D_{5d}} + a_{T_h} + 2a_I + a_{I_h} = \binom{10}{4} = 210$$

$$N_{C_3} = 4a_{C_3} + 2a_{D_3} + 2a_{C_{3v}} + a_{D_{3d}} + 2a_{T_h} = \binom{2}{2}\binom{6}{2} = 15$$

$$N_i = 60a_{C_i} + 30a_{C_{2h}} + 15a_{D_{2h}} + 10a_{D_{3d}} + 5a_{T_h} = \binom{10}{4} = 210$$

$$N_\sigma = 4a_{C_s} + 4a_{C_{2v}} + 2a_{C_{2h}} + 4a_{C_{3v}} + 3a_{D_{2h}} + 2a_{D_{3d}} + a_{T_h} = \binom{4}{0}\binom{8}{4} + \binom{4}{2}\binom{8}{3} + \binom{4}{4}\binom{8}{2} = 434$$

$$N_{S_6} = a_{D_{3d}} + 2a_{T_h} = \binom{1}{1}\binom{3}{1} = 3,$$

$$N_{S_{10}} = N_{C_5} = 0$$

$a_{C_1} = 975,\quad a_{C_2} = 43,\ a_{C_3} = 2,\ a_{D_2} = 1, a_{C_i} = 2,\ a_{D_3} = 1,\ a_{C_s} = 96, a_{C_{2v}} = 9,\ a_{C_{2h}} = 2,\ a_{C_{3v}} = 1,$

$a_{D_{2h}} = 1,\ a_{D_{3d}} = 1, a_{T_h} = 1$. the other symmetries are forbidden.

$$PCV\left(C_{20}H_{12}X_8\right) = \left(125970,\ 210,\ 15,\ 0,\ 210,\ 3,\ 0,\ 434\right)$$

$$IICV\left(C_{20}H_{12}X_8\right) = \left(975, 43, 96, 2, 2, 1, 9, 2, 0, 1, 1, 0, 1, 0, 0, 0, 0, 1, 0, 1, 0, 0\right)$$

For $q=9,\ 20\text{-}q=11$

$$N_E = 120a_{C_1} + 60a_{C_s} + 40a_{C_3} + 20a_{C_{3v}} = \binom{20}{9} = 167960$$

$$N_{C_3} = 4a_{C_3} + 2a_{C_{3v}} = \binom{2}{0}\binom{6}{3} = 20$$

$$N_\sigma = 4a_{C_s} + 4a_{C_{3v}} = \binom{4}{1}\binom{8}{4} + \binom{4}{3}\binom{8}{3} = 504$$

$$N_{C_2} = N_i = N_{C_5} = N_{S_6} = N_{S_{10}} = 0$$

$a_{C_s} = 124,\quad a_{C_{3v}} = 2,\ a_{C_3} = 4,\ a_{C_1} = 1336$ the other symmetries are forbidden,

$PCV\ (C_{20}H_{11}X_9) = (167960, 0, 20, 0, 0, 0, 0, 504)$

$IICV\ (C_{20}H_{11}X_9) = (1336,0,124,0,4,0,0,0,0,0,2,0,0,0,0,0,0,0,0,0,0,0)$

For $q=10,\ 20\text{-}q=10$

$$N_E = 120a_{C_1} + 60a_{C_2} + 60a_{C_s} + 60a_{C_i} + +40a_{C_3} + 30a_{C_{2v}} + 30a_{C_{2h}} + 20a_{C_{3v}} + 12a_{C_{5v}} + 8a_{D_{5d}} = \binom{20}{10} = 184756$$

$$N_{C_2} = 4a_{C_2} + 2a_{C_{2v}} + 2a_{C_{2h}} + 2a_{D_{5d}} = \binom{10}{5} = 252$$

$$N_{C_3} = 4a_{C_3} + 2a_{C_{3v}} = \binom{2}{1}\binom{6}{3} = 40$$

$$N_i = 60a_{C_i} + 30a_{C_{2h}} + 15a_{D_{2h}} + 12a_{C_{5i}} + 10a_{D_{3d}} + 6a_{D_{5d}} = \binom{10}{5} = 252$$

$$N_{C_5} = 4a_{C_5} + 2a_{D_5} + 2a_{C_{5v}} + 2a_{C_{5i}} + a_{D_{5d}} = \binom{4}{2} = 6$$

$$N_{S_6} = 0$$

$$N_{S_{10}} = 2a_{C_{5i}} + a_{D_{5d}} = \binom{2}{1}, a_{C_{5i}} = 0, \quad a_{D_{5d}} = 2$$

$$N_{\sigma} = 4a_{C_s} + 4a_{C_{2v}} + 2a_{C_{2h}} + 4a_{C_{3v}} + 2a_{D_{5d}} + 4a_{C_{5v}} = \binom{4}{0}\binom{8}{3} + \binom{4}{2}\binom{8}{2} + \binom{4}{4}\binom{8}{1} = 532$$

$$a_{C_1} = 1448, \quad a_{C_2} = 54, \ a_{C_3} = 8, \ a_{C_i} = 2, \ a_{C_s} = 112, \ a_{C_{2v}} = 12, \ a_{C_{2h}} = 4, \ a_{C_{3v}} = 4, \ a_{C_{5d}} = 2, \ a_{C_{5v}} = 2$$

$$PCV(C_{20}H_{10}X_{10}) = (184756, \ 252, \ 40, \ 252, \ 0, \ 2, \ 532)$$

$$IICV(C_{20}H_{10}X_{10}) = (1448, 54, 112, 2, 8, 0, 12, 4, 0, 0, 4, 0, 0, 0, 2, 0, 0, 0, 2, 0, 0, 0)$$

The collection of *PCVs* and *IICVs* calculated in the range $1 \leq q \leq 20$ generates a permutomers count matrix $PCM(MX)$ and an itemized isomer count matrix $IICM(MX)$ which satisfy the generalized dot product:

$$IICM\left[MX\right]_{q=0}^{q=20} \times W_{I_h} = PCM\left[MX\right]_{q=0}^{q=20} \qquad (51)$$

explicitly written in eq.52 which summarizes the results of the symmetry itemized enumeration of homosubstituted DDH and DDH homo hetero-analogues. The 22 entries *IICVs* collected to form the 21 x 22 *IICM* of eq.52 possess the elements $a_{G_j} > 0$ indicating the number of isomers occurring with G_j-allowed symmetries and the elements $a_{G_j} = 0$ indicating distinct types of G_j-forbidden symmetries. As example for $q=2$ and n-q=18 the *IICV*=(0 1 1 0 0 0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 0). These entries aligned in the order of the set of subgroups of I_h given in eq.25 predict the occurrence of C_2 chiral and $C_s+2C_{2v}+D_{3d}$ achiral isomers for the series $C_{20}H_{18}X_2$ and $(CH)_{18}X_2$. The numbers and types of occurring symmetries for distinct coisomeric series of homosubstituted DDH derivatives ($C_{20}H_{20-q}X_q$) and DDH homo hetero-analogues $(CH)_{20-q}X_q$ are summarized in table 2.

$IICM(C_{20}H_{20-q}X_q/(CH)_{20-q}X_q)$

$q,n-q$	C_1	C_2	C_s	C_i	C_3	D_2	C_{2v}	C_{2h}	C_5	D_3	C_{3v}	C_{3i}	D_{2h}	D_5	C_{5v}	C_{5i}	T	D_{3d}	D_{5d}	T_h	I	I_h
0,20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1,19	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
2,18	0	1	1	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
3,17	5	0	8	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
4,16	28	8	13	0	1	0	3	1	0	0	2	0	1	0	0	0	1	0	0	0	0	0
5,15	112	0	33	0	1	0	0	0	0	0	1	0	0	0	2	0	0	0	0	0	0	0
6,14	284	23	47	0	2	0	8	3	0	1	1	1	0	0	0	0	0	1	0	0	0	0
7,13	603	0	81	0	6	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0
8,12	975	43	96	2	2	1	9	2	0	1	1	0	1	0	0	0	0	1	0	1	0	0
9,11	1336	0	124	0	4	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0
10,10	1448	54	112	2	8	0	12	4	0	0	4	0	0	0	2	0	0	0	2	0	0	0

×

SSG-*I_h*	E	15C2	20C3	24C5	***i***	20S6	24S10	15σ
C1	120	0	0	0	0	0	0	0
C2	60	4	0	0	0	0	0	0
Cs	60	0	0	0	0	0	0	4
Ci	60	0	0	0	60	0	0	0
C3	40	0	4	0	0	0	0	0
D2	30	6	0	0	0	0	0	0
C2v	30	2	0	0	0	0	0	4
C2h	30	2	0	0	30	0	0	2
C5	24	0	0	4	0	0	0	0
D3	20	4	2	0	0	0	0	0
C3v	20	0	2	0	0	0	0	4
C3i	20	0	2	0	20	2	0	0
D2h	15	3	0	0	15	0	0	3
D5	12	4	0	2	0	0	0	0
C5v	12	0	0	2	0	0	0	4
C5i	12	0	0	2	12	0	2	0
T	10	2	4	0	0	0	0	0
D3d	10	2	1	0	10	1	0	2
D5d	6	2	0	1	6	0	1	2
Th	5	1	2	0	5	2	0	1
I	2	2	2	2	0	0	0	0
Ih	1	1	1	1	1	1	1	1

(52)

= $PCM(C_{20}H_{20-q}X_q/(CH)_{20-q}X_q)$

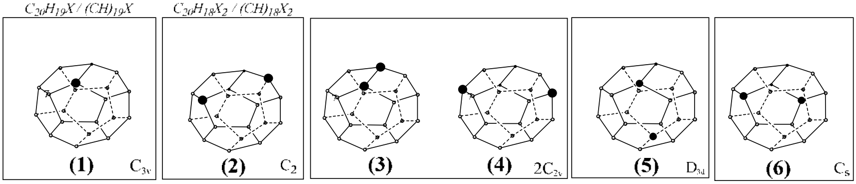
$q,n-q$	N_E	N_{C_2}	N_{C_3}	N_{C_5}	N_i	N_{S_6}	$N_{S_{10}}$	N_σ
0,20	1	1	1	1	1	1	1	1
1,19	20	0	2	0	0	0	0	4
2,18	190	10	1	0	10	0	0	14
3,17	1140	0	6	0	0	0	0	36
4,16	4845	45	12	0	45	0	0	77
5,15	15504	0	6	4	0	0	0	144
6,14	38760	120	15	0	120	3	0	232
7,13	77520	0	30	0	0	0	0	336
8,12	125970	210	15	0	210	3	0	434
8,11	167960	0	20	0	0	0	0	504
10,10	184756	252	40	252	0	2	0	532

Table 2. Numbers of isomers and types of occurring symmetries predicted for homo substituted DDH derivatives($C_{20}H_{20\text{-}q}X_q$) and DDH homo hetero-analogues $(CH)_{20\text{-}q}X_q$.

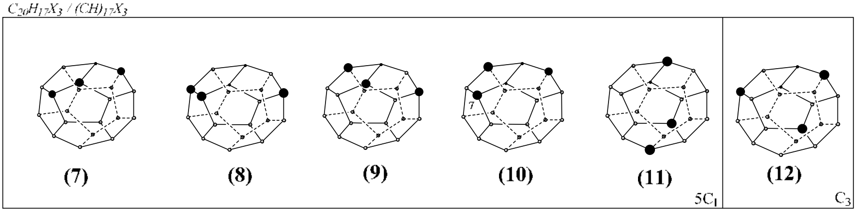
q,n-q	$C_{20}H_{20\text{-}q}X_q$	$(CH)_{20\text{-}q}X_q$	A_c	A_{ac}	A_{dia}	*Occurring Symmetries*
0,20	$C_{20}H_{20}$	$(CH)_{20}$	0	1	1	I_h
1,19	$C_{20}H_{19}X$	$(CH)_{19}X$	0	1	1	C_{3V}
2,18	$C_{20}H_{18}X_2$	$(CH)_{18}X_2$	1	4	5	$C_2+C_s+2C_{2v}+D_{3d}$
3,17	$C_{20}H_{17}X_3$	$(CH)_{17}X_3$	6	9	15	$5C_1+C_3+8C_s+C_{3v}$
4,16	$C_{20}H_{16}X_4$	$(CH)_{16}X_4$	38	20	58	$28C_1+C_2+C_3+T+13C_s+3C_{2v}+C_{2h}+2C_{3v}+D_{2h}$
5,15	$C_{20}H_{15}X_5$	$(CH)_{15}X_5$	113	36	149	$112C_1+C_3+33C_s+C_{3v}+2C_{5v}$
6,14	$C_{20}H_{14}X_6$	$(CH)_{14}X_6$	310	61	371	$284C_1+23C_2+2C_3+D_3+$ $47Cs+8C_{2v}+3C_{2h}+C_{3v}+C_{3i}+D_{3d}$
7,13	$C_{20}H_{13}X_7$	$(CH)_{13}X_7$	609	84	693	$603C_1+6C_s+81C_s+3C_{3v}$
8,12	$C_{20}H_{12}X_8$	$(CH)_{12}X_8$	1022	113	1135	$975C_1+43C_2+2C_3+D_2+D_3$ $+96C_s+2C_i+9C_{2v}+2C_{2h}+C_{3v}+D_{2h}+D_{3d}+T_h$
9,11	$C_{20}H_{11}X_9$	$(CH)_{11}X_9$	1340	126	1466	$1336C_1+4C_3+124C_s+2C_{3v}$
10,10	$C_{20}H_{10}X_{10}$	$(CH)_{10}X_{10}$	1510	138	1648	$1448C_1+54C_2+8C_3+$ $112C_s+2C_i+12C_{2v}+4C_{2h}+4C_{3v}+2C_{5v}+2D_{5d}$

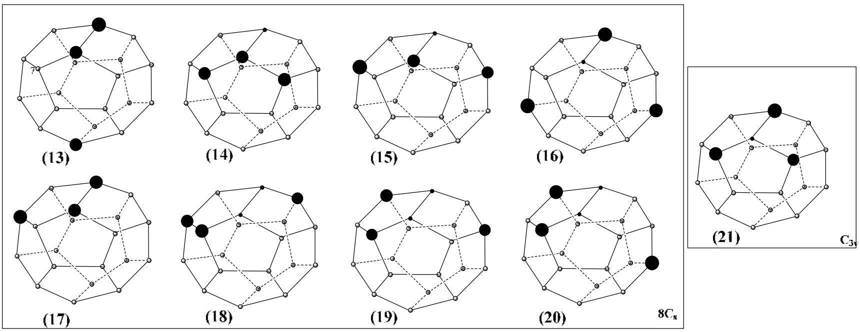
These results predict one C_{3v}-isomer for $C_{20}H_{19}X/(CH)_{19}X$; 5-isomers including one C_2 chiral and $C_s+2C_{2v}+D_{3d}$ achiral isomers for $C_{20}H_{18}X_2/(CH)_{18}X_2$; $5C_1+C_3$ chiral and $8C_s+C_{3v}$ achiral isomers for $C_{20}H_{17}X_3/(CH)_{17}X_3$; then $28C_1+C_2+C_3+T$ chiral and $13C_s+3C_{2v}+C_{2h}+2C_{3v}+D_{2h}$-achiral isomers for $C_{20}H_{16}X_4/(CH)_{16}X_4$; $112C_1+C_3$ chiral and $33C_s+C_{3v}+2C_{5v}$ achiral isomers for $C_{20}H_{15}X_5/(CH)_{15}X_5$; $284C_1+23C_2+2C_3+D_3$ chiral and $47C_s+8C_{2v}+3C_{2h}+C_{3v}+C_{3i}+D_{3d}$ achiral isomers for $C_{20}H_{14}X_6$ $/(CH)_{14}X_6$; $603C_1+6C_3$-chiral and $81C_s+3C_{3v}$ for $C_{20}H_{13}X_7/(CH)_{13}X_7$; $975C_1+43C_2+2C_3+D_2+D_3$ chiral and $96C_s+2C_i+9C_{2v}+2C_{2h}+C_{3v}+D_{2h}+D_{3d}+T_h$ achiral isomers for $C_{20}H_{12}X_8/(CH)_{12}X_8$; $1336C_1+4C_3$ chiral and $124C_s+2C_{3v}$ achiral isomers for $C_{20}H_{11}X_9/(CH)_{11}X_9$; $1448C_1+54C_2+8C_3$ chiral and $112C_s+2C_i+12C_{2v}+4C_{2h}+4C_{3v}+2C_{5v}+2D_{5d}$ achiral isomers for $C_{20}H_{10}X_{10}/(CH)_{10}X_{10}$. The illustrations of these results are depicted in fig.1 by the graphs **1-107** reproducing some selected symmetries occuring with reduced isomers numbers. In this representation the isomers belonging to the same symmetry point group are drawn in one single box with underneath identifying numbers and their figure inventory is given in the lower right corner. We notice for the sake of comparison the following remarks: (1) data in columns 4, 5 and 6 results of bipartite enumeration (given in part I) and those of column 7 obtained from this pattern inventory satisfy equations 48, 49 and 50. (2). We notice that the scalar of the summands of partition equations are similar to the numbers of homopolysubstituted DDH derivatives with achiral substituents predicted by the USCI-methods of Fujita.[7,19]

$C_{20}H_{19}X$ / $(CH)_{19}X$ *$C_{20}H_{18}X_2$ / $(CH)_{18}X_2$*



$C_{20}H_{17}X_3$ / $(CH)_{17}X_3$





$C_{20}H_{16}X_4/(CH)_{16}X_4$

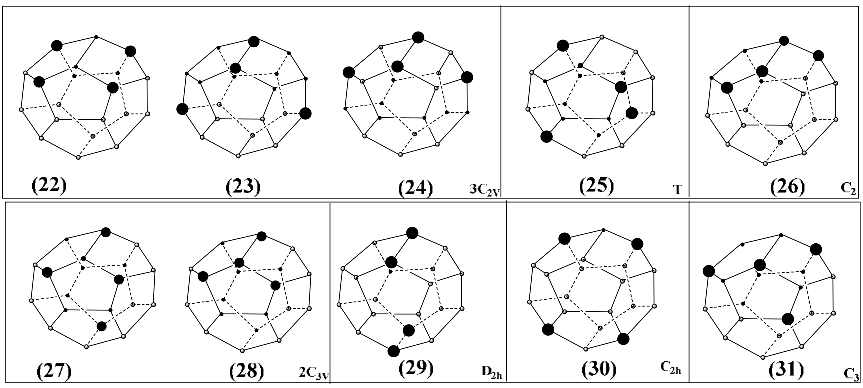
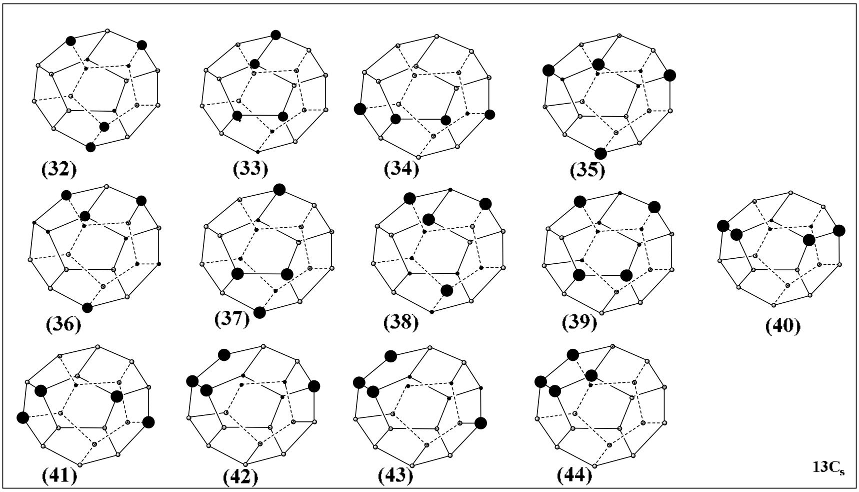
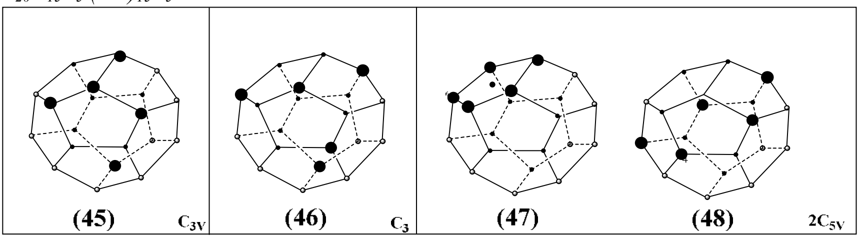


Figure 1 continued

$C_{20}H_{16}X_4/(CH)_{16}X_4$



$C_{20}H_{15}X_5/(CH)_{15}X_5$



$C_{20}H_{14}X_6/(CH)_{14}X_6$

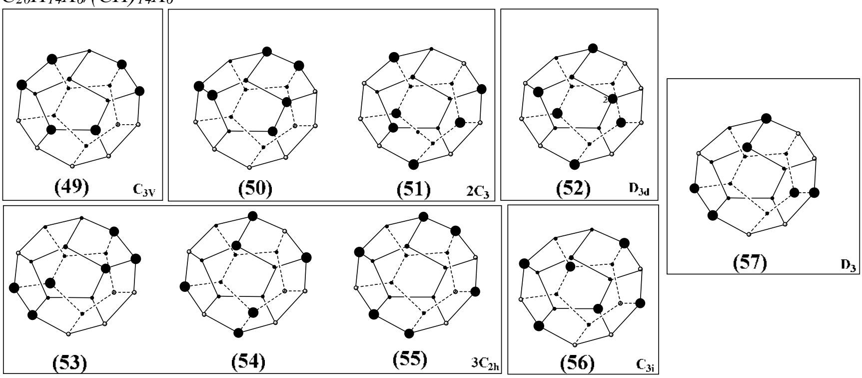
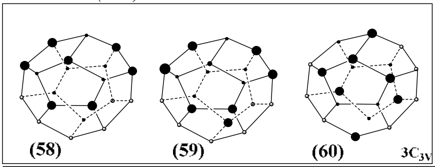
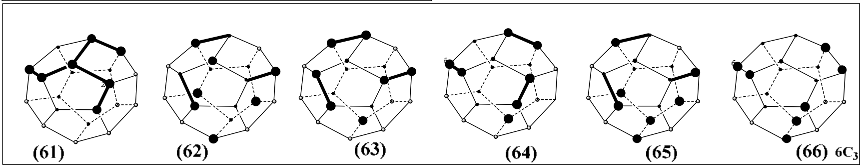


Figure 1 continued

$C_{20}H_{13}X_7$/ $(CH)_{13}X_7$

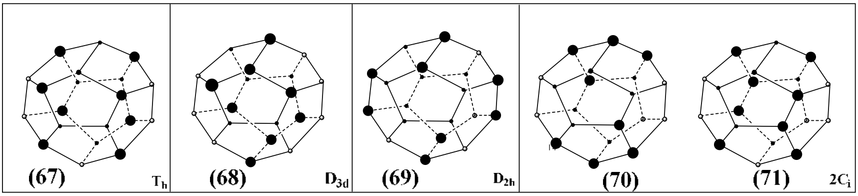


(58) (59) (60) $3C_{3V}$

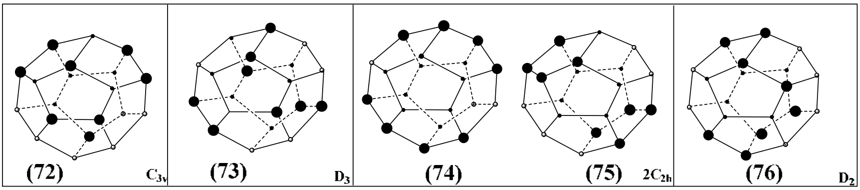


(61) (62) (63) (64) (65) (66) $6C_3$

$C_{20}H_{12}X_8$/ $(CH)_{12}X_8$:

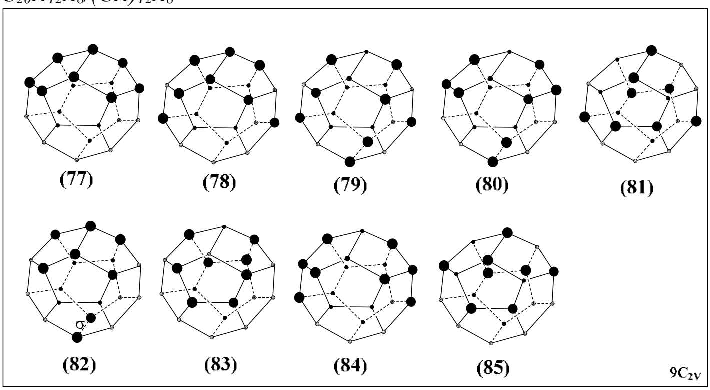


(67) T_h (68) D_{3d} (69) D_{2h} (70) (71) $2C_i$

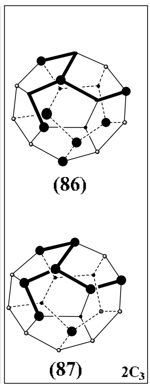


(72) C_{3v} (73) D_3 (74) (75) $2C_{2h}$ (76) D_2

$C_{20}H_{12}X_8$/$(CH)_{12}X_8$



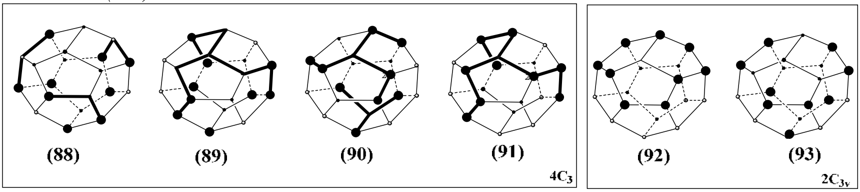
(77) (78) (79) (80) (81) (82) (83) (84) (85) $9C_{2V}$



(86) (87) $2C_3$

Figure 1 continued, end.

$C_{20}H_{11}X_9$ / $(CH)_{11}X_9$:



$C_{20}H_{10}X_{10}$ / $(CH)_{10}X_{10}$

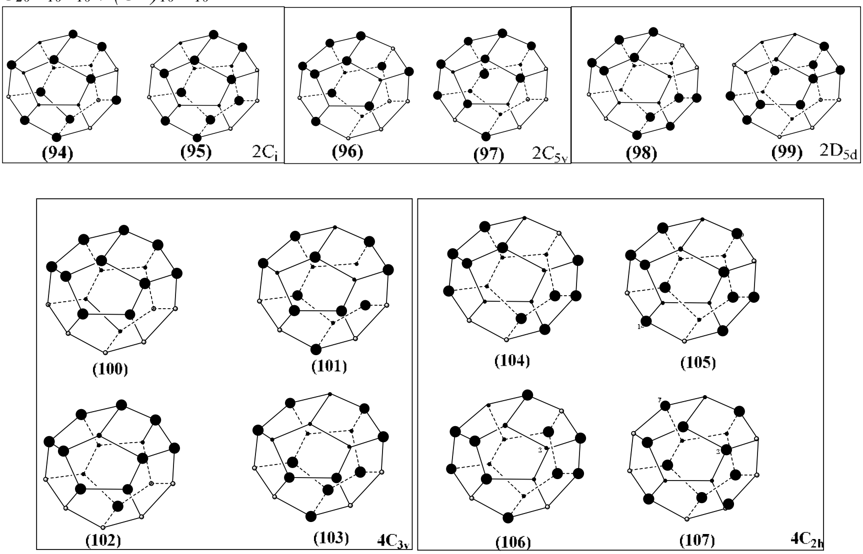


Figure 1. Graphs of homopolysubstituted DDH derivatives $C_{20}H_{20-q}X_q$ and DDH homo-hetero-analogues $(CH)_{20-q}X_q$.

Example 2: Symmetry itemized enumeration of di, tri, tetra, penta, hexa and dodeca-heteropo lysubstituted DDH derivatives $C_{20}H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ and their corresponding hetero hetero-analogues $(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ given in table 3.

Table 3. Molecular formulas of di, tri, tetra, penta, hexa and dodeca-heteropolysubstituted DDH derivatives $C_{20}H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ and their DDH hetero hetero-analogues $(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$

*k	$C_{20}H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}/(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$	k	$C_{20}H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}/(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$
2	$C_{20}H_{18}XY$ / $(CH)_{18}XY$	3	$C_{20}H_{17}XYZ$ / $(CH)_{17}XYZ$
	$C_{20}H_{17}X_2Y$ / $CH)_{17}X_2Y$		$C_{20}H_{16}X_2YZ$ / $(CH)_{16}X_2YZ$
	$C_{20}H_{16}X_3Y$ / $(CH)_{16}X_3Y$		$C_{20}H_{15}X_2Y_2Z$ / $(CH)_{15}X_2YZ$
	$C_{20}H_{16}X_2Y_2$ / $(CH)_{16}X_2Y_2$		$C_{20}H_{15}X_3YZ$ / $(CH)_{15}X_3YZ$
	$C_{20}H_{15}X_3Y_2$ / $(CH)_{15}X_3Y_2$		$C_{20}H_{14}X_3Y_2Z$ / $(CH)_{14}X_3Y_2Z$
	$C_{20}H_{14}X_3Y_3$ / $CH)_{14}X_3Y_3$		$C_{20}H_{14}X_4YZ$ / $(CH)_{14}X_4YZ$
	$C_{20}H_8X_6Y_6$ / $CH)_8X_6Y_6$		

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

To solve the enumeration problem for each DDH derivative MX=$C_{20}H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ or $(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ aforementioned having an integer sequence of partial degrees of heteropolysubstitution $q_0,\dots q_i,\dots,q_k$ we have first to find compatible pairs of integer sequences $(p'_0,...,p'_i,...,p'_k)\leftrightarrow(q'_0,...,q'_i,...,q'_k)$, $(p''_0,...,p''_i,...,p''_k)\leftrightarrow(q''_0,...,q''_i,...,q''_k)$ and $(p'''_0,...,p'''_i,...,p'''_k)$ $\leftrightarrow(q'''_0,...,q'''_i,...,q'''_k)$. Such data given in table 3 of part I are introduced in eqs.38-45 for the computation of symmetry itemized isomers numbers a_{G_j} of MX as follows:

For given $C_{20}H_{18}XY/(CH)_{18}XY$, we note $(q_0,q_1,q_2)=(18,1,1)$,

$(p'_0,p'_1,p'_2)\leftrightarrow(q'_0,q'_1,q'_2)$=(0,1,1)$\leftrightarrow$(6,0,0) and $(p''_0,p''_1,p''_2)\leftrightarrow(q''_0,q''_1,q''_2)$ = (2,1,1)$\leftrightarrow$(8,0,0)

$$\left.\begin{aligned} N_E &= 120a_{C_1}+60a_{C_s}+20a_{C_{3v}} = \binom{20}{18,1,1} = 380 \\ N_{C_3} &= 2a_{C_{3v}} = \binom{2}{0,1,1}\binom{6}{6,0,0} = 2 \\ N_\sigma &= 4a_{C_s}+4a_{C_{3v}} = \binom{4}{2,1,1}\binom{8}{8,0,0} = 12 \end{aligned}\right\}\Rightarrow a_{C_1}=2, a_{C_s}=2,\ a_{C_{3v}}=1,$$

$N_{C_2}=N_{C_5}=N_i=N_{S_{10}}=N_{S_6}=0$ and their a_{G_j} values are nil.

In accordance with the selection rules the symmetries forbidden to $C_{20}H_{18}XY/(CH)_{18}XY$ are:

$G_j = a_{C_2}, a_{C_i}, a_{C_3}, a_{D_2}, a_{C_{2v}}, a_{C_{2h}}, a_{C_5}, a_{D_3}, a_{C_{3i}}, a_{D_{2h}}, a_{D_5}, a_{C_{5v}}, a_{C_{5i}}, a_T, a_{D_{3d}}, a_{D_{5d}}, a_{T_h}, a_I, a_{I_h}$

while $G_j = (C_1, C_s, C_{3v})$ are allowed symmetries.

$PCV(C_{20}H_{18}XY) = (380, 0, 2, 0, 0, 0, 0, 0, 0, 12)$

$IICV(C_{20}H_{18}XY) = (2, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$

For $C_{20}H_{17}X_2Y$ / $(CH)_{17}X_2Y$,

$(q_0, q_1, q_2) = (17,2,1)$, $(p''_0, p''_1, p''_2) \leftrightarrow (q''_0, q''_1, q''_2)$ =(1,2,1)↔(8,0,0), (3,0,1) ↔ (7,1,0) then

$$N_E = 120a_{C_1} + 60a_{C_s} = \binom{20}{17,2,1} = 3420$$

$N_{C_2} = N_{C_3} = N_{C_5} = N_i = N_{S_{10}} = N_{S_6} = 0$ indicate forbidden symmetries.

$$N_\sigma = 4a_{C_s} = \binom{4}{1,2,1}\binom{8}{2,0,0} + \binom{4}{3,0,1}\binom{8}{7,1,0} = 44$$

Then we compute $a_{C_1} = 23,\ a_{C_s} = 11$ allowed symmetries.

$PCV(C_{20}H_{17}X_2Y) = (3420, 0, 0, 0, 0, 0, 0, 44)$

$IICV(C_{20}H_{17}X_2Y) = (23, 0, 11, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$

For $C_{20}H_{16}X_3Y$ / $(CH)_{16}X_3Y$

$(q_0, q_1, q_2) = (16,3,1)$, $(p'_0, p'_1, p'_2) \leftrightarrow (q'_0, q'_1, q'_2)$=(1,0,1)↔(5,1,0),

$(p''_0, p''_1, p''_2) \leftrightarrow (q''_0, q''_1, q''_2)$ = (2,1,1) ↔ (7,1,0), (0,3,1) ↔ (8,0,0)

$$N_E = 120a_{C_1} + 60a_{C_s} + 40a_{C_3} + 20a_{C_{3v}} = \binom{20}{16,3,1} = 19380$$

$$N_{C_3} = 4a_{C_3} + 2a_{C_{3v}} = \binom{2}{1,0,1}\binom{6}{5,1,0} = 12$$

$$N_\sigma = 4a_{C_s} + 4a_{C_{3v}} = \binom{4}{2,1,1}\binom{8}{7,1,0} + \binom{4}{0,3,1}\binom{8}{8,0,0} = 100$$

$a_{C_1} = 149, a_{C_s} = 23,\ a_{C_3} = 2, a_{C_{3v}} = 2$

$N_{C_2} = N_{C_5} = N_i = N_{S_{10}} = N_{S_6} = 0$, their a_{G_j} values are nil.

$PCV(C_{20}H_{17}X_3Y) = (19380, 0, 12, 0, 0, 0, 0, 0, 0, 100)$

$IICV(C_{20}H_{16}X_3Y) = (149, 0, 23, 0, 2, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$

For $C_{20}H_{16}X_2Y_2$ / $(CH)_{16}X_2Y_2$, $(q_0,q_1,q_2)=(16,2,2)$

$(p''_0, p''_1, p''_2)\leftrightarrow(q''_0,q''_1,q''_2)$=(2,2,0)↔(7,0,1) ; (0,2,2)↔(8,0,0) ; (2,0,2)↔(7,1,0) ; (4,0,0)↔ (6,1,1)

$$N_E = 120a_{C_1} + 60a_{C_2} + 60a_{C_s} + 60a_{C_i} + 30a_{C_{2v}} + 30a_{C_{2h}} = \binom{20}{16,2,2} = 29070$$

$$N_E = 120a_{C_1} + 60a_{C_2} + 60a_{C_s} + 60a_{C_i} + 30a_{C_{2v}} + 30a_{C_{2h}} = 29070$$

$$N_{C_2} = 4a_{C_2} + 2a_{C_{2v}} + 2a_{C_{2h}} = \binom{10}{8,1,1} = 90$$

$$N_i = 30a_{C_{2h}} + 60a_{C_i} = \binom{10}{8,1,1} = 90$$

$$N_\sigma = 4a_{C_s} + 4a_{C_{2v}} + 2a_{C_{2h}} = \binom{4}{2,2,0}\binom{8}{7,0,1} + \binom{4}{0,2,2}\binom{8}{8,0,0} + \binom{4}{2,0,2}\binom{8}{7,1,0} + \binom{4}{4,0,0}\binom{8}{6,1,1} = 158$$

$$N_{C_3} = N_{C_5} = N_{S_6} = N_{S_{10}} = 0$$

$$PCV\left(C_{20}H_{16}X_2Y_2\right) = \left(29070, 90, 0, 0, 90, 0, 0, 158\right)$$

$a_{C_1} = 214$, $a_{C_2} = 19$, $a_{C_s} = 33$, $a_{C_i} = 1$, $a_{C_{2v}} = 6$, $a_{C_{2h}} = 1$ the other symmetries are forbidden.

$$IICV(C_{20}H_{16}X_2Y_2) = \left(214, 19, 33, 1, 0, 0, 6, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0\right)$$

For $C_{20}H_{15}X_3Y_2$ / $(CH)_{15}X_3Y_2$, $(q_0,q_1,q_2)=(15,3,2)$,

$(p'_0, p'_1, p'_2)\leftrightarrow(q'_0,q'_1,q'_2)$=**(**0,0,2**)↔(**5,1,0**),**

$(p''_0, p''_1, p''_2)\leftrightarrow(q''_0,q''_1,q''_2)$=(1,1,2)↔(7,1,0) ; (3,1,0) ↔ (6,1,1) ; (1,3,0) ↔ (7,0,1)

$$N_E = 120a_{C_1} + 60a_{C_s} + 40a_{C_3} + 20a_{C_{3v}} = \binom{20}{15,3,2} = 155040$$

$$N_{C_2} = N_{C_5} = N_i = N_{S_{10}} = N_{S_6} = 0$$

$$N_\sigma = 4a_{C_s} + 4a_{C_{3v}} = \binom{4}{1,1,2}\binom{8}{7,1,0} + \binom{4}{3,1,0}\binom{8}{6,1,1} + \binom{4}{1,3,0}\binom{8}{7,0,1} = 352$$

$$N_{C_3} = 4a_{C_3} + 2a_{C_{3v}} = \binom{2}{0,0,2}\binom{6}{5,1,0} = 6$$

$$PCV(C_{20}H_{15}X_3Y_2) = \left(155040, 0, 6, 0, 0, 0, 0, 352\right)$$

$a_{C_1} = 1248$, $a_{C_s} = 87$, $a_{C_{3v}} = 1$ $a_{C_3} = 1$ the other symmetries are forbidden.

$IICV\left(C_{20}H_{15}X_3Y_2\right)=\left(1248,0,87,0,1,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0\right)$

For $C_{20}H_{14}X_3Y_3$ / $(CH)_{14}\ X_3Y$,

$(q_0,q_1,q_2)=(14,3,3)$, $(p'_0,p'_1,p'_2)\leftrightarrow(q'_0,q'_1,q'_2)$=(2,0,0)↔(4,1,1),

$(p''_0,p''_1,p''_2)\leftrightarrow(q''_0,q''_1,q''_2)$=(2,1,1)↔(6,1,1), (0,3,1) ↔ (7,0,1) , (0,1,3) ↔ (7,1,0),

$$N_E=120a_{C_1}+60a_{C_s}+40a_{C_3}+20a_{C_{3v}}=\binom{20}{15,3,3}=775200$$

$$N_{C_2}=N_{C_5}=N_i=N_{S_{10}}=N_{S_6}=0$$

$$N_\sigma=4a_{C_s}=\binom{4}{2,1,1}\binom{8}{6,1,1}+\binom{4}{0,3,1}\binom{8}{7,0,1}+\binom{4}{0,1,3}\binom{8}{7,1,0}=732$$

$$N_{C_3}=4a_{C_3}+2a_{C_{3v}}=\binom{2}{2,0,0}\binom{6}{4,1,1}=30$$

$PCV\left(C_{20}H_{15}X_3Y_3\right)=\left(775200,0,30,0,0,0,0,732\right)$

$a_{C_1}=6366,\ a_{C_s}=183,\ a_{C_{3v}}=1\ \ a_{C_3}=7$ the other symmetries are forbidden

$IICV\left(C_{20}H_{15}X_3Y_3\right)=\left(6366,0,183,0,1,0,0,0,0,0,7,0,0,0,0,0,0,0,0,0,0,0,0\right)$

For $C_{20}H_{17}XYZ$ / $(CH)_{17}XYZ$, $(q_0,q_1,q_2,q_3)=17,1,1,1$

$(p''_0,p''_1,p''_2,p''_3)\leftrightarrow(q''_0,q''_1,q''_2,q''_3)$ = (1,1,1,1) ↔ (8,0,0,0)

$$N_E=120a_{C_1}+60a_{C_s}=\binom{20}{17,1,1,1}=6840$$

$$N_\sigma=4a_{C_s}=\binom{4}{1,1,1,1}\binom{8}{8,0,0,0}=24$$

$$N_{C_2}=N_{C_3}=N_{C_5}=N_i=N_{S_{10}}=N_{S_6}=0$$

$PCV\left(C_{20}H_{17}XYZ\right)=\left(6840,0,0,0,0,0,0,0,0,24\right)$

$a_{C_1}=54,\ a_{C_s}=6$ the other symmetries are forbidden.

$IICV\left(C_{20}H_{17}XYZ\right)=\left(54,0,0,0,6,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0\right)$

For $C_{20}H_{16}X_2YZ$ / $(CH)_{16}X_2YZ$, $q_0,q_1,q_2,q_3=(16,2,1,1)$,

$(p''_0,p''_1,p''_2,p''_3)\leftrightarrow(q''_0,q''_1,q''_2,q''_3)$ = (0,2,1,1) ↔ (8,0,0,0) , (2,0,1,1) ↔ (7,1,0,0)

$$N_E = 120a_{C_1} + 60a_{C_s} = \binom{20}{16,2,1,1} = 58140$$

$$N_\sigma = 4a_{C_s} = \binom{4}{0,2,1,1}\binom{8}{8,0,0,0} + \binom{4}{2,0,1,1}\binom{8}{7,1,0,0} = 108$$

$$N_{C_2} = N_{C_3} = N_{C_5} = N_i = N_{S_{10}} = N_{S_6} = 0$$

$a_{C_1} = 471,\ a_{C_s'} = 27$ for allowed symmetries the others are forbidden.

$$PCV(C_{20}H_{16}X_2YZ) = (58140, 0, 0, 0, 0, 0, 0, 0, 0, 108)$$

$$IICV(C_{20}H_{16}X_2YZ) = (471, 0, 0, 0, 27, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

For $C_{20}H_{15}X_3YZ$ / $(CH)_{15}X_3YZ$, $q_0, q_1, q_2, q_3, =15,3,1,1$

$(p_0'', p_1'', p_2'', p_3'') \leftrightarrow (q_0'', q_1'', q_2'', q_3'') = (1,1,1,1) \leftrightarrow (7,1,0,0)$. Then we compute:

$$N_E = 120a_{C_1} + 60a_{C_s} = \binom{20}{15,3,1,1} = 310080$$

$$N_\sigma = 4a_{C_s} = \binom{4}{1,1,1,1}\binom{8}{7,1,0,0} = 192$$

$$N_{C_2} = N_{C_3} = N_{C_5} = N_i = N_{S_{10}} = N_{S_6} = 0$$

$a_{C_1} = 2562,\ a_{C_s} = 48$ the other symmetries are forbidden.

$$PCV(C_{20}H_{15}X_3YZ) = (310080, 0, 0, 0, 0, 0, 0, 192)$$

$$ICV(C_{20}H_{15}X_3YZ) = (2562, 0, 0, 0, 48, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

For $C_{20}H_{15}X_2Y_2Z$ / $(CH)_{15}X_2Y_2Z$, $q_0, q_1, q_2, q_3 = 15,2,2,1$.

$(p_0'', p_1'', p_2'', p_3'') \leftrightarrow (q_0'', q_1'', q_2'', q_3'') = (3,0,0,1) \leftrightarrow (6,1,1,0); (1,2,0,1) \leftrightarrow (7,0,1,0),$

$(1,0,2,1) \leftrightarrow (7,1,0,0)$

$$N_E = 120a_{C_1} + 60a_{C_s} = \binom{20}{15,2,2,1} = 465120$$

$$N_\sigma = 4a_{C_s} = \left[\binom{4}{3,0,0,1}\binom{8}{6,1,1,0} + \binom{4}{1,2,0,1}\binom{8}{7,0,1,0} + \binom{4}{1,0,2,1}\binom{8}{7,1,0,0}\right] = 416$$

$$N_{C_2} = N_{C_3} = N_{C_5} = N_i = N_{S_{10}} = N_{S_6} = 0$$

$a_{C_1} = 3824,\ a_{C_s} = 104$, the other symmetries are forbidden.

$$PCV(C_{20}H_{15}X_2Y_2Z) = (465120, 0, 0, 0, 0, 416)$$

For $C_{20}H_{14}X_3Y_2Z\,/\,(CH)_{14}X_3Y_2Z$, $q_0, q_1, q_2, q_3 = 14,3,2,1$

$\left(p''_0, p''_1, p''_2, p''_3\right) \leftrightarrow (q''_0, q''_1, q''_2, q''_3) = (2,1,0,1) \leftrightarrow (6,1,1,0)$; $(0,3,0,1) \leftrightarrow (7,0,1,0)$;
$(0,1,2,1) \leftrightarrow (7,1,0,0)$

$$N_E = 120a_{C_1} + 60a_{C_s} = \binom{20}{14,3,2,1} = 2325600$$

$$N_\sigma = 4a_{C_s} = \left[\binom{4}{2,1,0,1}\binom{8}{6,1,1,0} + \binom{4}{0,3,0,1}\binom{8}{7,0,1,0} + \binom{4}{0,1,2,1}\binom{8}{7,1,0,0}\right] = 800$$

$$N_{C_2} = N_{C_3} = N_{C_5} = N_i = N_{S_{10}} = N_{S_6} = 0$$

$a_{C_1} = 19280$, $a_{C_s} = 200$ the other symmetries are forbidden.

$$PCV(C_{20}H_{14}X_3Y_2Z) = (2325600,\ 0,\ 0,\ 0,\ 0,\ 800)$$

$$IICV\left(C_{20}H_{14}X_3Y_2Z\right) = (19280, 0, 200, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

For $(C_{20}H_{14}X_4Y\,Z)\,/\,(C_{20}H_{14}X_4Y\,Z)$, $q_0, q_1, q_2, q_3 = 14,4,1,1$

$\left(p''_0, p''_1, p''_2, p''_3\right) \leftrightarrow (q''_0, q''_1, q''_2, q''_3) = (0,2,1,1) \leftrightarrow (7,1,0,0)$, $(2,0,1,1) \leftrightarrow (6,2,0,0)$,

$$N_E = 120a_{C_1} + 60a_{C_s} = \binom{20}{14,4,1,1} = 1162800$$

$$N_\sigma = 4a_{C_s} = \left[\binom{4}{0,2,1,1}\binom{8}{7,1,0,0} + \binom{4}{2,0,1,1}\binom{8}{6,2,0,0}\right] = 432$$

$$N_{C_2} = N_{C_3} = N_{C_5} = N_i = N_{S_{10}} = N_{S_6} = 0$$

$a_{C_1} = 9636$, $a_{C_s} = 108$ are allowed symmetries the others are forbidden.

$$PCV(C_{20}H_{14}X_4Y\,Z) = (1162800,\ 0,\ 0,\ 0, 0,\ 432)$$

$$IICV(C_{20}H_{14}X_4Y\,Z) = (9636, 0, 108, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

For $C_{20}H_8X_6Y_6/CH)_8X_6Y_6$, $(q_0,q_1,q_2)=(8,6,6)$; $\left(p'_0, p'_1, p'_2\right) \leftrightarrow \left(q'_0, q'_1, q'_2\right) = (2,0,0) \leftrightarrow (2,2,2)$,

$\left(p''_0, p''_1, p''_2\right) \leftrightarrow \left(q''_0, q''_1, q''_2\right) = (4,0,0) \leftrightarrow (2,3,3)$, $(0,4,0) \leftrightarrow (4,1,3)$; $(0,0,4) \leftrightarrow (4,3,1)$; $(2,2,0) \leftrightarrow (3,2,3)$;

$(0,2,2) \leftrightarrow (4,2,2)$; $(2,0,2) \leftrightarrow (3,3,2)$

$\left(p'''_0, p'''_1, p'''_2\right) \leftrightarrow \left(q'''_0, q'''_1, q'''_2\right) = (1,0,0) \leftrightarrow (1,1,1)$

$$N_E = \begin{bmatrix} 120a_{C_1} + 60a_{C_2} + 60a_{C_s} + 60a_{C_i} + 30a_{C_3} \\ +30a_{C_{2v}} + 30a_{C_{2h}} + 20a_{C_{3v}} + 20a_{C_{3i}} + 20a_{D_3} \end{bmatrix} = \binom{20}{8,6,6} = 116\ 396\ 280$$

$$N_{C_2} = 4a_{C_2} + 2a_{C_{2v}} + 2a_{C_{2h}} + 4a_{D_3} = \binom{10}{4,3,3} = 4200$$

$$N_{C_i} = 60_{C_i} + 30_{C_{2h}} + 20a_{C_{3i}} = \binom{10}{4,3,3} = 4200$$

$$N_{C_3} = 4a_{C_3} + 4a_{D_3} + 4a_{C_{3v}} + 4a_{C_{3i}} = \binom{2}{2,0,0}\binom{6}{2,2,2} = 90$$

$$N_{S_6} = 2a_{C_{3i}} = \binom{1}{1,0,0}\binom{3}{1,1,1} = 6$$

$$N_\sigma = 4a_{C_s} + 2a_{C_{2h}} + 2a_{C_{2v}} + 4a_{C_{3v}} = \begin{bmatrix} \binom{4}{4,0,0}\binom{8}{2,3,3} + \binom{4}{0,4,0}\binom{8}{4,1,3} + \binom{4}{0,0,4}\binom{8}{4,3,1} \\ \binom{4}{2,2,0}\binom{8}{2,3,3} + \binom{4}{0,2,2}\binom{8}{4,2,2} + \binom{4}{2,0,2}\binom{8}{3,3,2} \end{bmatrix} = 10360$$

$N_{S_{10}} = N_{C_5} = 0$, forbidden symmetries are C_5, D_5, C_{5v}, C_{5i}, T, D_{5d}, D_2, D_{2h}, D_{3d}, T_h, I, I_h then we compute for allowed symmetries: $a_{C_1} = 968140$, $a_{C_2} = 1017$, $a_{C_s} = 2533$, $a_{C_i} = 63$, $a_{C_3} = 18$, $a_{C_{2v}} = 48$, $a_{C_{2h}} = 12$, $a_{C_{3v}} = 3$, $a_{C_{3i}} = 3$, $a_{D_3} = 3$.

$PCV(C_{20}H_8X_6Y_6) =$ (116 396 280, 4200, 90, 0, 4200, 6, 0, 10360)

$IICV(C_{20}H_8X_6Y_6) =$ (968140,1017, 2533, 63, 18, 0, 48, 12, 0, 3, 3, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)

The *PVCs* and *IICVs* computed and collected to form the permutomers count matrix (*PCM*) and the itemized isomers count matrix (*IICM*) for coisomeric heteropolysubstituted DDH derivatives $(C_{20}H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k})$ and DDH hetero hetero-analogues $(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k})$ are summarized in eq.53.

$IICM\left(C_{20}H_{q0}X_{q1}....Y_{q_i}...Z_{qk}\right)/\left((CH)_{q0}X_{q1}....Y_{qi}...Z_{qk}\right)$

$C_{20}H_{q0}X_{q_1}....Y_{q_i}...Z_{q_k}$	C_1	C_2	C_s	C_i	C_3	D_2	C_{2v}	C_{2h}	C_5	D_3	C_{3v}	C_{3i}	D_{2h}	D_5	C_{5v}	C_{5i}	T	D_{3d}	D_{5d}	T_h	I	I_h
$C_{20}H_{18}XY$	2	0	2	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
$C_{20}H_{17}X_2Y$	23	0	11	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
$C_{20}H_{16}X_3Y$	149	0	23	0	2	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0
$C_{20}H_{16}X_2Y_2$	214	19	33	1	0	0	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$C_{20}H_{15}X_3Y_2$	1248	0	87	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
$C_{20}H_{14}X_3Y_3$	6366	0	183	0	7	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
$C_{20}H_{17}XYZ$	54	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
$C_{20}H_{16}X_2YZ$	471	0	27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$C_{20}H_{15}X_3YZ$	2560	0	46	0	2	0	0	0	0	0	2	0	0	0	0	0	0	1	0	1	0	0
$C_{20}H_{15}X_2Y_2Z$	3824	0	104	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$C_{20}H_{14}X_3Y_2Z$	19280	0	200	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$C_{20}H_{14}X_4YZ$	9636	0	108	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$C_{20}H_8X_6Y_6$	968140	1017	2533	63	18	0	48	12	0	3	3	3	0	0	0	0	0	0	0	0	0	0

$\times$

SSG-I_h	E	$15C_2$	$20C_3$	$24C_5$	***i***	$20S_6$	$24S_{10}$	15σ
C_1	120	0	0	0	0	0	0	0
C_2	60	4	0	0	0	0	0	0
C_s	60	0	0	0	0	0	0	4
C_i	60	0	0	0	60	0	0	0
C_3	40	0	4	0	0	0	0	0
D_2	30	6	0	0	0	0	0	0
C_{2v}	30	2	0	0	0	0	0	4
C_{2h}	30	2	0	0	30	0	0	2
C_5	24	0	0	4	0	0	0	0
D_3	20	4	2	0	0	0	0	0
C_{3v}	20	0	2	0	0	0	0	4
C_{3i}	20	0	2	0	20	2	0	0
D_{2h}	15	3	0	0	15	0	0	3
D_5	12	4	0	2	0	0	0	0
C_{5v}	12	0	0	2	0	0	0	4
C_{5i}	12	0	0	2	12	0	2	0
T	10	2	4	0	0	0	0	0
D_{3d}	10	2	1	0	10	1	0	2
D_{5d}	6	2	0	1	6	0	1	2
T_h	5	1	2	0	5	2	0	1
I	2	2	2	2	0	0	0	0
I_h	1	1	1	1	1	1	1	1

$=$ $PCM\left(C_{20}H_{q0}X_{q1}....Y_{q_i}...Z_{qk}\right)/\left((CH)_{q0}X_{q1}....Y_{qi}...Z_{qk}\right)$

$C_{20}H_{q0}X_{q_1}....Y_{q_i}...Z_{q_k}$	N_E	N_{C_2}	N_{C_3}	N_{C_5}	N_i	N_{S_6}	$N_{S_{10}}$	N_σ
$C_{20}H_{18}XY$	380	0	2	0	0	0	0	12
$C_{20}H_{17}X_2Y$	3420	0	0	0	0	0	0	44
$C_{20}H_{16}X_3Y$	19380	0	12	0	0	0	0	100
$C_{20}H_{16}X_2Y_2$	29070	90	0	0	9	0	0	158
$C_{20}H_{15}X_3Y_2$	155040	0	6	0	0	0	0	352
$C_{20}H_{14}X_3Y_3$	775200	0	30	0	0	0	0	732
$C_{20}H_{17}XYZ$	6840	0	0	0	0	0	0	84
$C_{20}H_{16}X_2YZ$	68140	0	0	0	0	0	0	108
$C_{20}H_{15}X_3YZ$	310080	0	0	0	0	0	0	192
$C_{20}H_{15}X_2Y_2Z$	465120	0	0	0	0	0	0	416
$C_{20}H_{14}X_3Y_2Z$	2325600	0	0	0	0	2	0	800
$C_{20}H_{14}X_4YZ$	1162800	0	0	0	0	0	0	432
$C_{20}H_8X_6Y_6$	116396280	4200	90	0	4200	6	0	10360

(53)

The numbers and types of occurring symmetries predicted for coisomeric heteropolysubstituted DDH derivatives and DDH hetero hetero-analogues of the series $C_{20}H_{q_0}X_{q_1}Y_{q_2}/(CH)_{q_0}X_{q_1}Y_{q_2}$ and $C_{20}H_{q_0}X_{q_1}Y_{q_2}Z_{q_3}/(CH)_{q_0}X_{q_1}Y_{q_2}Z_{q_3}$ are detailed by the terms of partition equations given in column 7 of table 4. The a_{G_j} values reported in these partitions satisfy eqs. 48-50 which establish the compliance of bipartite and symmetry itemized enumeration methods.

Table 4. Numbers and types of occurring symmetries predicted for coisomeric series $C_{20}H_{q_0}X_{q_1}Y_{q_2}/(CH)_{q_0}X_{q_1}Y_{q_2}$ and $(CH)_{q_0}X_{q_1}Y_{q_2}Z_{q_3}/(CH)_{q_0}X_{q_1}Y_{q_2}Z_{q_3}$.

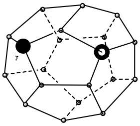
q_0,q_1,q_2	$C_{20}H_{q_0}X_{q_1}Y_{q_2}$	$(CH)_{q_0}X_{q_1}Y_{q_2}$	A_c	A_{ac}	A_{dia}	*Partition of occurring Symmetries*
18,1,1	$C_{20}H_{18}XY$	$(CH)_{18}XY$	2	3	5	$2C_1+C_{3v}+2C_s$
17,2,1	$C_{20}H_{17}X_2Y$	$(CH)_{17}X_2Y$	23	11	34	$23C_1+11C_s$
16,3,1	$C_{20}H_{17}X_3Y$	$(CH)_{16}X_3Y$	151	25	176	$149C_1+23C_s+2C_3+2C_{3v}$
16,2,2	$C_{20}H_{16}X_2Y_2$	$(CH)_{16}X_2Y_2$	233	41	274	$214C_1+19C_2+33C_s+C_i+6C_{2v}+C_{2h}$
15,3,2	$C_{20}H_{15}X_3Y_2$	$(CH)_{15}X_3Y_2$	1249	88	1337	$1248C_1+87C_s+C_3+C_{3v}$
14,3,3	$C_{20}H_{14}X_3Y_3$	$(CH)_{14}X_3Y_3$	1373	184	1557	$6366C_1+183C_s+7C_3+C_{3v}$
q_0,q_1,q_2,q_3	$C_{20}H_{q_0}X_{q_1}Y_{q_2}Z_{q_3}$	$(CH)_{q_0}X_{q_1}Y_{q_2}Z_{q_3}$	A_c	A_{ac}	A_{dia}	*Partition of occurring Symmetries*
17,1,1,1	$C_{20}H_{17}XYZ$	$(CH)_{17}XYZ$	54	6	60	$54C_1+6C_s$
16,2,1,1	$C_{20}H_{16}X_2YZ$	$(CH)_{16}X_2YZ$	471	27	498	$96C_1+18C_s$
15,3,1,1	$C_{20}H_{15}X_3YZ$	$(CH)_{15}X_3YZ$	2562	48	2610	$2560C_1+46C_s+2C_3+2C_{3v}$
15,2,2,1	$C_{20}H_{15}X_2Y_2Z$	$(CH)_{15}X_2Y_2Z$	3824	104	3928	$3824C_1+104C_s$
14,4,1,1	$C_{20}H_{14}X_4YZ$	$(CH)_{14}X_4YZ$	9636	108	9744	$9636C_1+108C_s$
14,3,2,1	$C_{20}H_{14}X_3Y_2Z$	$(CH)_{14}X_3Y_2Z$	19280	200	19480	$19280C_1+200C_s$
8,6,6	$C_{20}H_8X_6Y_6$	$(CH)_8X_6Y_6$	969178	2662	971840	$968140C_1+1017C_2+2533C_s+18C_3+3C_{3v}+3C_{3v}+3D_3+48C_{2v}+12C_{2h}+63C_i$

The denumerants of I_h symmetry applied to the aforementioned series predict the occurrences of $2C_1+C_{3v}+2C_s$ isomers for $C_{20}H_{18}XY/(CH)_{18}XY$; $23C_1+11C_s$ isomers for $C_{20}H_{17}X_2Y/(CH)_{17}X_2Y$; $149C_1+23C_s+2C_3+2C_{3v}$ isomers for $C_{20}H_{17}X_3Y/(CH)_{16}X_3Y$. $214C_1+19C_2+33C_s+C_i+6C_{2v}+C_{2h}$ isomers for $C_{20}H_{16}X_2Y_2/(CH)_{16}X_2Y_2$, $1248C_1+87C_s+C_3+C_{3v}$ isomers for $C_{20}H_{15}X_3Y_2/(CH)_{15}X_3Y_2$, $6366C_1+183C_s+7C_3+C_{3v}$ isomers for $C_{20}H_{14}X_3Y_3/(CH)_{14}X_3Y_3$, $54C_1+6C_s$ isomers for $C_{20}H_{17}XYZ/(CH)_{17}XYZ$, $96C_1+18C_s$ isomers for $C_{20}H_{16}X_2YZ/(CH)_{16}X_2YZ$, $2560C_1+46C_s+2C_3+2C_{3v}$ isomers for $C_{20}H_{15}X_3YZ/(CH)_{15}X_3YZ$, $3824C_1+104C_s$ isomers for $C_{20}H_{15}X_2Y_2Z/(CH)_{15}X_2Y_2Z$, $9636C_1+108C_s$ isomers for $C_{20}H_{14}X_4YZ/(CH)_{14}X_4YZ$, $19280C_1+200C_s$ isomers for $C_{20}H_{14}X_3Y_2Z/(CH)_{14}X_3Y_2Z$ and $968140C_1+1017C_2+2533C_s+18C_3+3C_{3v}+3C_{3v}+3D_3+48C_{2v}+12C_{2h}+63C_i$ isomers for $C_{20}H_8X_6Y_6/(CH)_8X_6Y_6$. We notice for the sake of comparison that the scalar of the summands of these partition equations are similar to the numbers of DDH derivatives of G_j subsymmetries predicted by the USCI-methods of Fujita. [7,19] The data reported in columns 4, 5 and 6 obtained from bipartite enumeration (part I) and those of column 7 obtained from this pattern inventory satisfy equations 48, 49 and 50. These results are illustrated by 57 graphs drawn in fig.2 with underneath identifying numbers (**108**) - (**164**) and distinct symmetries indicated in the lower right corner of the boxes.

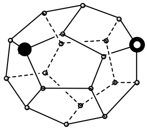
6 Conclusion

A six-steps algorithm including: (1)-the determination of permutations induced by 8 conjugacy classes of symmetry operations of the I_h group acting on DDH skeleton; (2)-the transformation of these permutations into generic formulas for deriving permutomers count vector $PCV(MX)$ characterizing the series of substituted DDH derivatives or DDH heteroanalogues; (3)-the determination of 22 non-redundant subgroups of I_h ; (4)-the determination of a 22x8 matrix $W_{I_h} = [w_{G_j,g_i}]$ whose elements w_{G_j,g_i} are the weights of the subgroups G_j of I_h; (5)-the construction of eight associated Sylvester's denumerants of type $N_{g_\ell} = \sum_{G_j} a_{G_j} w_{G_j,g_\ell}$ equating each permutomers number N_{g_ℓ} as a sum of symmetry adapted isomers numbers a_{G_j} scaled by the weights w_{G_j,g_i} of 22 subgroups of $I_{h,}$. (6) -The resolution of eight associated partition equations yields 22 a_{G_j} values collected to form the entries of the itemized isomers count vector IICV(MX) both enumerating substituted DDH derivatives and DDH heteroanalogues. This novel method provides : (1) A direct and systematic decomposition of the numbers A_c and A_{ac} of chiral and achiral isomers skeletons (obtained in part I) as sum total of $a_{G_j^c}$ chiral and $a_{G_j^{ac}}$ achiral symmetry itemized isomers numbers, respectively ; (2) A complete list of all possible permutomers of DDH derivatives and heteroanalogues. (3) A correspondence between Polya's numbers of diastereoisomers and symmetry adapted isomers numbers. This enumeration procedure is useful for stereochemical investigations and molecular modelling of such I_h based compounds.

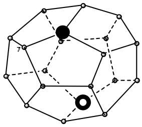
$C_{20}H_{18}XY$ / $(CH)_{18}XY$



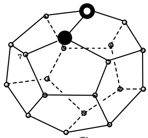
(108)



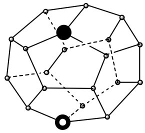
(109) **$2C_1$**



(110) **C_{3v}**

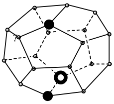


(111) C_s

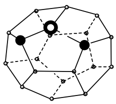


(112) **$2C_s$**

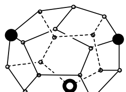
$C_{20}H_{17}X_2Y$ / $(CH)_{17}X_2Y$



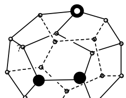
(113)



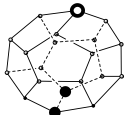
(114)



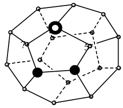
(115)



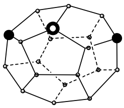
(116)



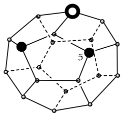
(117)



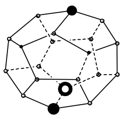
(123)



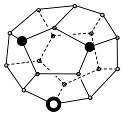
(118)



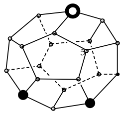
(119)



(120)

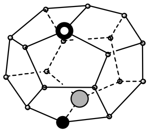


(121)

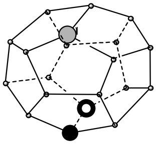


(122) **$11C_s$**

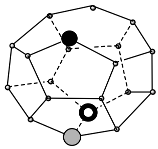
$C_{20}H_{17}XYZ$ / $(CH)_{17}XYZ$



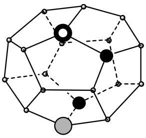
(124)



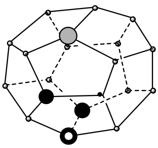
(125)



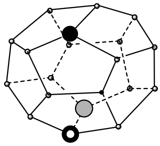
(126)



(127)

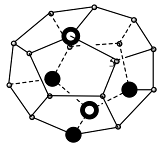


(128)

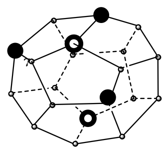


(129) **6Cs**

$C_{20}H_{15}X_3Y_2$ / $(CH)_{15}X_3Y_2$



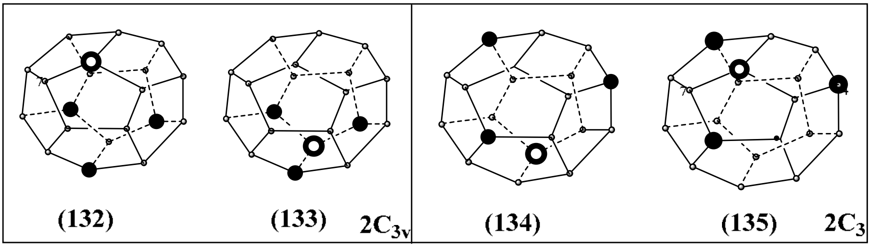
(130) **C_{3v}**



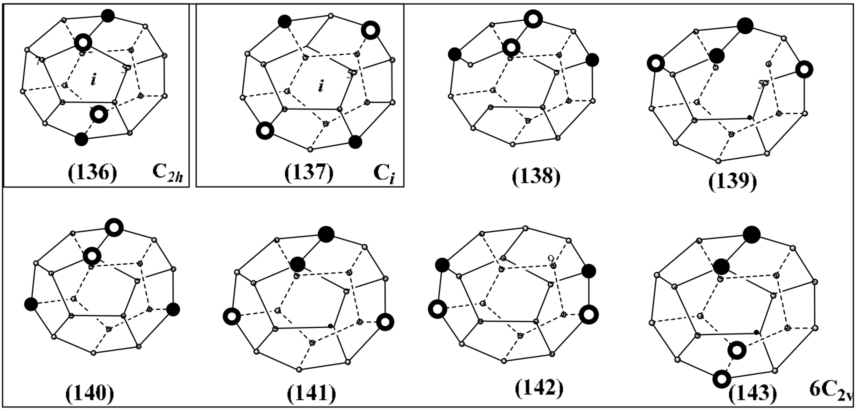
(131) **C_3**

Figure 2 continued

$C_{20}H_{16}X_3Y$ / $(CH)_{16}X_3Y$



$C_{20}H_{16}X_2Y_2$ / $(CH)_{16}X_2Y_2$



$C_{20}H_{15}X_3YZ$ / $(CH)_{15}X_3YZ$

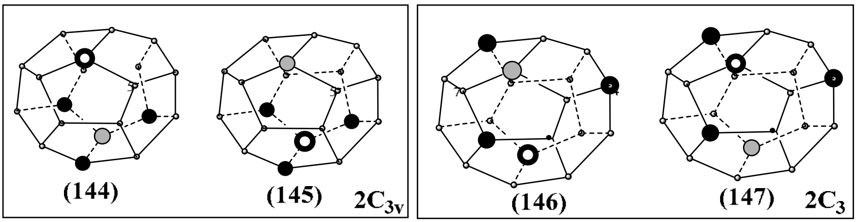
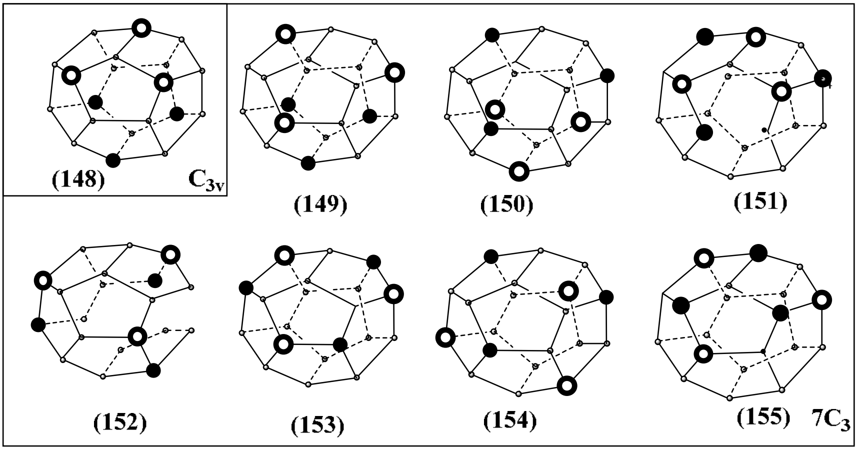


Figure 2 continued, end.

$C_{20}H_{14}X_3Y_3$ / $(CH)_{14}X_3Y_3$



$C_{20}H_8X_6Y_6$ /$(CH)_8X_6Y_6$

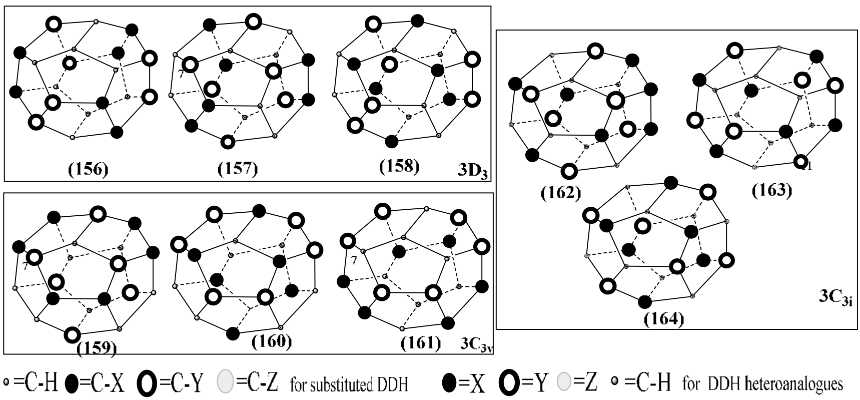


Figure 2. Graphs of coisomeric heteropolysubstituted DDH derivatives and DDH-hetero-hetero analogues of the series $C_{20}H_{q_0}X_{q_1}Y_{q_2}$ / $(CH)_{q_0}X_{q_1}Y_{q_2}$ and $(CH)_{q_0}X_{q_1}Y_{q_2}Z_{q_3}$ / $(CH)_{q_0}X_{q_1}Y_{q_2}Z_{q_3}$.

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