MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **86** (2021) 59-83

ISSN 0340 - 6253

Bipartite Enumeration of Substituted Dodecahedrane Derivatives and Heteroanalogues. I.

Robert Martin Nemba*, T. Makon

Faculty of Sciences, Laboratory of Physical and Theoretical Chemistry, Yaoundé I University, P. O. Box 812 Yaoundé, Cameroon
nembarobertmartin@yahoo.com

(Received January 5, 2021)

Abstract

Permutations representations controlling the chirality-chirality fittingness and the diastereoisomerism of dodecahedrane (DDH) skeleton in I_h symmetry are derived and transformed by means of binomial and multinomial theorems into generic formulas for bipartite enumeration of enantiomers pairs and achiral skeletons of coisomeric series of: (a) homopolysubstituted DDH derivatives($C_{20}H_{20-q}X_q$) and DDH homo hetero-analogues ($(CH)_{20-q}X_q$) and (b) of heteropolysubstituted DDH derivatives ($C_{20}H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$)and DDH hetero hetero-analogues ($(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$) where X,…,Y and Z are achiral substituents.

1 Introduction

Dodecahedrane(DDH) a polycyclic hydrocarbon symbolized by the molecular formula $C_{20}H_{20}$ has been synthesized by Leo Paquette in 1982 [1-5]. Its structure is shaped like a polyhedron of twelve regular 5-gonal faces and due to this geometrical feature, it belongs to the series of polyhedrane and is the third member of the family of Platonic hydrocarbons which include tetrahedrane, cubane, dodecahedrane and icosahedrane.[6] The discovery of this non naturally occurring cage hydrocarbon has opened a great deal of interest for the preparation of its derivatives [7-11]and the investigation of their applications in medicine. [12] Partial and total substitutions of hydrogen atoms of DDH skeleton reported in the literature[13] yield a variety of

---

* Corresponding author.

homo and hetero-polysubstituted DDH derivatives while successive substitutions of methine groups by trivalent heteroatoms give rise to DDH heteroanalogues[14]. These 2 modes of substitutions give rise to a set of 4 structurally distinct series of DDH derivatives which include:

(1)- Homopolysubstituted DDH derivatives $C_{20}H_{20-q}X_q$ obtained by replacing among 20 positions *qH* by *qX* achiral substituents of the same kind.

(2)- Homogeneous DDH heteroanalogues or DDH homo hetero-analogues$(CH)_{20-q}X_q$ issued from substitutions replacing among 20 positions in accord with the obligatory minimum valency restriction (OMV=3) [15], *qCH* groups by *qX* trivalent heteroatoms of the same kind.

(3)- Heteropolysubstituted DDH derivatives $C_{20}H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ obtained by substitutions keeping q_0H hydrogen atoms among 20 positions and replacing the remaining others by $q_1X, ..., q_iY, ..., q_kZ$ achiral substituents *of* different kinds.

(4)- Heterogeneous DDH heteroanalogues or DDH hetero hetero-analogues obtained by substitutions keeping $q_0(CH)$ groups among 20 positions and replacing in accord with the OMV=3 the remaining others by $q_1X, ..., q_iY, ..., q_kZ$ trivalent heteroatoms of different kinds.

The expansion of such molecular series needs stereo chemical investigations including enumeration problems. Fujita has developed the USCI and the RPCI-methods for combinatorial enumeration of DDH derivatives [16-17] and some structural studies are reported. [18-22] This paper presents the determination of permutations representations controlling the chirality and the achirality fittingness of DDH skeleton under the I_h group action and their transformations into generic expressions for combinatorial bipartite enumeration of A_c enantiomer pairs and A_{ac} achiral skeletons of substituted DDH derivatives and DDH heteroanalogues.

2 Mathematical formulation

2.1 Location of symmetry elements of DDH skeleton

Let us represent the cage structure of DDH by a hydrogen depleted stereograph given in fig 1. where 20 black vertices joined together by 30 edges symbolize carbon atoms and C-C bonds respectively. The 20 vertices and 30 edges are distributed throughout 12 regular 5-gonal faces displayed by pair in staggered conformation. Each carbon atom having a sp^3 hybridization state is bonded to 3 neighboring carbon and 1 hydrogen atoms. This saturation of the carbon skeleton allows the formation of a tridimensional carbon cluster shaped as an ultra-symmetric dodecahedron named dodecahedrane which belongs to the icosahedral group I_h including 120 symmetry operations distributed among 8 conjugacy classes reported in eq.1.

$$I_h = \left\{E, 15C_2, 10\left(C_3^1, C_3^2\right), 6\left(C_5^1, C_5^2, C_5^3, C_5^4\right), i, 10\left(S_6^1, S_6^5\right), 6\left(S_{10}^1, S_{10}^3, S_{10}^7, S_{10}^9\right), 15\sigma\right\} \quad (1)$$

The locations of symmetry elements of dodecahedrane are depicted in fig.1.

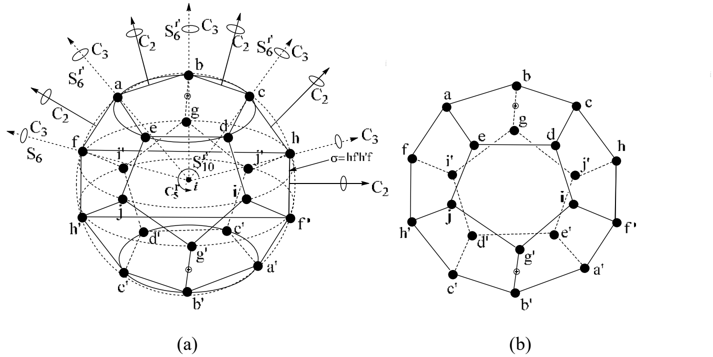

Figure 1. Hydrogen depleted 3D-graphs or stereographs of dodecahedrane where black vertices symbolize CH groups indicated by alphabetical labels. (a) Locations of symmetry elements (b) Presentation of opposite pairs of 5-gonal faces in staggered conformation.

Six 5-fold rotation axes $(6C_5^{r'})$ colinear with 6 10-fold rotoreflection axes $6S_{10}^{r'}$ intersect the inversion centre i and join the centres of 6 pairs of opposite pentagonal faces displayed in staggered conformation and depicted by 5-tuples of alphabetical letters given hereafter: (*abcde-a'b'c'd'e'*), (*aejh'f-a'e'j'hf'*), (*dejg'i-d'e'j'gi'*), (*cdif'h-c'd'i'fh'*), (*b'c'h'jg'-bchj'g*), (*abgi'f-a'b'g'if'*). The 15 pairs of opposite edges depicted in fig.1 by 4 tuples of alphabetical letters reported in table 1 define the 15σ mirror planes of the molecule.

Table 1. The 15 pairs of opposite edges defining the 15σ mirror planes of DDH.

ab-a'b'	*bc-b'c'*	*cd-c'd'*	*de-d'e'*	*ea-e'a'*
ej-e'j'	*jh'-j'h*	*h'f-f'h*	*af-a'f'*	*d'i'-di*
i'f-if'	*c'h'-ch*	*jg'-j'g*	*g'i-gi'*	*g'b'-gb*

The $15C_2$ rotation axes intersect the midpoints of 15 pairs of opposite edges abovementioned. Then 10 3-fold rotation axes ($10C_3^{r'}$) and their 10 colinear 6-fold rotoreflections axes ($10S_6^{r'}$) are located on the lines intersecting 10 pairs of opposite vertices *aa', bb', cc', dd', ee', ff', gg', hh', ii'* and *jj'*. The inversion centre i is located on the centre of DDH skeleton.

2.2 Permutations of 20H or 20C of DDH under the I_h group action.

The application to a set of atoms of symmetry operations belonging to a conjugacy class generates congruent permutations (i.e. subsets of equivalent cyclic permutations of atoms). This congruence of permutations is used for the sake of brevity to derive distinct sets of permutations of 20H or 20C of DDH skeleton induced by 120 symmetry operations of I_h.

(a) Permutations induced by the identity operation E

The identity operation E fixes each hydrogen atoms in an invariant position and gives rise to 20 unit cycle permutations or permutations of class 1^{20}:

$$E \xrightarrow{20H \text{ or } 20C} (a)(b)(c)(d)(e)(f)(g)(h)(a')(b')(c')(d')(e')(f')(g')(h()\sim 1^{20} \quad (2)$$

(b) Permutation induced by $C_3^r = (C_3^1, C_3^2)$ rotations and 6-fold rotoreflections $S_6^{r'} = (S_6^1, S_6^5)$

The projection of 20CH of DDH among two parallel planes containing respectively 10 substitution sites located on the northern (N) and southern (S) moieties of DDH (see fig 2) is used to derive permutations induced by 3-fold rotations $C_3^r = (C_3^1, C_3^2)$. The C_3^1 and C_3^2 rotations about the *aa'* axis keep invariant the opposite vertices *a* and *a'* generating 2 unit-cycles permutations (1^2) and simultaneously divide the 18 remaining others (*b,c,d,e,f,g,h,i,j,b',c',d',e',f', g', h',i',j'*) into six 3-cycles permutations (3^6) as given in eq.3-4:

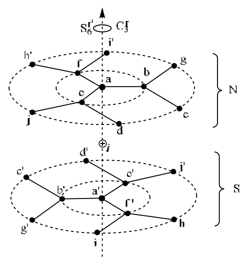

Figure 2. Projection about the C_3 rotation axis aa' of 20CH groups distributed among 2 parallel planes containing respectively 10 substitution sites located on the northern (N) and southern (S) moieties of DDH.

$$C_3^1 \xrightarrow{20H \text{ or } 20C} (a)(a')(b,e,f)-(d,h',g)-(c,j,i')-(b',e',f')-(d',h,g')-(c',j',i)\sim[1^2 3^6] \quad (3)$$

$$C_3^2 \xrightarrow{20H \text{ or } 20C} (a)(a')(b,f,e)-(c,i',j)-(g,h',d)-(b',f',e')-(c',i,j')-(g',h,d')\sim[1^2 3^6] \quad (4)$$

These 2 conjugated symmetry operations yield 2 permutations of class $[1^2 3^6]$ and 10 3-fold rotation axes *aa', bb', cc', dd', ee', ff', gg', hh', ii'* and *jj'* generate $10 \times 2 \times [1^2 3^6]$.

The associated 6-fold rotoreflections $S_6^{r'} = (S_6^1, S_6^5)$ about the aa' axis generates the transposition (*a,a'*) ~2^1 and simultaneously divide the 18 remaining vertices *b,c,d,e,f,g,h,i,j,b',c', d',e',f', g',h',i',j'* into 3 6-cycles permutations $(b,f',e,b',f,e')(c,i,j,c',i',j')(g,h,d,g',h',d') \sim 6^3$ and $(b,e',f,b',e,f')(c,j',i',c',j,i)(d,h,g,d',h',g') \sim 6^3$,respectively. The rotoreflections S_6^1 and S_6^5 applied to 20 H or 20 C of DDH yield respectively the term $(2^1 6^3)$ including 1 transposition and 3 6-cycles permutations given in eq.5-6.

$$\begin{array}{c}(a,b,c,d,e,f,g,h,i,j,a',b',c',d',e',f',g',h',i',j') \\ \downarrow S_6^1 \\ (a,a')(b,f',e,b',f,e')(c,i,j,c',i',j')(g,h,d,g',h',d') \sim [2^1 3^6]\end{array} \qquad (5)$$

$$\begin{array}{c}(a,b,c,d,e,f,g,h,i,j,a',b',c',d',e',f',g',h',i',j') \\ \downarrow S_6^5 \\ (a,a')(b,e',f,b',e,f')(c,j',i',c',j,i)(d,h,g,d',h',g') \sim [2^1 3^6]\end{array} \qquad (6)$$

Therefore $10S_6^{r'} = 10(S_6^1, S_6^5)$ performed about the *aa', bb', cc', dd', ee', ff', gg', hh', ii' and jj'* axes yield the term $10 \times 2 \times [2^1 6^3]$ corresponding to 20 composite permutations of class $[2^1 6^3]$.

(c) Permutations induced by C_5^r rotations and $S_{10}^{r'}$ rotoreflections

In DDH six 5-fold rotation axes $6C_5^r = 6(C_5^1, C_5^2, C_5^3, C_5^4)\ 1 \le r \le 4$ colinear with their six associated 10-fold rotoreflection axes $6S_{10}^{r'} = 6(S_{10}^1, S_{10}^3, S_{10}^7, S_{10}^9)$ are located on the lines intersecting the centres of opposite pairs of 5-gonal faces *(abcde-a'b'c'd'e'); (aejh'f-a'e'j'hf');(dejg'i-d'e'j'gi');(cdif'h-c'd'i'fh');(b'c'h'jg'-bchj'g);(abgi'f-a'b'g'if')* displayed in staggered conformation. The projection of 20CH of DDH among two parallel planes containing respectively 10 substitution sites displayed at the corners of 2 pairs of regular 5-gons located on the northern (N) and southern (S) moieties of DDH (see fig 3)

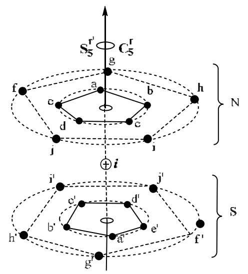

Figure 3. Projection about the C_5^r rotation axis of 20CH distributed among 2 parallel planes containing respectively 10 substitution sites located on the northern (N) and southern (S) moieties of DDH.

is used to derive permutations induced by C_5^r and $S_{10}^{r'}$. The 5-fold rotations $C_5^{r'} = (C_5^1, C_5^2, C_5^3, C_5^4)$ performed about the axis passing through the centres of 2 pairs of opposite 5-gonal faces (*abcde-a'b'c'd'e'*) and (*fghij-f'g'h'i'j'*) generates permutations of class [5^4] including 4-5 cycles permutations. An example is given in eq.7 for C_5^1.

$$\begin{gathered}(a,b,c,d,e,f,g,h,i,j,a',b',c',d',e',f',g',h',i',j')\\ \downarrow C_5^1 \\ (a,b,c,d,e)(a',b',c',d',e')(f',g',h',i',j')(f,g,h,i,j) \sim [5^4]\end{gathered} \tag{7}$$

Hence each C_5^r generates 4 [5^4] congruent permutations and $6C_5^r$ yield 24 [5^4].

The S_{10}^1 rotoreflection collinear to C_5^1 generates 2 10-cycles permutations denoted [10^2] in eq.8 :

$$\begin{gathered}(a,b,c,d,e,f,g,h,i,j,a',b',c',d',e',f',g',h',i',j')\\ \downarrow S_{10}^1 \\ (a,d',b,e',c,a',d,b'e,c')(f,i',g,j',h,f',i,g',j,h') \sim \left[10^2\right]\end{gathered} \tag{8}$$

Therefore 6 $S_{10}^{r'}$ yield 24 congruent 10-cycles permutations 24[10^2].

(d) Permutations induced by C_2 rotations

The C_2 rotation performed about the axis bisecting the mid-points of the opposite edges *ab* and *a'b'* yields 10 transpositions of 20H and 20C given in eq.9 and denoted [2^{10}] .

$$\begin{gathered}(a,b,c,d,e,f,g,h,i,j,a',b',c',d',e',f',g',h',i',j')\\ \downarrow C_2 \\ (a,\ b)(a',\ b')(c,\ f)(h,\ h')(f',\ c')(j',\ j)(e,\ g)(e',g')(d,\ i')(i,\ d') \sim [2^{10}]\end{gathered} \tag{9}$$

15 C_2 rotations yield the term 15 sets of permutations of class [2^{10}] .

(e) Permutations induced by σ mirror planes

Each σ mirror plane keeps invariant 4 vertices located on opposite edges and simultaneously inverts the positions of 16 remaining others. This operation gives rise to a permutation of class $\left[1^4 2^8\right]$ including 4 unit cycles permutations and 8 transpositions. An example is given below for σ located on the opposite edges *ab-a'b'*:

$$(a,b,c,d,e,f,g,h,i,j,a',b',c',d',e',f',g',h',i',j') \quad \downarrow \sigma \quad (a)(b)(a')(b')(c,f)(h,h')(f',c')(j',j)(e,g)(e',g')(d,i')(i,d') \sim [1^4 2^8] \tag{10}$$

15 σ mirror planes yield 15 x $[1^4 2^8]$.

(f) Permutations induced by the inversion centre *i*

The operation *i* inverts the positions of 10 pairs of opposite vertices and generates 10 transpositions indicated in eq.11 and denoted by the term $[2^{10}]$.

$$(a,b,c,d,e,f,g,h,i,j,a',b',c',d',e',f',g',h',i',j') \quad \downarrow i \quad (a,a')(b,b')(c,c')(d,d')(e,e')(f,f')(g,g')(h,h')(i,i')(j,j') \sim [2^{10}] \tag{11}$$

The I_h group action on DDH skeleton i.e. the set of permutations of 20H and 20C of DDH induced by 120 symmetry operations of I_h, partitioned among 8 conjugacy classes is summarized in table 2.

Table 2. Summary of permutations of 20H or 20C for DDH under the I_h group action including 120 symmetry operations partitioned among 8 conjugacy classes.

Classes of Symmetry operations	Symmetry operations of conjugacy classes	Number of axes	Total number of symmetry operations	Classes of permutations	Total number of permutations
$\{E\}$	E	-	1	$[1^{20}]$	$[1^{20}]$
$\{C_2\}$	C_2	15	15	$[2^{10}]$	$15[2^{10}]$
$\{C_3^r\}$	(C_3^1, C_3^2)	10	20	$[1^2 3^6]$	$20[1^2 3^6]$
$\{S_6^{r'}\}$	(S_6^1, S_6^5)	10	20	$[2^1 6^3]$	$20[2^1 6^3]$
$\{C_5^r\}$	$(C_5^1, C_5^2, C_5^3, C_5^4)$	6	24	$[5^4]$	$24[5^4]$
$\{S_{10}^{r'}\}$	$(S_{10}^1, S_{10}^3, S_{10}^7, S_{10}^9,)$	6	24	$[10^2]$	$24[10^2]$
$\{\sigma\}$	σ	-	15	$[1^4 2^8]$	$15[1^4 2^8]$
$\{ i \}$	i	-	1	$[2^{10}]$	$[2^{10}]$

2.3 Permutations representations controlling the chirality-achirality fittingness of DDH

The I_h group action on 20H or 20 C of DDH is the set P of distinct permutations induced by 8 conjugacy classes of symmetry operations of I_h given in column 6 of table 2.

$$P=\left[1^{20}\right],\,24\left[5^{4}\right],\,20\left[1^{2}3^{6}\right],\,15\left[2^{10}\right],\,15\left[1^{4}.2^{8}\right],\,\left[2^{10}\right],\,24\left[10^{2}\right],\,20\left[2^{1}.6^{3}\right] \qquad (12)$$

Noting that P includes P_{ro} and P_{rr} the subsets of permutations induced by rotations and rotoreflections given hereafter.

$$P_{ro}=\left[1^{20}\right],\,24\left[5^{4}\right],\,20\left[1^{2}3^{6}\right],\,15\left[2^{10}\right] \qquad (13)$$

$$P_{rr}=15\left[1^{4}.2^{8}\right],\,\left[2^{10}\right],\,24\left[10^{2}\right],\,20\left[2^{1}.6^{3}\right] \qquad (14)$$

we define $\overline{P_{ro}}H_{20}$ as the averaged weight of permutations induced by 60 rotations of I_h including $E,15C_2,20C_3,24C_5$:

$$\begin{aligned}\overline{P_{ro}}H_{20}&=\frac{1}{60}\left(P^{(E)}H_{20}+20P^{(C_3)}H_{20}+15P^{(C_2)}H_{20}+24P^{(C_5)}H_{20}\right)\\&=\frac{1}{60}\left([1^{20}]+20[1^{2}3^{6}]+15[2^{10}]+24[5^{4}]\right)\end{aligned} \qquad (15)$$

and $\overline{P_{rr}}H_{8}$ as the averaged weight of permutations induced by 60 rotoreflections of I_h including $i,\ 15\sigma\ ,20S_6,\ 24S_{10}$:

$$\begin{aligned}\overline{P_{rr}}H_{20}&=\frac{1}{60}\left(P^{(i)}H_{20}+20P^{(S_6)}H_{20}+24P^{(S_{10})}H_{20}+15P^{(\sigma)}H_{20}\right)\\&=\frac{1}{60}\left([2^{10}]+24[5^{4}]+20[2^{1}6^{3}]+15[1^{4}2^{8}]\right)\end{aligned} \qquad (16)$$

Definition 1 : *The permutations representation controlling the chirality fittingness for DDH of I_h symmetry denoted $\Delta_c H_{20}$ is the half value of the positive difference between $\overline{P_{ro}}H_{20}$ and $\overline{P_{rr}}H_{20}$ the averaged weights of permutations of 20H or 20 C induced by 60 rotations and 60 rotoreflections*.

$$\Delta_c H_{20}=\frac{1}{2}\left(\overline{P_{ro}}H_{20}-\overline{P_{rr}}H_{20}\right)=\frac{1}{120}\left[\begin{array}{l}\left(\left[1^{20}\right]+15\left[2^{10}\right]+20\left[1^{2}3^{6}\right]+24\left[5^{4}\right]\right)\\-\left(\left[2^{10}\right]+24\left[5^{4}\right]+20\left[2^{1}6^{3}\right]+15\left[1^{4}2^{8}\right]\right)\end{array}\right] \qquad (17)$$

Definition 2 : *The permutations representation controlling the achirality fittingness for DDH of* I_h *symmetry denoted* $\Delta_{ac}H_{20}$ *is equal to* $\overline{P_{rr}}H_{20}$ *the averaged weight of permutations of 20H or 20C induced by 60 rotoreflections including i, 15σ ,20*S_6*, 24*S_{10}*.*

$$\Delta_{ac}H_{20} = \overline{P_{rr}}H_{8} = \frac{1}{60}\left(\left[2^{10}\right] + 24\left[5^{4}\right] + 20\left[2^{1}6^{3}\right] + 15\left[1^{4}2^{8}\right]\right) \tag{18}$$

The permutations representation controlling the diastereoisomerism of DDH skeleton denoted $\Sigma_{dia}H_{20}$ is given in eq.19:

$$\Sigma_{dia}H_{20} = \frac{1}{2}\left(\overline{P_{ro}}H_{20} + \overline{P_{rr}}H_{20}\right) = \frac{1}{120}\left[\begin{array}{c}\left(\left[1^{20}\right] + 16\left[2^{10}\right] + 20\left[1^{2}3^{6}\right] + 24\left[5^{4}\right]\right) \\ +\left(24\left[10^{2}\right] + 20\left[2^{1}6^{3}\right] + 15\left[1^{4}2^{8}\right]\right)\end{array}\right] \tag{19}$$

3 Enumeration of distinct homogeneous arrangements of achiral substituents in DDH

Let us consider : (a)-homopolysubstituted DDH derivatives $C_{20}H_{20-q}X_q$ and their DDH heteroanalogues $(CH)_{20-q}X_q$ as compounds issued from the placements in distinct ways of q achiral substituents of the same kind X among 20 substitution sites submitted to permutations induced by 120 symmetry operations of I_h and (b)-heteropolysubstituted DDH derivatives $C_{20}H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ and their DDH heteroanalogues $(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ as compounds resulting from the placements in distinct ways of q_0H, q_1X,..,q_iY,...,q_kZ achiral substituents of different kinds among 20 substitution sites submitted to permutations induced by 120 symmetry operations of I_h. We notice that $C_{20}H_{20-q}X_q$ and $(CH)_{20-q}X_q$ have the same homogeneous arrangements of achiral substituents. Similarly, $C_{20}H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ and $(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ are issued from the same heterogeneous arrangements of achiral substituents. Such series of chemical compounds having in their structure the same mode of arrangements of atoms or groups of atoms are coisomeric molecules [23] i.e. pair of molecules possessing the same isomers numbers.

3.1 The numbers of permutomers of substituted 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 of different kinds among 20 substitution sites of DDH permuted by distinct symmetry operations $g_\ell \in I_h$. For $g_\ell = E, C_2, C_3, C_5, i, S_6, S_{10}, \sigma$ one obtains a set of permutomers numbers $N_{g_\ell} = N_E, N_{C_2}, N_{C_3}, N_{C_5}, N_{i,}, N_{S_6}, N_{S_{10}}, N_\sigma$ which are derived as follows:

The number N_{g_ℓ} of permutomers of homopolysubstituted DDH derivatives $C_{20}H_{20-q}X_q$ / DDH homo heteroanalogues $(CH)_{20-q}X_q$ or number of distinct ways of putting qX elements of the same kind among 20 positions submitted to ℓ-cycles permutations of class $\ell^{\frac{20}{\ell}}$ induced by a symmetry operation $g_\ell \in I_h$ is derived from the binomial coefficient $N_{g_\ell} = \begin{pmatrix} \frac{20}{\ell} \\ \frac{q}{\ell} \end{pmatrix}$. For distinct classes of permutations given hereafter*:*

$$[1^{20}] \rightarrow N_E = \begin{pmatrix} 20 \\ q \end{pmatrix}, \ \ell = 1 \qquad (20)$$

$$[2^{10}] \rightarrow N_{C_2} = \begin{pmatrix} 10 \\ \frac{q}{2} \end{pmatrix}, \ell = 2 \qquad (21)$$

$$[5^4] \rightarrow N_{C_5} = \begin{pmatrix} 4 \\ \frac{q}{5} \end{pmatrix}, \ \ell = 5 \qquad (22)$$

$$[10^2] \rightarrow N_{S_{10}} = \begin{pmatrix} 2 \\ \frac{q}{10} \end{pmatrix}, \ \ell = 10 \qquad (23)$$

For the cycle structure $[1^2 3^6]$ we have to put $\alpha = 0,1,2$ substituents X among 2 invariant positions and $(q-\alpha)X$ among 18 remaining positions submitted to six 3-cycles permutations. *The number N_{C_3} of permutomers or number of distinct placements of substituents of the same kind X among 20 positions submitted to a composite permutation of class $[1^2 3^6]$ comprising 2* *unit cycles and 6 3-cycles permutations is obtained from the sum over α of the product of binomial coefficients $T(2,\alpha)$ and $T\left(6,\frac{q\text{-}\alpha}{3}\right)$ given in eq.24*

$$[1^2.3^6] \rightarrow N_{C_3} = \sum_{\alpha=0}^{2} \binom{2}{\alpha} \binom{6}{\frac{q\text{-}\alpha}{3}} \tag{24}$$

For the cycle structure [$1^4.2^8$], we have to put $\alpha' = 0,1,3,4$ substituents X among 4 invariant positions and $(q-\alpha')X$ among 16 remaining positions submitted to transpositions.

The number N_σ of distinct placements of q substituents of the same kind X among 20 positions submitted to a composite permutation of class [$1^4.2^8$] *comprising 4 unitary cycles and 8 transpositions is obtained from the sum over α' of the product of binomial coefficients $T(4,\alpha')$ and $T\left(8,\frac{q\text{-}\alpha'}{2}\right)$ given in eq.25.*

$$[\ 1^4.2^8\ ] \rightarrow N_\sigma = \sum_{\alpha=0}^{4} T(4,\alpha)\, T\left(8,\frac{q\text{-}\alpha}{2}\right) = \sum_{\alpha'=0}^{4} \binom{4}{\alpha'} \binom{8}{\frac{q\text{-}\alpha'}{2}} \tag{25}$$

For the cycle structure [$2^1 6^3$], we have to put $\alpha'' = 0,2$ substituents X among 2 invertible positions and $(q-\alpha'')X$ among 18 remaining positions submitted to 6-cycle permutations.

The number N_{S_6} of distinct placements of qX substituents of the same kind among 20 positions submitted to a composite permutation of class [$2^1 6^3$] *comprising 1 transposition and 3 6-cycles permutations is obtained from the sum over a'' of the product of binomial coefficients $T(1,\alpha'')$ and $T\left(3,\frac{q\text{-}2\alpha''}{6}\right)$ given in eq.26.*

$$[2^1.6^3] \rightarrow N_{S_6} = \sum_{\alpha''=0,1} \binom{1}{\alpha''} \binom{3}{\frac{q-2\alpha''}{6}} \tag{26}$$

3.2 Enumeration of heterogeneous arrangements of substituents in dodecahedrane

The numbers N_{g_ℓ} *of permutomers* $C_{20}H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ *and* $(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ *issued from distinct heterogeneous arrangements of* q_0H *and k types of substituents of different kinds X,..., Y, ..., Z with partial degrees of substitution* $q_1,...,q_i,...,q_k$ *among 20 substitution sites of DDH submitted to* ℓ*-cycles permutations of class* $\ell^{\frac{20}{\ell}}$ *are obtained from the multinonomial theorem.*

For classes of classes of permutations [1^{20}], [2^{10}], [5^4] and [10^2] the N_{g_ℓ} values are derived from eqs.27-30 :

$$[\,1^{20}] \rightarrow N_E = \binom{20}{q_0,,q_i,,q_k},\ \ell = 1 \tag{27}$$

$$[\,2^{10}] \rightarrow N_{C_2} = N_i = \binom{10}{\frac{q_0}{2},,,\frac{q_i}{2},,,\frac{q_k}{2}},\ \ell{=}2 \tag{28}$$

$$[\,5^4] \rightarrow N_{C_5} = \binom{4}{\frac{q_0}{5},,,\frac{q_i}{5},,,\frac{q_k}{5}},\quad \ell = 5 \tag{29}$$

$$[\,10^2] \rightarrow N_{S_{10}} = \binom{2}{\frac{q_0}{10},,,\frac{q_i}{10},,,\frac{q_k}{10},},\ \ell{=}10 \tag{30}$$

The numbers N_{g_ℓ} of permutomers issued from composite permutations of classes [$1^2 3^6$], [$2^1 6^3$] and [$1^4 2^8$], are calculated as follows:

$$\left[1^2.3^6\right] \rightarrow N_{C_3} = \sum_{\lambda}\binom{2}{p'_0,...,p'_i,...,p'_k}\binom{6}{q'_0,...,q'_i,...,q'_k} \tag{31}$$

$$[2^1.6^3] \rightarrow N_{S_6} = \sum_{\lambda}\binom{1}{p'''_0,...,p'''_i,...,p'''_k}\binom{3}{q'''_0,...,q'''_i,...,q'''_k} \tag{33}$$

with the restrictions $$\sum_{i=0}^{k} p'''_i = 1,\quad \sum_{i=0}^{k} q'''_i = 3,\quad q'''_i = \frac{q_i - 2p'''_i}{6} \tag{34}$$

$$[1^4 2^8] \rightarrow \boldsymbol{N}_\sigma = \sum_\lambda \binom{4}{p''_0,\dots,p''_i,\dots,p''_k}\binom{8}{q''_0,,\dots,q''_i,,\dots,,q''_k} \qquad (35)$$

with the restrictions $\sum_{i=0}^{k} p''_i = 4, \quad \sum_{i=0}^{k} q''_i = 8, \quad q''_i = \dfrac{q_i - p''_i}{3}$ (36)

3.3 Generalized equations for bipartite enumeration of chiral and achiral skeletons of homopolysubstituted DDH and DDH homo hetero-analogues

By replacing the right hand side terms of eqs.17-18 with equivalent algebraic expressions previously indicated in eqs.20-26, we convert $\Delta_c H_{20}$ and $\Delta_{ac} H_{20}$ into $A_c(20,q)$ and $A_{ac}(20,q)$ which are the generalized formulas for a direct bipartite combinatorial enumeration of chiral and achiral skeletons of coisomeric series of DDH homopolysubstituted derivatives $C_{20}H_{20\text{-}q}X_q$ and their corresponding homo hetero-analogues $(CH)_{20\text{-}q}X_q$.

$$A_c(20,q) = \frac{1}{120}\left[\binom{20}{q} + 24\binom{4}{\frac{q}{5}} + 20\sum_{\alpha=0}^{2}\binom{2}{\alpha}\binom{6}{\frac{q-\alpha}{3}} + 14\binom{10}{\frac{q}{2}} - 15\sum_{\alpha'=0}^{4}\binom{4}{\alpha'}\binom{8}{\frac{q-\alpha'}{2}} - 24\binom{2}{\frac{q}{10}} - 20\sum_{\alpha''=0}^{1}\binom{1}{\alpha''}\binom{3}{\frac{q-2\alpha''}{6}}\right] \qquad (37)$$

The expansion of eq.14 generate eq.14':

$$A_c(20,q) = \frac{1}{120}\left[\begin{array}{l} \binom{20}{q} + 24\binom{4}{\frac{q}{5}} + 20\binom{6}{\frac{q}{3}} + 40\binom{6}{\frac{q-1}{3}} + 20\binom{6}{\frac{q-2}{3}} + 14\binom{10}{\frac{q}{2}} - 15\binom{8}{\frac{q}{2}} \\ -60\binom{8}{\frac{q-1}{2}} - 90\binom{8}{\frac{q-2}{2}} - 60\binom{8}{\frac{q-3}{2}} - 15\binom{8}{\frac{q-4}{2}} - 24\binom{2}{\frac{q}{10}} \\ -20\binom{3}{\frac{q}{6}} - 20\binom{3}{\frac{q-2}{6}} \end{array}\right] \qquad (37')$$

The number of achiral isomers is obtained from eq.38:

$$A_{ac}(20,q) = \frac{1}{60}\left[\binom{10}{\frac{q}{2}} + 15\sum_{\alpha'=0}^{4}\binom{4}{\alpha'}\binom{8}{\frac{q-\alpha'}{2}} + 20\sum_{\alpha''=0,1}\binom{1}{\alpha''}\binom{3}{\frac{q-2\alpha''}{6}} + 24\binom{2}{\frac{q}{10}}\right] \qquad (38)$$

which is expanded to give eq.38':

$$A_{ac}(20,q) = \frac{1}{60}\left[\binom{10}{\frac{q}{2}} + 15\binom{8}{\frac{q}{2}} + 60\binom{8}{\frac{q-1}{2}} + 90\binom{8}{\frac{q-2}{2}} + 60\binom{8}{\frac{q-3}{2}} + 15\binom{8}{\frac{q-4}{2}} + 24\binom{2}{\frac{q}{10}} + 20\binom{3}{\frac{q}{6}} + 20\binom{3}{\frac{q-2}{6}}\right] \qquad (38')$$

3.4 Generalized equations for bipartite enumeration of heteropolysubstituted DDH derivatives $C_{20}H_{q_0}X_{q_1}\dots Y_{q_i}\dots Z_{q_k}$ and DDH hetero-hetero-analogues $(CH)_{q_0}X_{q_1}\dots Y_{q_i}\dots Z_{q_k}$.

By replacing the right hand side terms of eqs.17-18 with equivalent algebraic expressions we convert $\Delta_c H_{20}$ and $\Delta_{ac} H_{20}$ with equivalent terms given in eqs.27-36 one obtains generalized formulas for bipartite enumeration of $A_c\left(20, q_0,\dots,q_i,\dots,q_k\right)$ chiral and $A_{ac}\left(20, q_0,\dots,q_i,\dots,q_k\right)$ achiral skeletons of coisomeric heteropolysubstituted DDH derivatives and DDH hetero hetero-analogues.

$$A_c\left(20, q_0, \dots,q_i,\dots,q_k\right)=\frac{1}{120}\left[\begin{array}{l}\binom{20}{q_0,\dots,q_i,\dots,q_k}+24\binom{4}{\frac{q_0}{5},\dots,\frac{q_i}{5},\dots,\frac{q_k}{5}}+14\binom{10}{\frac{q_0}{2},\dots,\frac{q_i}{2},\dots,\frac{q_k}{2}}\\ +20\sum_{\lambda}\binom{2}{p'_0,\dots,p'_i,\dots,p'_k}\binom{6}{q'_0,\dots,q'_i,\dots,q'_k}-15\sum_{\lambda}\binom{4}{p''_0,\dots,p''_i,\dots,p''_k}\binom{8}{q''_0,\dots,q''_i,\dots,q''_k}\\ -20\sum_{\lambda}\binom{1}{p'''_0,\dots,p'''_i,\dots,p'''_k}\binom{3}{q'''_0,\dots,q'''_i,\dots,q'''_k}-24\binom{2}{\frac{q_0}{10},\dots,\frac{q_i}{10},\dots,\frac{q_k}{10}}\end{array}\right] \quad (39)$$

and

$$A_{ac}\left(20, q_0, \dots,q_i,\dots,q_k\right)=\frac{1}{60}\left[\begin{array}{l}\binom{10}{\frac{q_0}{2},\dots,\frac{q_i}{2},\dots,\frac{q_k}{2}}+15\sum_{\lambda}\binom{4}{p''_0,\dots,p''_i,\dots,p''_k}\binom{8}{q''_0,\dots,q''_i,\dots,q''_k}\\ +20\sum_{\lambda}\binom{1}{p'''_0,\dots,p'''_i,\dots,p'''_k}\binom{3}{q'''_0,\dots,q'''_i,\dots,q'''_k}+24\binom{2}{\frac{q_0}{10},\dots,\frac{q_i}{10},\dots,\frac{q_k}{10}}\end{array}\right] \quad (40)$$

The sum of a pair of integer numbers (A_c, A_{ac}) derived from eqs.37-38 or eqs.39-40 is the number of diastereoisomers A_{dia} of the DDH derivative.

$$A_{dia} = A_c + A_a \quad (41)$$

For the sake of comparison with classical enumeration procedures we notice that A_{dia} matches up with the coefficients of Polya's generating function derived from cycles indices. [24-25]

4 Applications

Example 1: Bipartite enumeration of coisomeric skeletons of homopolysubstituted DDH derivatives $C_{20}H_{20-q}X_q$ and DDH homo hetero-analogues $(CH)_{20-q}X_q$. The numbers of chiral and achiral skeletons of the representatives of these 2 series where $0 \leq q \leq 20$ are obtained from eqs.37-38 as follows:

q=0

$$A_c(20,0)=\frac{1}{120}\left[\binom{20}{0}+24\binom{4}{0}+20\binom{6}{0}+14\binom{10}{0}-15\binom{8}{0}-24\binom{2}{0}-20\binom{3}{0}\right]=0$$

$$A_{ac}(20,0)=\frac{1}{60}\left[\binom{10}{0}+15\binom{8}{0}+24\binom{2}{0}+20\binom{3}{0}\right]=1$$

$q=1$

$$A_c(20,1)=\frac{1}{120}\left[\binom{20}{1}+40\binom{6}{0}-60\binom{8}{0}\right]=0$$

$$A_{ac}(20,1)=\frac{1}{60}\left(60\left[\binom{8}{0}\right]\right)=1$$

$q=2$

$$A_c(20,2)=\frac{1}{120}\left[\binom{20}{2}+20\binom{6}{0}+14\binom{10}{1}-15\binom{8}{1}-90\binom{8}{0}-20\binom{3}{0}\right]=1$$

$$A_{ac}(20,2)=\frac{1}{60}\left[\binom{10}{1}+15\binom{8}{1}+90\binom{8}{0}+20\binom{3}{0}\right]=4$$

$q=3$

$$A_c(20,3)=\frac{1}{120}\left[\binom{20}{3}+20\binom{6}{1}-60\binom{8}{1}-60\binom{8}{0}\right]=6$$

$$A_{ac}(20,3)=\frac{1}{60}\left[60\binom{8}{1}+60\binom{8}{0}\right]=9$$

$q=4$

$$A_c(20,4)=\frac{1}{120}\left[\binom{20}{4}+40\binom{6}{1}+14\binom{10}{2}-15\binom{8}{2}-90\binom{8}{1}-15\binom{8}{0}\right]=38$$

$$A_{ac}(20,4)=\frac{1}{60}\left[\binom{10}{2}+15\binom{8}{2}+90\binom{8}{1}+15\binom{8}{0}\right]=20$$

q=5

$$A_c(20,5)=\frac{1}{120}\left[\binom{20}{5}+24\binom{4}{1}+20\binom{6}{1}-60\binom{8}{2}-60\binom{8}{1}\right]=113$$

$$A_{ac}(20,5)=\frac{1}{60}\left[60\binom{8}{2}+60\binom{8}{1}\right]=36$$

q=6

$$A_c(20,6)=\frac{1}{120}\left[\binom{20}{6}+20\binom{6}{2}+14\binom{10}{3}-15\binom{8}{3}-90\binom{8}{2}-15\binom{8}{1}-20\binom{3}{1}\right]=310$$

$$A_{ac}(20,6)=\frac{1}{60}\left[\binom{10}{3}+15\binom{8}{3}+90\binom{8}{2}+15\binom{8}{1}+20\binom{3}{1}\right]=61$$

q=7

$$A_c(20,7)=\frac{1}{120}\left[\binom{20}{7}+40\binom{6}{2}-60\binom{8}{3}-60\binom{8}{2}\right]=609$$

$$A_{ac}(20,7)=\frac{1}{60}\left[60\binom{8}{3}+60\binom{8}{2}\right]=84$$

q=8

$$A_c(20,8)=\frac{1}{120}\left[\binom{20}{8}+20\binom{6}{2}+14\binom{10}{4}-15\binom{8}{4}-90\binom{8}{3}-15\binom{8}{2}-20\binom{3}{1}\right]=1022$$

$$A_{ac}(20,8)=\frac{1}{60}\left[\binom{10}{4}+15\binom{8}{4}+90\binom{8}{3}+15\binom{8}{2}+20\binom{3}{1}\right]=113$$

q=9

$$A_c(20,9)=\frac{1}{120}\left[\binom{20}{9}+20\binom{6}{3}-60\binom{8}{4}-60\binom{8}{3}\right]=1340$$

$$A_{ac}(20,9)=\frac{1}{60}\left[60\binom{8}{4}+60\binom{8}{3}\right]=126$$

q=10

$$A_c(20,10)=\frac{1}{120}\left[\binom{20}{10}+24\binom{4}{2}+40\binom{6}{3}+14\binom{10}{5}-15\binom{8}{5}-90\binom{8}{4}-15\binom{8}{3}-24\binom{2}{1}\right]=1510$$

$$A_{ac}(20,10)=\frac{1}{60}\left[\binom{10}{5}+15\binom{8}{5}+90\binom{8}{4}+15\binom{8}{3}+24\binom{2}{1}\right]=138$$

The numbers $A_c(20,q)$ of enantiomers pairs and $A_{ac}(20,q)$ of achiral isomers derived from this bipartite enumeration of homopolysubstituted dodecahedrane derivatives $C_{20}H_{20-q}X_q$ and their homo hetero-analogues $(CH)_{20-q}X_q$ where $0 \le q \le 20$ are collected to form a two column isomers count matrix ICM ($C_{20}H_{20-q}X_q$)/ICM($(CH)_{20-q}X_q$) with 21x2 entries given in eq.41. Due to the complementarity of the degrees of substitution q and 20-q we notice that the numbers of chiral and achiral isomers skeletons satisfy the equalities $A_c(q)=A_c(20\text{-}q)$ and $A_{ac}(q)=A_{ac}(20\text{-}q)$. Therefore, the ICM is a symmetric matrix written in compact notation as given in eq.41 where the last column reports Polya's numbers which are diastereoisomers numbers A_{dia} predicted for the series ($C_{20}H_{20\text{-}q}X_q$) and ($(CH)_{20\text{-}q}X_q$). Alkorta et al. (see reference 14) have found similar numbers of possible isomers for aza dodecahedranes which are DDH homo heteroanalogues symbolized by the molecular formula $(CH)_{20\text{-}q}N_q = C_{20\text{-}q}H_{20\text{-}q}N_q$ where q nitrogen heteroatoms replace q(CH) groups) and $0 \le q \le 20$.

$$ICM(C_{20}H_{20\text{-}q}X_q) = ICM(CH_{20\text{-}q}X_q) = \begin{pmatrix} q,20-q \\ 0,20 \\ 1,19 \\ 2,18 \\ 3,17 \\ 4,16 \\ 5,15 \\ 6,14 \\ 7,13 \\ 8,12 \\ 9,11 \\ 10,10 \end{pmatrix} \overbrace{\begin{pmatrix} A_c & A_{ac} \\ 0 & 1 \\ 0 & 1 \\ 1 & 4 \\ 6 & 9 \\ 18 & 20 \\ 113 & 36 \\ 310 & 61 \\ 609 & 84 \\ 1022 & 113 \\ 1340 & 126 \\ 1510 & 138 \end{pmatrix}}^{\text{Bipartite enumeration}} \Rightarrow \begin{pmatrix} x^q, x^{20-q} \\ x^0, x^{20} \\ x^1, x^{19} \\ x^2, x^{18} \\ x^3, x^{17} \\ x^4, x^{16} \\ x^5, x^{15} \\ x^6, x^{14} \\ x^7, x^{13} \\ x^8, x^{12} \\ x^9, x^{11} \\ x^{10} \end{pmatrix} \overbrace{\begin{pmatrix} A_{dia} \\ 1 \\ 1 \\ 5 \\ 15 \\ 38 \\ 149 \\ 371 \\ 693 \\ 1135 \\ 1466 \\ 1648 \end{pmatrix}}^{\text{Polya's numbers}} \quad (41)$$

Example 3: Bipartite enumeration of di, tri, tetra, penta, and hexa -heteropolysubstituted 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 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 this problem for coisomeric pairs of DDH derivatives $C_{20}H_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ / $(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ aforementioned we list the appropriate values of partial indices $q_0,...q_i,...,q_k$ satisfying the restriction $\sum_{i=0}^{k} q_i = 20$ and compute from eqs.32, 34 and 36 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 $(p'''_0,...,p'''_i,...,p'''_k) \leftrightarrow (q'''_0,...,q'''_i,...,q'''_k)$ indicating different choices of arrangements of substituents affordable from distinct classes of permutations. The data collected from such calculations are reported in table 4 and used in eqs.39-40.

Table 4. Compatible pairs of integer sequences $(p'_0, p'_1, p'_2) \leftrightarrow (q'_0,...,q'_i,...,q'_k)$, $(p''_0, p''_1, p''_2) \leftrightarrow (q''_0,...,q''_i,...,q''_k)$, $(p'''_0, p'''_1, p'''_2) \leftrightarrow (q'''_0,...,q'''_i,...,q'''_k)$ for heteropolysubstituted DDH derivatives $C_{20}H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ and DDH hetero hetero-analogues $(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ having k=2 or 3 kinds of achiral substituents(see table 3).

(q_0,q_1,q_2)	(p'_0, p'_1, p'_2)	(q'_0,q'_1,q'_2)	(p''_0, p''_1, p''_2)	(q''_0,q''_1,q''_2)	(p'''_0, p'''_1, p'''_2)	(q'''_0,q'''_1,q'''_2)
18,1,1	0,1 ,1	6,0,0	2,1,1	8,0,0	--	---
17,2,1	---------	-----	1,2,1	8,0,0	--	--
			3,0,1	7,1 ,0		
16,3,1	1,0,1	5,1,0	2,1,1	7,1,0	--	--
			0,3,1	8,0,0		
16,2,2			2,2,0	7,0,1		
			0,2,2	8,0,0	--	--
			2,0,2	7,1,0		
			4 ,0,0	6,1,1	----------	--------
15,3,2	0,0,2	5.1,0	1,1,2	7,1,0	---------	-------
			3,1,0	6,1,1		
			1,3,0	7,0,1		
14,3,3	2,0,0	4,1,1	2,1,1	6,1,1		
			0,3,1	7,0,1		
			0,1,3	7,1,0		
8,6,6	2,0,0	2,2,2	4,0,0	2,3,3	1,0,0	1 ,1,1
			0,4,0	4,1,3		
			0,0,4	4,3,1		
			2,2,0	3,2,3		
			0,2,2	4,2,2		
			2,0,2	3,3,2		
(q_0,q_1,q_2,q_3)	(p'_0, p'_1, p'_2, p'_3)	(q'_0,q'_1,q'_2,q'_3)	$(p''_0,p''_1,p''_2,p''_3)$	$(q''_0,q''_1,q''_2,q''_3)$	$(p'''_0,p'''_1,p'''_2,p'''_3)$	$(q'''_0,q'''_1,q'''_2,q'''_3)$
17,1,1,1			1,1,1,1	8,0,0,0		
16,2,1,1			0,2,1,1	8,0,0,0		
			2,0,1,1	7,1,0,0		
15,3,1,1	0,0,1,1	5,1,0,0	1,1,1,1	7,1,0,0		
15,2,2,1			3,0,0,1	6,1,1,0		
			1,2,0,1	7,0,1,0		
			1,0,2,1	7,1,0,0		
14,3,2,1			2.1,0,1	6,1,1,0		
			0,3,0,1	7,0,1,0		
			0,1,2,1	7,1,0,0		
14,4,1,1			0,2,1,1	7,1,0,0		
			2,0,1,1	6,2,0,0		

The integer sequences of $A_c\left(20,\, q_0,\ldots,q_i,\ldots,q_k\right)$ and $A_{ac}\left(20,\, q_0,\ldots,q_i,\ldots,q_k\right)$ calculated for these series are as follows:

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

$$A_c\left(20,\, 18,1,1\right)=\frac{1}{120}\left[\binom{20}{18,1,1}+20\binom{2}{0,1,1}\binom{6}{6,0,0}-15\binom{4}{2,1,1}\binom{8}{8,0,0}\right]=2$$

$$A_{ac}\left(20,\, 18,1,1\right)=\frac{1}{60}\left[15\binom{4}{2,1,1}\binom{8}{8,0,0}\right]=3$$

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

$$A_c\left(20,\, 17,2,1\right)=\frac{1}{120}\left[\binom{20}{17,2,1}-15\binom{4}{1,2,1}\binom{8}{8,0,0}-15\binom{4}{3,0,1}\binom{8}{7,1,0}\right]=23$$

$$A_{ac}\left(20,\, 17,2,1\right)=\frac{1}{60}\left[15\binom{4}{1,2,1}\binom{8}{8,0,0}+15\binom{4}{3,0,1}\binom{8}{7,1,0}\right]=11$$

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

$$A_c\left(20,\, 16,3,1\right)=\frac{1}{120}\left[\binom{20}{16,3,1}+20\binom{2}{1,0,1}\binom{6}{5,1,0}-15\binom{4}{2,1,1}\binom{8}{7,0,1}-15\binom{4}{0,3,1}\binom{8}{8,0,,0}\right]=151$$

$$A_{ac}\left(20,\, 16,3,1\right)=\frac{1}{60}\left[15\binom{4}{2,1,1}\binom{8}{7,1,0}+15\binom{4}{0,3,1}\binom{8}{8,0,,0}\right]=25$$

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

$$A_c\left(20,\, 16,2,2\right)=\frac{1}{120}\left[\binom{20}{16,2,2}+14\binom{10}{8,1,1}-15\left[\binom{4}{2,2,0}\binom{6}{7,0,1}+\binom{4}{0,2,2}\binom{8}{8,0,0}+\binom{4}{2,0,2}\binom{8}{7,1,0,}+\binom{4}{4,0,0}\binom{8}{6,1,1}\right]\right]=233$$

$$A_{ac}\left(20,\, 16,2,2\right)=\frac{1}{60}\left[\binom{10}{8,1,1}+15\left[\binom{4}{2,2,0}\binom{6}{7,0,1}+\binom{4}{0,2,2}\binom{8}{8,0,0}+\binom{4}{2,0,2}\binom{8}{7,1,0,}+\binom{4}{4,0,0}\binom{8}{6,1,1}\right]\right]=41$$

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

$$A_c\left(20,\, 15,3,2\right)=\frac{1}{120}\left[\binom{20}{15,3,2}+20\binom{2}{0,0,2}\binom{6}{5,1,0}-15\left[\binom{4}{1,1,2}\binom{8}{7,1,0}+\binom{4}{3,1,0}\binom{8}{6,1,1}+\binom{4}{1,3,0}\binom{8}{7,0,1}\right]\right]=1249$$

$$A_{ac}(20,\ 15,3,2)=\frac{15}{60}\left[\binom{4}{2,2,0}\binom{6}{7,0,1}+\binom{4}{0,2,2}\binom{8}{8,0,0}+\binom{4}{2,0,2}\binom{8}{7,1,0,}+\binom{4}{4,0,0}\binom{8}{6,1,1}\right]=88$$

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

$$A_c(20;\ 14,3,3)=\frac{1}{120}\left[\binom{20}{14,3,3}-15\left(\binom{4}{2,1,1}\binom{8}{6,1,1}+\binom{4}{0,3,1}\binom{8}{6,1,1}+\binom{4}{0,1,3}\binom{8}{0,1,3}\right)\right]=6373$$

$$A_{ac}(20;\ 14,3,3)=\frac{1}{60}\left[15\left(\binom{4}{2,1,1}\binom{8}{6,1,1}+\binom{4}{0,3,1}\binom{8}{6,1,1}+\binom{4}{0,1,3}\binom{8}{0,1,3}\right)\right]=184$$

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

$$A_c(20;\ 17,1,1,1)=\frac{1}{120}\left[\binom{20}{17,1,1,1}-15\binom{4}{1,1,1,1}\binom{8}{8,0,0}\right]=54$$

$$A_{ac}(20;\ 17,1,1,1)=\frac{1}{60}\left[15\binom{4}{1,1,1,1}\binom{8}{8,0,0}\right]=6$$

For $C_{20}H_{16}X_2YZ/(CH)_{16}X_2YZ$

$$A_c(20;\ 16,2,1,1)=\frac{1}{120}\left[\binom{20}{16,2,1,1}-15\left(\binom{4}{0,2,1,1}\binom{8}{8,0,,0,0}+\binom{4}{2,0,1,1}\binom{8}{7,1,0,0}\right)\right]=471$$

$$A_{ac}(20;\ 16,2,1,1)=\frac{1}{60}\left[15\left(\binom{4}{0,2,1,1}\binom{8}{8,0,,0,0}+\binom{4}{2,0,1,1}\binom{8}{7,1,0,0}\right)\right]=27$$

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

$$A_c(20;\ 15,3,1,1)=\frac{1}{120}\left[\binom{20}{15,3,1,1}+20\left(\binom{2}{0,0,1,1}\binom{6}{5,1,0,0}-15\binom{4}{1,1,1,1}\binom{8}{7,1,0,0}\right)\right]=2562$$

$$A_{ac}(20;\ 15,3,1,1)=\frac{1}{60}\left[15\left(\binom{4}{1,1,1,1}\binom{8}{7,1,0,0}\right)\right]=48$$

For $C_{20}H_{15}X_2Y_2Z/(CH)_{15}X_2Y_2Z$

$$A_c(20;\ 15,2,2,1)=\frac{1}{120}\left[\binom{20}{15,2,2,1}-15\left(\binom{4}{3,0,0,1}\binom{8}{6,1,1,0}+\binom{4}{1,2,0,1}\binom{8}{7,0,1,0}+\binom{4}{1,0,2,1}\binom{8}{7,1,0,0}\right)\right]=3824$$

$$A_{ac}\left(20;\ 15,2,2,1\right)=\frac{1}{60}\left[15\left(\binom{4}{3,0,0,1}\binom{8}{6,1,1,0}+\binom{4}{1,2,0,1}\binom{8}{7,0,1,0}+\binom{4}{1,0,2,1}\binom{8}{7,1,0,0}\right)\right]=104$$

For $C_{20}H_{14}X_3Y_2Z/(CH)_{14}X_3Y_2Z$

$$A_c\left(20;\ 15,3,2,1\right)=\frac{1}{120}\left[\binom{20}{15,3,2,1}-15\left(\binom{4}{2,1,0,1}\binom{8}{6,1,1,0}+\binom{4}{0,3,0,1}\binom{8}{7,0,1,0}+\binom{4}{0,1,2,1}\binom{8}{7,1,0,0}\right)\right]=19280$$

$$A_{ac}\left(20;\ 15,3,2,1\right)=\frac{1}{60}\left[15\left(\binom{4}{2,1,0,1}\binom{8}{6,1,1,0}+\binom{4}{0,3,0,1}\binom{8}{7,0,1,0}+\binom{4}{0,1,2,1}\binom{8}{7,1,0,0}\right)\right]=200$$

For $C_{20}H_{14}X_4YZ/(CH)_{14}X_4YZ$

$$A_c\left(20;\ 14,4,1,1\right)=\frac{1}{120}\left[\binom{20}{14,4,1,1}-15\left(\binom{4}{0,2,1,1}\binom{8}{7,1,0,0}+\binom{4}{2,0,1,1}\binom{8}{6,2,0,0}\right)\right]=9636$$

$$A_{ac}\left(20;\ 14,4,1,1\right)=\frac{1}{60}\left[15\left(\binom{4}{0,2,1,1}\binom{8}{7,1,0,0}+\binom{4}{2,0,1,1}\binom{8}{6,2,0,0}\right)\right]=108$$

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

$$A_c\left(20;\ 8,6,6\right)=\frac{1}{120}\left[\begin{array}{l}\binom{20}{8,6,6}+20\binom{2}{2,0,0}\binom{6}{2,2,2}+14\binom{10}{4,3,3}-20\binom{1}{1,0,0}\binom{3}{1,1,1}\\ -15\left[\begin{array}{l}\binom{4}{4,0,0}\binom{8}{2,3,3}+\binom{4}{0,4,0}\binom{8}{4,1,3}+\binom{4}{0,0,4}\binom{8}{4,3,1}\\+\binom{4}{2,2,0}\binom{8}{3,2,1}+\binom{4}{2,0,2}\binom{8}{3,3,2}+\binom{4}{0,2,2}\binom{8}{4,2,2}\end{array}\right]\end{array}\right]=969178$$

$$A_{ac}\left(20;\ 8,6,6\right)=\frac{1}{60}\left[20\binom{1}{1,0,0}\binom{3}{1,1,1}+\binom{10}{4,3,3}+15\left[\begin{array}{l}\binom{4}{4,0,0}\binom{8}{2,3,3}+\binom{4}{0,4,0}\binom{8}{4,1,3}+\binom{4}{0,0,4}\binom{8}{4,3,1}\\+\binom{4}{2,2,0}\binom{8}{3,2,1}+\binom{4}{2,0,2}\binom{8}{3,3,2}+\binom{4}{0,2,2}\binom{8}{4,2,2}\end{array}\right]\right]=2662$$

The results of these calculations are summarized in columns 5, 6 and 7 of table 5 where we report the numbers A_c, A_{ac} and A_{dia} of enantiomers pairs, achiral isomers and diastereoisomers skeletons predicted for the above mentioned heteropolysubstituted DDH derivatives and DDH hetero hetero-analogues.

Table 5. Numbers A_c, A_{ac} and A_{dia} of enantiomers pairs, achiral isomers and diastereoisomers skeletons predicted for the above mentioned heteropolysubstituted DDH derivatives and DDH hetero hetero-analogues.

k	$q_0,..,q_i,,q_k$	*Heteropolysubstituted dodecahedranes*	*Dodecahedrane hetero hetero-analogues*	A_c	A_{ac}	A_{dia}
2	*18,1,1*	$C_{20}H_{18}XY$	$(CH)_{18}XY$	*2*	*3*	*5*
	17,2,1	$C_{20}H_{17}X_2Y$	$(CH)_{17}X_2Y$	*23*	*11*	*34*
	16,3,1	$C_{20}H_{16}X_3Y$	$(CH)_{16}X_3Y$	*151*	*25*	*176*
	16,2,2	$C_{20}H_{16}X_2Y_2$	$(CH)_{16}X_2Y_2$	*233*	*41*	*274*
	15,3,2	$C_{20}H_{15}X_3Y_2$	$(CH)_{15}X_3Y_2$	*1249*	*88*	*1337*
	14,3,3	$C_{20}H_{14}X_3Y_3$	$(CH)_{14}X_3Y_3$	*6373*	*184*	*6557*
	8,6,6	$C_{20}H_8X_6Y_6$	$(CH)_8X_6Y_6$	*969178*	*2662*	*971840*
3	17,1,1,1	$C_{20}H_{16}XYZ$	$(CH)_{17}XYZ$	*54*	*6*	*60*
	16,2,1,1	$C_{20}H_{16}X_2YZ$	$(CH)_{16}X_2YZ$	*471*	*27*	*498*
	15,3,1,1	$C_{20}H_{15}X_3YZ$	$(CH)_{15}X_3YZ$	*2562*	*48*	*2610*
	15,2,2,1	$C_{20}H_{15}X_2Y_2Z$	$(CH)_{15}X_2Y_2Z$	*3824*	*104*	*3928*
	14,4,1,1	$C_{20}H_{14}X_4YZ$	$CH)_{14}X_4YZ$	*9636*	*108*	*9744*
	14,3,2,1	$C_{20}H_{14}X_3Y_2Z$	$(CH)_{14}X_3Y_2Z$	*19280*	*200*	*19480*

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

These results predict the occurrences for di-heteropolysubstitution of DDH with $k=2$, of (A_c,A_{ac})=(2,3)-isomers for the series $C_{20}H_{18}XY/(CH)_{18}XY$; for tri-heteropolysubstitution of DDH with $k=2$ in the series $C_{20}H_{17}X_2Y/(CH)_{17}X_2Y$ (A_c,A_{ac}) = (23,11) isomers and with $k=3$ in the series $C_{20}H_{16}XYZ/$ $(CH)_{16}XYZ$, (A_c,A_{ac})=(54,6)-isomers. For tetra-heteropolysubstitution with $k=2$ in the series $(CH)_{16}X_3Y/C_{20}H_{16}X_3Y$ and $C_{20}H_{16}X_2Y_2/(CH)_{16}X_2Y_2$, (A_c,A_{ac}) = (151,25), (233,41) respectively while for $k=3$ in the series $C_{20}H_{16}X_2YZ/(CH)_{16}X_2YZ$, (A_c,A_{ac})= (471,27)-isomers. For Penta-heteropolysubstitution of DDH where $k=2$ in the series $C_{20}H_{15}X_3Y_2/(CH)_{20}X_3Y_2$ (A_c,A_{ac})=(1249, 88) and for $k=3$ in the series $C_{20}H_{15}X_3YZ/(CH)_{15}X_3YZ$ and $C_{20}H_{15}X_2Y_2Z/$ $(CH)_{15}X_2Y_2Z$ one obtains (A_c,A_{ac})= (2562,48) and (3824,104) isomers skeletons respectively. For hexa-heteropolysubstitution of DDH where $k=2$ in the series $C_{20}H_{14}X_3Y_3/(CH)_{14}X_3Y_3$, (A_c,A_{ac}) = (6373,184) and with $k=3$ in the series $C_{20}H_{14}X_4YZ/(CH)_{14}X_4YZ$ and $C_{20}H_{14}X_3Y_2Z/$ $(CH)_{14}X_3Y_2Z$ (A_c,A_{ac})= (9638, 104), (19280, 200) isomer skeletons respectively. For dodeca-heteropoly substitution of DDH with $k=2$ in the series $C_{20}H_8X_6Y_6/(CH)_8X_6Y_6$, (A_c,A_{ac})=(969178, 2662). The continuation of this work presents in part II the partition of A_c, and A_{ac} into symmetry adapted isomers numbers illustrated by chemical graphs.

5 Concluding remarks

Permutations representations controlling the chirality and the achirality fittingness of 20 substitution sites of DDH submitted to the I_h group action are transformed from binomial and multinomial theorems into generic formula for bipartite enumeration of enantiomers pairs and achiral skeletons of homo and heteropolysubstituted DDH derivatives, DDH homo hetero-analogues and DDH hetero hetero-analogues. This mathematical procedure is a 6 steps-algorithm including:

1-The determination of $\overline{P_{ro}}$ and $\overline{P_{rr}}$ the averaged weights of permutations induced by 60 rotations and 60 rotoreflections of I_h acting on 20 substitutions sites located in a spherical orbit.

2-The construction of permutations representations Δ_c, Δ_{ac} and Σ_{dia} controlling the chirality-achirality fittingness and the diastereoisomerism of DDH derivatives.

3- The formulation of algebraic expressions (eqs.20-26 and eqs.27-36) for counting homogeneous and heterogeneous arrangements of substituents among 20 substitutions sites of DDH.

4- For heteropolysubstituted DDH derivatives $C_{20}H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ and DDH hetero hetero-analogues $(CH)_{q_0}X_{q_1}....Y_{q_i}...Z_{q_k}$ the resolution of partition eqs.32,34,36 is required to obtain pairs of integer sequences $(p_0', p_1', p_2') \leftrightarrow (q_0',...,q_i',...,q_k'), (p_0'', p_1'', p_2'') \leftrightarrow (q_0'',...,q_i'',...,q_k''), (p_0''', p_1''', p_2''')$ $\leftrightarrow (q_0''',...,q_i''',...,q_k''')$ compatible with $(q_0, q_1, ..., q_i, ..., q_k)$.

5- The transformation of Δ_c and Δ_{ac} into generic formulae for computing A_c chiral and A_{ac} achiral isomers skeletons for distinct coisomeric series of DDH derivatives and DDH hetero hetero-analogues (eqs.37-38 and eqs.39-40).

6-The computation of integer sequences (A_c, A_{ac}) satisfying the restriction $A_c + A_{ac} = A_{dia}$ which is used to verify the compliance of diastereoisomers numbers derived from bipartite enumeration with Pólya's coefficients derived from cycle indices.

The above mentioned bipartite enumeration algorithm has two advantages: (a) to perform direct and selective computations of integer sequences (A_c, A_{ac}) of enantiomers pairs and achiral skeletons for simple and complex 3D-structures exhibited by coisomeric series of I_h-based DDH derivatives and DDH heteroanalogues. (b) to circumvent the unwieldiness of classical enumeration methods which require the transformation of cycle indices into enumerating generating functions expanded with high powers series. Such a pattern inventory using permutations representations and combinatorial algebra has a pedagogical approach needed for stereo chemical studies and molecular design of topologically spherical molecules. The continuation of this work presents in part II the formulation and applications of the denumerants of I_h group for symmetry itemized enumeration of dodecahedrane derivatives and heteroanalogues.

References

[1] R. J. Ternansky, D. W. Balogh, L. A. Paquette, Dodecahedrane, *J. Am. Chem. Soc.* **104** (1982) 4503–4504.

[2] L. A. Paquette, R. J. Ternansky, D. W. Balogh, G. Kentgen, Total synthesis of dodecahedrane, *J. Am. Chem. Soc.* **105** (1983) 5446–5450.

[3] IUPAC name:hexadecahydro-5,2,1,6,3,[2,3]butanediyl[1,4]diylidenedipentaleno[2,1,6-cde:2',1',6'-gha]pentalene *CAS number*: 4493-23-6.

[4] P. E. Eaton, Towards dodecahedrane, *Tetrahedron* **35** (1979) 2189–2223.

[5] W. D. Fessner, B. A. R. C. Murty, H. Prinzbach, The pagodane route to dodecahedranes thermal, reductive, and oxidative transformations of pagodanes, *Angew. Chem. Int. Ed. Engl.* **26** (1987) 451–452.

[6] L. A. Paquette, The chemical transliteration of Plato's universe, *Rev. Proc. Natl. Acad. Sci.* **79** (1982) 4495–4500.

[7] L. A. Paquette, D. W. Ballogh, U. D. Kountz, C. G. G. Christoph, Crystal and molecular structure of a pentagonal dodecahedrane, *Science* **211** (1981) 575–576.

[8] F. L. Liu, DFT study on a molecule $C_{25}H_{20}$ with a dodecahedrane cage and a penta prismane cage sharing the same pentagon, *J. Mol. Struct. (Theochem*) **681** (2004) 51–55.

[9] L. A. Paquette, Y. Miyahara, Directed alkyl substitution of the dodecahedrane nucleus. The 1,4-dimethyl, 1,6-dimethy, and 1,4,16-trimethyl derivatives. Indanododecahedrane by stepwise dehydrogenation of a benzylated secoderivative, *J. Org. Chem.* **52** (1987) 1265–1272.

[10] G. Banfalvia, Dodecahedrane minibead polymers, *RSC. Adv*. **4** (2014) 3003–3008.

[11] R. J. Cross, M. Saunders, H. Prinzbach, Putting helium inside dodecahedrane. *Org. Lett.* **1** (1999) 1479–1481.

[12] J. C. Weber, L.A. Paquette, Synthesis of amino-substituted dodecahedranes, seco dodecahedranes and homododecahedranes and their antiviral relationship to 1-amino adamantane, *J. Org. Chem*. **53** (1988) 5315–5320.

[13] F. Wahl, A. Weiler, P. Landenberger, E. Sackers, T. Voss, A. Haas, M. Lieb, D. Hunkler, J. Wörth, L. Knothe, H. Prinzbach, Towards per functionalized dodecahedranes- En route to C20 Fullerene, *Chem. Eur. J.* **12** (2006) 6255–6267.

[14] I. Alkorta, J. Elguero, I Rozas, A. T. Balaban, Theoretical studies of aza analogues of platonic hydrocarbons. Part III. Dodecahedrane and its aza derivatives, *J. Mol. Struct. (Theochem)* **228** (1991) 47–60.

[15] S. Fujita, *Symmetry and Combinatorial Enumeration in Chemistry*, Springer, Berlin, 1991.

[16] S. Fujita, Unit subduced cycle indices with and without chirality fittingness for I_h group. An Application to systematic enumeration of dodecahedrane derivatives., *Bull. Chem. Soc. Jpn*. **63** (1990) 2759–2769.

[17] S. Fujita, Enumeration of three dimensional structures derived from a dodecahedrane skeleton under a restriction condition. II. The restricted partial cycle index (RPCI) method based on restricted subduced cycle indices, *J. Comput. Chem.* **11** (2012) 140–148.

[18] D. Moran, F. Stahl, E. D. Jemmis, H. F. Schaefer, P. R. von Schleyer, Structures, stabilities and ionization potentials of dodecahedrane endohedral complexes, *J. Phys. Chem. A* **106** (2002) 5144–5154.

[19] G. G. Christoph, P. Engel, R. Usha, D. W. Balogh, L.A. Paquette, Comparative X-ray crystal structure analysis of C_{2v} dimethyl monoseco dodecahedrane and D_{3d} dimethyl dodecahedrane. The remarkable consequence of a missing framework bond on molecular topology, *J. Am. Chem. Soc.* **104** (1982) 784–791.

[20] F. L. Liu, Theoretical study of the coplanar double edge dodecahedrane $C_{35}H_{30}$, *Phys. Chem. Chem. Phys.* **6** (2004) 906–909.

[21] S. Lee, Y. J. Cho, K. Lee, Five regioisomers of dimethyl dodecahedrane derivatives: A hybrid DFT B3LYP study, *J. Chem.* **2017** (2017) 1–7.

[22] Y. G. Lee, S. Lee, K. H. Lee, DFT study for substitution patterns of $C_{20}H_{18}X_2$ regioisomers (X=F, Cl, Br or OH), *Bull. Korean Chem. Soc.* **33** (2012) 641–646.

[23] A. T. Balaban, Valence isomers of heteroannulennes or of substtituted annulenes. Coisomeric Multigraphs., *Rev. Roum. Chim.* **19** (19/74) 1323–1342.

[24] G. Polya, R. C. Read, *Combinatorial Enumeration of Graphs, Groups and Chemical Compounds*, Springer, Berlin, 1987.

[25] A. T. Balaban (Ed.), *Chemical Applications of Graph Theory*, Academic Press, London, 1976.