MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **89** (2023) 301–323
ISSN: 0340–6253
doi: 10.46793/match.89-2.301N

Linear Spaces of Permutomers and Symmetry Itemized Isomers Numbers of C_{2V}-Based Cuneane Derivatives and Heteroanalogues. II

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(Received February 28, 2022)

Abstract

In application of part I this paper presents (a) 4- and 5-dimensional permutomers and symmetry itemized isomers count vectors (PCV_s and $IICV_s$). (b) the collection of these vectors in the form of permutomers count matrices (PCMs) and itemized isomers count matrices ($IICM_s$) (c) the structure of the V_4 and V_5 multidimensional vector spaces of isomers numbers of substituted C_{2v}-based cuneane derivatives and cuneane heteroanalogues.

1 Introduction

The chemistry of cage shaped eight carbon hydrocarbons and their derivatives has been developed since the successful synthesis of cubane [1, 2]. Cuneane or Pentacyclo $[3.3.0.0^{2,4}.0^{3,7}.0^{6,8}]$ octane, a saturated C_8H_8 hydrocarbon belongs to this group of chemical compounds. It is obtined

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from cubane by metal-ion catalyzed σ- bond rearrangement [3, 5]. Some cuneane derivatives more stable than the corresponding cubanes manifest liquid crystal properties [6]. NMR studies [7] have shown that the geometry of cuneane molecule is a hexahedron of C_{2V} symmetry which displays one pair of edge fused 5-gonal faces, one pair of edge-fused 4-gonal faces and 2 3-gonal faces at eclipsed position.

2 Classification of coisomeric substituted cuneane derivatives and cuneane heteroanalogues

Let us consider the substitutions replacing hydrogen atoms by achiral substituents or the replacements of CHgroups by trivalent heteroatoms as arrangements in distinct ways of objects of the same kind or different kinds among 8 positions of cuneane molecule submitted to permutations induced by the C_{2V} group. Substituted cuneane derivatives and cuneane heteroanalogues derived from such arrangements may be classified into 4 groups as follows:

1- Homosubstituted cuneane derivatives with the molecular formula $C_8H_{8-q}X_q$ (or $C_8H_{q_0}X_{q_1}$) issued from homogeneous arrangements of q achiral substituents of the same kind X among 8 substitution positions occupied by hydrogen atoms submitted to permutations induced by distinct symmetry operations of C_{2V}.

2- Cuneane homo-heteroanalogues $(CH)_{8-q}X_q$ (or $(CH)_{q_0}X_{q_1}$) issued from homogeneous arrangements putting in accord with the obligatory minimum valency (OMV) restriction (OMV=3), qX trivalent heteroatoms of the same kind among 8 CH positions permuted by distinct symmetry operations of C_{2V}.

3- Heteropolysubstituted cuneane derivatives $C_8H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ issued from heterogeneous arrangements of q_0H and $q_1X, ...q_iY, ..., q_kZ$ and achiral substituents of different kinds among 8 substitution sites permuted by distinct symmetry operations of C_{2V}.

4- cuneane hetero-heteroanalogues $(CH)_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ are obtained from heterogeneous arrangements putting in accord with the obligatory minimum valency restriction (OMV=3)$q_0 H$and $q_1 X, ...q_i Y, ..., q_k Z$ trivalent heteroatoms of different kinds among 8CH positions permuted by distinct symmetry operations of C_{2V}. We recall that throughout this study the indices of the molecular formula have the following significance:

I-q_0 is the number of unsubstituted hydrogen atoms while the indices $(q_1, ...q_i, ..., q_k)$ are partial degrees of substitution i.e. numbers of non hydrogen achiral substituents of different kinds X, Y,.....,Z.

II-The sub-indices $1 \leq i \leq k$ indicate the substitution order i which is the number of distinct types of non H substituents.

III-The set of indices $(q_0, q_1, ...q_i, ..., q_k)$ satisfy the restriction

$$\sum_{i=0}^{k} q_i = 8 \tag{1}$$

The mathematical properties presented in part I are applied in this paper to derive 4- and 5-dimensional permutomers and symmetry itemized isomers count vectors (PCVs and IICVs) and construct the structure of V_4 and V_5 multidimensional vector spaces of isomers numbers of substituted C_{2V}-based cuneane derivatives and cuneane heteroanalogues.

3 Formulation of the denumerants of C_{2v} group for symmetry itemized enumeration of cuneane derivatives and heteroanalogues

3.1 1 Permutations of carbon and hydrogen atoms of cuneane under the C_{2v} group action

Let us represent the structure of cuneane by a tridimensional hydrogen depleted graph given in fig.1 where 8 black vertices of degree 3 symbolize carbon atoms indicated by alphabetical labels of the set $C_8 = (a, b, c, d, a', b', c', d')$. These 8 interconnected carbon atoms are attached to 8 hydrogen atoms (not indicated in the graph) which compose the set H_8. These attachments form a cluster of 8CH groups which gives rise to a

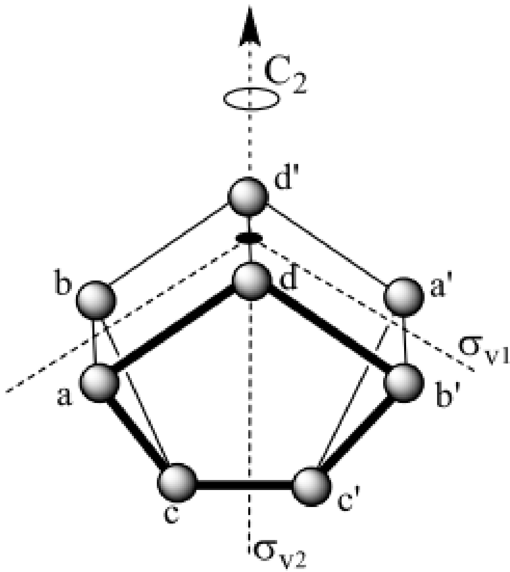

Figure 1. 3D-hydrogen depleted graph of cuneane

unicage shaped hydrocarbon of C_{2v} symmetry with 4 symmetry operations given in eq.2.

$$C_{2V} = E, C_2, \sigma_{v_1}; \sigma_{v_2} \tag{2}$$

The C_{2v} group action on cuneane skeleton consisting to apply the abovementioned symmetry operations $g_i \epsilon C_{2v}$ to the cluster of 8 CH groups generates the permutations representations $P^{C_{2v}}H_8$ and $P^{C_{2v}}C_8$ given in eqs.1 and 4, respectively.

$$P^{C_{2v}}\boldsymbol{H}_8 = P^E\boldsymbol{H}_8, P^{C_2}\boldsymbol{H}_8, P^{\sigma_{v_1}}\boldsymbol{H}_8, P^{\sigma_{v_2.}}\boldsymbol{H}_8 \tag{3}$$

$$P^{C_{2v}}\boldsymbol{C}_8 = P^E\boldsymbol{C}_8, P^{C_2}\boldsymbol{C}_8, P^{\sigma_{v_1}}\boldsymbol{C}_8, P^{\sigma_{v_2.}}\boldsymbol{C}_8 \tag{4}$$

The right hand side terms of eqs.3 and 4 are permutations induced by 4 distinct conjugacy classes of symmetry operations of C_{2v}. These permutations are written in cycle structure notation[8] as follows :

$$P^{E}\boldsymbol{H}_8 = 1^8,\ P^{C_2}\boldsymbol{H}_8 = 2^4,\ P^{\sigma_{v1}}\boldsymbol{H}_8 = 2^4, P^{\sigma_{v2}}\boldsymbol{H}_8 = 1^2 2^3 \tag{5}$$

$$P^{E}\boldsymbol{C}_8 = 1^8,\ P^{C_2}\boldsymbol{C}_8 = 2^4,\ P^{\sigma_{v1}}\boldsymbol{C}_8 = P^{\sigma_{v2}}\boldsymbol{C}_8 = 1^2 2^3 \tag{6}$$

One may notice that the right-hand side terms in eqs.5-6 are equivalent. Therefore $P^{C_{2v}}H_8$ and $P^{C_{2v}}C_8$ have the same cycle structure notations as follows:

$$P^{C_{2v}}H_8 \equiv P^{C_{2v}}C_8 = \left[1^8\right], \left[2^4\right], \left[1^2 2^3\right], \left[1^2 2^3\right] \tag{7}$$

Hence, cuneane substituted derivatives and cuneane heteroanalogues issued from equivalent sets of arrangements regulated by the permutations given in eq.7 are coisomeric structures [9].

3.2 Permutational isomers numbers of homo-and hete-ropolysubstituted cuneane derivatives and cuneane heteroanalogues

Let $(N_E, N_{C_2}, N_{\sigma_{v_1}}, N_{\sigma_{v_2}})$ denote permutomers numbers of cuneane substituted derivatives or corresponding cuneane heteroanalogues issued from arrangements regulated by the terms given in eq.7. Such numbers are calculated as follows :

Rule 1 : Permutational isomers numbers $N_E, N_{C_2}, N_{\sigma_{v_1}}, N_{\sigma_{v_2}}$ for a homopolysubstituted C_{2v}-based cuneane derivative $C_8H_{8-q}X_q$ or its cuneane homo hetero-analogue $(CH)_{8-q}X_q$ are numbers of distinct ways of putting q achiral substituents of the same kind X among 8 positions submitted to permutations of classes $1^8, 2^4, 1^2 2^3$ and$1^2 2^3$. They are derived from binomial theorem as follows :

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

$$2^4 \to N_{C2} = \binom{4}{q/2} \tag{9}$$

$$1^2.2^3 \rightarrow N_{\sigma_{v_1}} = N_{\sigma_{v_2}} = \sum_{\alpha=0}^{2} \binom{2}{\alpha} \binom{3}{4q-\alpha)/2} \tag{10}$$

Rule 2 : Permutational isomers numbers $(N_E, N_{C_2}, N_{\sigma_{v_1}}, N_{\sigma_{v_2}})$ for a heteropolysubstituted cuneane derivative $C_8H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ or its cuneane hetero hetero-analogues $(CH)_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ are numbers of placements in distinct ways of $q_0H$and $q_1X, ...q_0Y, ..., q_kZ$ achiral substituents of diffe-rent kinds among 8 positions submitted to permutations of classes $1^8, 2^4, 1^22^3$ and 1^22^3. These numbers are derived from multinomial theorem as follows:

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

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

$$1^2.2^4 \rightarrow N_{\sigma_{V_1}} = N_{\sigma_{V_2}} = \sum_{\lambda} \binom{2}{p_0', ..., p_i', ..., p_k'} \binom{3}{q_0', ..., q_i', ..., q_k'} \tag{13}$$

with the restrictions

$$\sum_{i=0}^{k} p_i' = 2, \quad \sum_{i=0}^{k} q_i' = 3, \quad q_i' = \frac{q_i - p_i'}{2} \tag{14}$$

The numbers $N_E, N_{C_2}, N_{\sigma_{v_1}}, N_{\sigma_{v_2}}$ derived from eqs.8-10 or eqs.11-13 are collected to form a 4 entries permutomers count vector (PCV) for a substituted cuneane which is expressed as follows :

$$PCV(MX) = (N_E, N_{C_2}, N_{\sigma_{v_1}}, N_{\sigma_{v_2}}) \tag{15}$$

where = $C_8H_{8-q}X_q$, $(CH)_{8-q}X_q$, $(CH)_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ or $C_8H_{q_0}X_{q_1}...$ $Y_{q_i}...Z_{q_k}$.

3.3 The Sylvester's denumerants of C_{2V} group applied to cuneane

The Sylvester's denumerants [10,11]of C_{2v} group (see eq.16 part I) applied for deriving symmetry itemized isomers numbers $a_{c_1}, a_{c_2}, a_{c_s}, a_{c'_s}, a_{c_{2v}}$ are given as follows:

-For a homopolysubstituted cuneane derivative and its cuneane homo-hetero-analogue $(CH)_{8-q}X_q$

$$N_E = (4a_{c_1} + 2a_{c_2} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}}) = \binom{8}{q} \tag{16}$$

$$N_{C_2} = (2a_{c_2} + a_{c_{2v}}) = \binom{4}{q/2} \tag{17}$$

$$N_{\sigma_{v_1}} = N_{\sigma_{v_2}} = 2a_{c_s} + a_{c_{2v}} = 2a_{c'_s} + a_{c_{2v}} = \sum \binom{2}{\alpha}\binom{3}{(q-\alpha)/2} \tag{18}$$

For a heteropolysubstituted cuneane derivative $C_8H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ and its cuneane hetero heteroanalogue $(CH)_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$:

$$N_E = (4a_{c_1} + 2a_{c_2} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}}) = \binom{8}{q_0, ...q_i, ...q_k} \tag{19}$$

$$N_{C_2} = (2a_{c2} + a_{c_{2v}}) = \binom{4}{q_0/2, ...q_i/2, ...q_k/2} \tag{20}$$

$$N_{\sigma_{v_1}} = N_{\sigma_{v_2}} = 2a_{c_s} + a_{c_{2v}} = 2a_{c'_s} + a_{c_{2v}} = \sum_{\lambda} \binom{2}{p_0, ..., p_i, ..., p_k}\binom{3}{q'_0, ..., q'_i, ..., q'_k} \tag{21}$$

$$q'_i = \frac{q_i - p_i}{2}, \sum_i p_i = 2, and \sum_i q'_i = 3 \tag{22}$$

4 Applications to symmetry itemized enumeration and construction of the linear spaces of C_{2v}-based isomers numbers for coisomeric series of substituted cuneane derivatives and heteroanalogues

Example 1 : Symmetry itemized enumeration and determination of linear spaces of isomers numbers of homopolysubstituted C_{2v}-based cuneane derivatives $C_8H_{8-q}X_q$ and cuneane homo heteroanalogues $(CH)_{8-q}X_q$ where $1 \leq q \leq 8$. By applying eqs.8-10 and 16-18 to these series one derives the PCV_s and the denumerants generating the linear mapping between PCV_s and $IICV_s$ ($PCVs \rightarrow IICVs$) calculated for each degree of substitution q. These vectors are collected to form the PCM and the IICM representing the V_4 and V_5 linear spaces of permutomers and symmetry itemized isomers numbers for these coisomeric series. The calculations are as follows : For q=1 in the series C_8H_7X and $(CH)_7X$,

$N_E = 4a_{c_1} + 2a_{c_2} + 2a_{c_s} + 2a_{c_s'} + a_{c_{2v}} = \binom{8}{1}$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N_{\sigma_1} = 2a_{c_s} + a_{c_{2v}} = \binom{2}{1}\binom{3}{0} = 2$

$N_{\sigma_{v_2}} = 2a_{c_s'} + a_{c_{2v}} = \binom{2}{1}\binom{3}{0} = 2$

$a_{c_1} = 1, a_{c_2} = 0, a_{c_s} = 1, a_{c_{2v}} = 0, a_{c_s'} = 1,$

$IICV(C_8H_7X) = (1, 0, 1, 1, 0) \rightarrow PCV(C_8H_7X) = (8, 0, 2, 2)$

For q=2 in the series C_8H_7X and $(CH)_6X_2$,

$N_E = 4a_{c_1} + 2a_{c_2} + 2a_{c_s'} + a_{c_{2v}} = \binom{8}{2} = 28$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = \binom{4}{1} = 4$

$N_{\sigma_1} = 2a_{cs} + a_{c_{2v}} = \binom{2}{0}\binom{3}{1} + \binom{2}{2}\binom{3}{0} = 4$

$N_{\sigma_{v2}} = 2a_{c's} + a_{c_{2v}} = \binom{2}{0}\binom{3}{1} + \binom{2}{2}\binom{3}{0} = 4$

$a_{c_1} = 5, a_{c_2} = 1, a_{c_s} = 1, a_{c_s'} = 1, a_{c_{2v}} = 2,$

$PCV(C_8H_6X_2) = (28, 4, 4, 4) \rightarrow IICV(C_8H_7X) = (5, 1, 1, 1, 2)$

For q=3 in the series $C_8H_5X_3$ and $(CH)_5X_3$

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c_s'} + a_{c_{2v}} = \binom{8}{3} = 56$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N_{\sigma_1} = 2a_{c_s} + a_{c_{2v}} = \binom{2}{1}\binom{3}{1} = 6$

$N_{\sigma_{v_2}} = 2a_{c_s}^{\gamma_1} + a_{c_{2v}}^{\gamma_2} = \binom{2}{1}\binom{3}{1} = 6$

$a_{c_1} = 2, a_{c_2} = 0, a_{c_s} = 3, a_{c_s'} = 3, a_{c_{2v}} = 0,$

$PCV(C_8H_5X_3) = (56, 0, 6, 6) \rightarrow IICV(C_8H_5X_3) = (2, 0, 1, 1, 0)$

For q=4 in the series $C_8H_4X_4$ and $(CH)_4X_4$

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c's} + a_{c_{2v}} = \binom{8}{4} = 70$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = \binom{4}{2} = 6$

$N_{\sigma_1} = 2a_{c_s} + a_{c_{2v}} = \binom{2}{0}\binom{3}{1} + \binom{2}{2}\binom{3}{1} = 6$

$N_{\sigma_{v2}} = 2a_{c's} + a_{c_{2v}} = \binom{2}{0}\binom{3}{1} + \binom{2}{2}\binom{3}{1} = 6$

$a_{c_1} = 14, a_{c_2} = 2, a_{cs} = 2, a_{c's} = 2, a_{c_{2v}} = 2,$

$PCV(C_8H_4X_4) = (70, 6, 6, 6) \rightarrow IICV(C_8H_4X_4) = (14, 2, 2, 2, 2)$

For q=8 in the series C_8X_8 ,

$N_E = \binom{8}{8}, N_{C_2} = N_{\sigma_{v1}} = \binom{4}{4} = 1, N_{\sigma_{v2}} = \binom{2}{2}\binom{3}{3} = 1$

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c_s'} + a_{c_{2v}} = 1$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 1$

$N_{\sigma_1} = 2a_{c_s} + a_{c_{2v}} = 1$

$N_{\sigma_{v_2}} = 2a_{c's} + a_{c_{2v}} = 1$

$a_{c_1} = a_{c_2} = a_{cs} = a_{c_s'} = 0, a_{c_{2v}} = 1$

PCV(C_8X_8 or X_8)=(1, 1, 1, 1)→ IICV(C_8X_8 or X_8)=(0, 0, 0, 0, 1),

We collect 4-dimensional PCV_s and 5-dimensional IICVs to form the PCM and the IICM that construct the V_4 and V_5 associated vector spaces of permutomers numbers and symmetry itemized isomers numbers for these coisomeric series as follows:

$$PCM\begin{pmatrix} C_8H_{q_0}X_{q_1} \\ or \\ (CH)_{q_0}X_{q_1} \end{pmatrix} = \begin{pmatrix} q_0,q_1 \\ 8,0 \\ 7,1 \\ 6,2 \\ 5,3 \\ 4,4 \end{pmatrix} \underbrace{\begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v_1}} & N_{\sigma_{v_2}} \\ 1 & 1 & 1 & 1 \\ 8 & 0 & 2 & 2 \\ 28 & 4 & 4 & 4 \\ 56 & 0 & 6 & 6 \\ 70 & 0 & 6 & 6 \end{pmatrix}}_{V_4} \rightarrow IICM\begin{pmatrix} C_8H_{q_0}X_{q_1} \\ or \\ (CH)_{q_0}X_{q_1} \end{pmatrix} = \begin{pmatrix} q_0,q_1 \\ 8,0 \\ 7,1 \\ 6,2 \\ 5,3 \\ 4,4 \end{pmatrix} \underbrace{\begin{pmatrix} a_{c_1} & a_{c_2} & a_{c_s} & a_{c_s'} & a_{c_{2v}} \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 5 & 1 & 1 & 1 & 2 \\ 11 & 0 & 3 & 3 & 0 \\ 14 & 2 & 2 & 2 & 2 \end{pmatrix}}_{V_5}$$

The row vectors entries of the PCM and IICM are interpreted as follows : for coisomeric series $C_8H_{q_0}X_{q_1}$) and $(CH)_{q_0}X_{q_1}$ where (q_0, q_1)=(8,0), (7,1), (6,2), (5,3), (4,4) the linear mappings between 4 entries PCVs and 5 entries $IICV_s$ are :

(1, 1, 1, 1)→(0,0,0,0,1) ; (8, 0, 2, 2)→(1,0,1,1,0) ;

(28, 4, 4, 4)→(5,1,1,1,2); (56, 0, 6, 6)→(11,0,3,3,0);

(70, 6, 6, 6)→(14,2,2,2,2).

These transformations of 4-tuples of permutomers numbers N_E, N_{C_2}, $N_{\sigma_{v1}}, N_{\sigma_{v2}}$ into 5-tuples of symmetry itemized isomers numbers a_{cs}, a_{c_2}, $a_{cs}, a_{c's}, a_{c_{2v}}$ predict the occurrences of :

$(0,0,0,0,C_{2v})$; $(C_1,0,C_s,C'_s,0)$; $(5C_1,C_2,C_s,C'_s,2C_{2v})$;

$(11C_1,0,3C_s,3C'_s,0)$; $(14C_1,2C_2,2C_s,2C'_s,2C_{2v})$ isomers for coisomeric series $C_8H_8/C_8X_8, (C_8H_7X)/(CH)_7X, C_8H_6X_2/(CH)_6X_2$, $C_8H_5X_3/(CH)_5X_3, (C_8H_4X_4)/(CH)_4X_4))$, respectively.

The illustration of these results is given in fig.2.

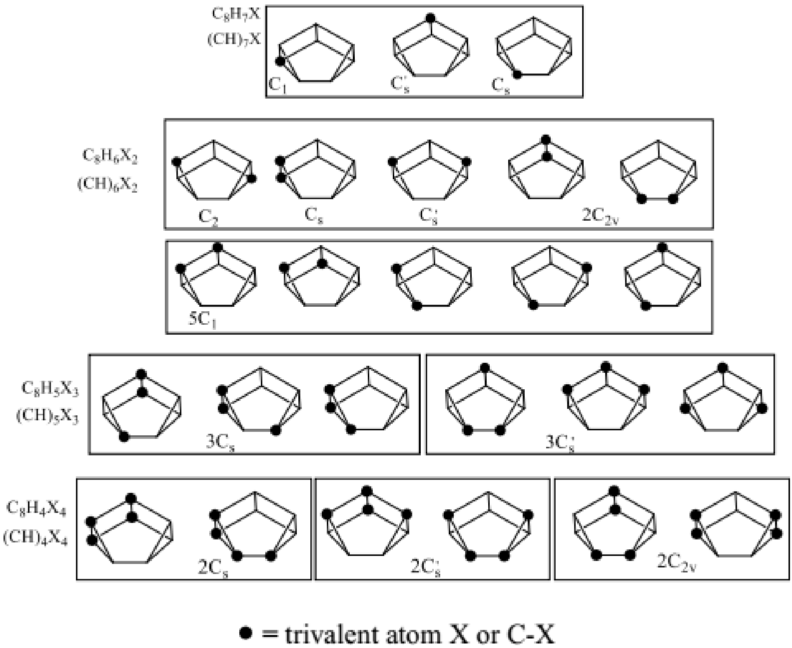

Figure 2. Graphs of $C_1 + C_s + C'_s$, $5C_1 + C_2 + C_s + C'_s + 2C_{2v}$, $3C_s + 3C'_s$,$2C_s + 2C'_s + 2C_{2v}$ isomers of homopolysubstituted cuneanes and cuneane homo-heteroanalogues for coisomeric series $(C_8H_7X)/(CH)_7X, C_8H_6X_2/(CH)_6X_2$, $C_8H_5X_3/(CH)_5X_3, (C_8H_4X_4)/(CH)_4X_4))$.

Example 2: Symmetry itemized enumeration and vector spaces of isomers numbers of coisomeric series of heteropolysubstituted C_{2v}-based cuneane derivatives and their cuneane hetero-heteroanalogues symbolized by the molecular formulas given in table 1 hereafter and where $\sum_{i=0}^{k} q_i = 8$.

Table 1. Molecular formulas of coisomeric series of heteropolysubstituted C_{2v}-based cuneane derivatives and their cuneane hetero-heteroanalogues .

$C_8H_{q0}X_{q1}Y_{q2}/(CH)_{q0}X_{q1}Y_{q2})$	$C_8H_{q0}V_{q1}W_{q3}X_{q1}Y_{q4}Z_{q5}/$ $(CH)_{q0}V_{q1}W_{q3}X_{q1}Y_{q4}Zq_5$
$C_8H_{q0}X_{q1}Y_2Z_{q3}/(CH)_{q0}X_{q1}Y_{q2}Z_{q3}$	$C_8H_{q0}U_{q1}V_{q2}W_{q3}X_{q4}Y_{q5}Zq_6/$ $(CH)_{q0}U_{q1}V_{q2}W_{q3}X_{q4}Y_{q5}Z_{q6}$
$C_8H_{q0}W_{q1}X_{q2}Y_{q3}Z_{q4}/(CH)_{q0}W_{q1}X_{q2}Y_{q3}Z_{q4}$	$C_8H_{q0}T_{q1}U_{q2}V_{q3}W_{q4}X_{q5}Y_{q6}Z_{q7}/$ $(CH)_{q0}T_{q1}U_{q2}V_{q3}W_{q4}X_{q5}Y_{q6}Z_{q7}$

By applying eqs.16-18 and 19-21 to these series one obtains the PCV_s and the denumerants calculated for each sequence of substitution indices $(q_0, q_1, ..., q_K)$. The resolution of these denumerants generates the $IICV_s$ and the linear mappings $PCV_s \rightarrow IICV_s$ for distinct heteropolysubstitutions. The calculations are as follows :

In the series $C_8H_{q_0}X_{q_1}Y_{q_2}/(CH)_{q_0}X_{q_1}Y_{q_2})$ where $(q_0, q_1, q_2) = (6, 1, 1)$, $(5, 2, 1), (4, 3, 1), (4, 2, 2), (3, 3, 2)$, the denumerants solved are:

For $q_0, q_1, q_2 = (6, 1, 1)$ in C_8H_6XY

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{6,1,1} = 56$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N^{\gamma}_{\sigma_1} = 2a_{c_s} + a_{c_{2v}} = \binom{2}{0,1,1}\binom{3}{3,0,0} = 2$

$N_{\sigma_{v_2}} = 2a_{c'_s} + a_{c_{2v}} = \binom{2}{0,1,1}\binom{3}{3,0,0} = 2$

$a_{c_1} = 2, a_{c_2} = 0, a_{cs} = 1, a_{c'_s} = 1, a_{c_{2v}} = 0,$

$PCV(C_8H_6XY) = (56, 0, 2, 2) \rightarrow IICV(C_8H_6XY) = (13, 0, 1, 1, 0)$

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

$N_E = 4a_{c_1} + 2a_{cs} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{5,2,1} = 168$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N_{\sigma_1} = 2a_{c_s} + a_{c_{2v}} = \binom{2}{1,0,1}\binom{3}{2,1,0} = 6$

$N_{\sigma_{v_2}} = 2a_{c'_s} + a_{c_{2v}} = \binom{2}{1,0,1}\binom{3}{2,1,0} = 6$

$a_{c_1} = 39, a_{c_2} = 0, a_{cs} = a_{c's} = 3, a_{c_{2v}} = 0,$

$PCV(C_8H_5X_2Y) = (168, 0, 6, 6) \rightarrow IICV(C_8H_5X_2Y) = (39, 0, 3, 3, 0)$

For $q_0, q_1, q_2 = (4, 3, 1)$ in $C_8H_4X_3Y$

$N_E = 4a_{c_1} + 2a_{cs} + 2a_{c's} + a_{c_{2v}} = \binom{8}{4,3,1} = 280$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N_{\sigma_1} = 2a_{c_s} + a_{c_{2v}} = \binom{2}{0,1,1}\binom{3}{2,1,0} = 6$

$N_{\sigma_{v_2}} = 2a_{c'_s} + a_{c_{2v}} = \binom{2}{0,1,1}\binom{3}{2,1,0} = 6$

$a_{c_1} = 67, a_{c_2} = 0, a_{cs} = a_{c's} = 3, a_{c_{2v}} = 0,$

$PCV(C_8H_4X_3Y) = (280, 0, 6, 6) \rightarrow IICV(C_8H_4X_3Y) = (67, 0, 3, 3, 0)$

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

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{4,2,2} = 420$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = \binom{4}{2,1,1} = 12$

$N_{\sigma_1} = 2a_{c_s} + a_{c_{2v}} = \binom{2}{0,0,0}\binom{3}{1,1,1} + \binom{2}{0,2,0}\binom{3}{2,0,1} + \binom{2}{0,0,2}\binom{3}{2,1,0} = 12$

$N_{\sigma_{v2}} = 2a_{c'_s} + a_{c_{2v}} = \binom{2}{2,0,0}\binom{3}{1,1,1} + \binom{2}{0,2,0}\binom{3}{2,0,1} + \binom{2}{0,0,2}\binom{3}{2,1,0} = 12$

$a_{c_1} = 97, a_{c_2} = a_{c_s} = a_{c'_s} = 5, a_{c_{2v}} = 2,$

$PCV(C_8H_4X_2Y_2) = (420, 12, 12, 12) \rightarrow IICV(C_8H_4X_2Y2) = (97, 5, 5, 5, 2)$

For $q_0, q_1, q_2 = (3, 3, 2)$ in $C_8H_3X_3Y_2$

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{4,2,2} = 420$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = \binom{4}{2,1,1} = 12$

$N_{\sigma_1} = 2a_{c_s} + a_{c_{2v}} = \binom{2}{2,0,0}\binom{3}{1,1,1} + \binom{2}{0,2,0}\binom{3}{2,0,1} + \binom{2}{0,0,2}\binom{3}{2,1,0} = 12$

$N_{\sigma_{v_2}} = 2a_{c'_s} + a_{c_{2v}} = \binom{2}{2,0,0}\binom{3}{1,1,1} + \binom{2}{0,2,0}\binom{3}{2,0,1} + \binom{2}{0,0,2}\binom{3}{2,1,0} = 12$

$a_{c_1} = 134, a_{c_2} = 0, a_{cs} = a_{c's} = 6, a_{c_{2v}} = 0,$

$PCV(C_8H_3X_3Y_2) = (560, 0, 12, 12) \rightarrow IICV(C_8H_3X_3Y2) = (134, 0, 6, 6, 0)$

We collect 4-dimensional PCV_s and 5-dimensional $IICV_s$ to form the PCM and the IICM composing the V_4 and V_5 associated vector spaces of permutomers and symmetry itemized isomers numbers for these coisomeric series as follows:

$$PCM \begin{pmatrix} C_8H_{q_0}X_{q_1}Y_{q_2} \\ or \\ (CH)_{q_0}X_{q_1}Y_{q_2} \end{pmatrix} = \begin{pmatrix} q_0q_1q_2 \\ 6,1,1 \\ 5,2,1 \\ 4,3,1 \\ 4,2,2 \\ 3,3,2 \end{pmatrix} \underbrace{\begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v_1}} & N_{\sigma_{v_2}} \\ 56 & 0 & 2 & 2 \\ 168 & 0 & 6 & 6 \\ 280 & 0 & 6 & 6 \\ 420 & 12 & 12 & 12 \\ 560 & 0 & 12 & 12 \end{pmatrix}}_{V_4}$$

$$\downarrow$$

$$IICM \begin{pmatrix} C_8H_{q_0}X_{q_1}Y_{q_2} \\ or \\ (CH)_{q_0}X_{q_1}Y_{q_2} \end{pmatrix} = \begin{pmatrix} q_0,q_1,q_2 \\ 6,1,1 \\ 5,2,1 \\ 4,3,1 \\ 4,2,2 \\ 3,3,2 \end{pmatrix} \underbrace{\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 13 & 0 & 1 & 1 & 0 \\ 39 & 0 & 3 & 3 & 0 \\ 67 & 0 & 3 & 3 & 0 \\ 97 & 5 & 5 & 5 & 2 \\ 134 & 0 & 6 & 6 & 0 \end{pmatrix}}_{V_5}$$

For coisomeric series $C_8H_{q_0}X_{q_1}Y_{q_2}$ and $(CH)_{q_0}X_{q_1}Y_{q_2})$ where q_0, q_1, q_2 = (6,1,1), (5,2,1), (4,3,1), ((4,2,2) (3,3,2) the data of linear mappings between 4 entries PCV_s and 5 entries IICVs are as follows : (56, 0, 2, 2)→(13,0,1,1,0); (168, 0, 6, 6)→(39,0,3,3,0); (280,0,6,6)→(67,0,3,3,0); (420,12,12,12)→(97,5,5,5,2) ;(560,0,12,12)→(134,0,6,6,0). These transformations of 4-tuples of permutomers numbers $N_E, N_{C_2}, N_{\sigma_{v_1}}, N_{\sigma_{v_2}}$ into 5-tuples of symmetry itemized isomers numbers $a_{c_s}, a_{c_2}, a_{c_s}, a_{c'_s}, a_{c_{2v}}$ predict the occurrences of $(13C_1, 0, C_s, C'_s, 0)$; $(39C_1, 0, 3C_s, 3C'_s, 0)$; $(67C_1, 0, 3C_s, 3C'_s, 0)$; $(97C_1, 5C_2, 5C_s, 5C'_s, 2C_{2v})$; $(134C_1, 0, 6C_s, 6C'_s, 0)$ isomers for $C_8H_6XY, C_8H_5X_2Y, C_8H_4X_3Y, C_8H_4X_2Y_2, C_8H_3X_3Y_2$ and their corresponding hetero-heteroanalogues $(CH)_6XY, (CH)_5X_2Y, (CH)_4X_3Y, (CH)_4X_2Y_2, (CH)_3X_3Y_2$. The graphs depicting $13C_1 + C_s + C'_s$, $3C_s + 3C'_s$, $3C_s + 3C'_s$, $5C_2 + 5C_s + 5C'_s + 2C_{2v}$ skeletons of coisomeric series $C_8H_6XY/(CH)_6XY, C_8H_5X_2Y/(CH)_5X_2Y, C_8H_4X_3Y/(CH)_4X_3Y$ and $C_8H_4X_2Y_2/(CH)_4X_2Y_2$ are given in Fig. 3.

In the series $C_8H_{q_0}X_{q_1}Y_{q_2}Zq_3/(CH)_{q_0}X_{q_1}Y_{q_2}Zq_3)$ where $(q_0, q_1, q_2, q_3) = (5,1,1,1), (4,2,1,1), (3,3,1,1), (3,2,2,1), (2,2,2,2)$, the denumerants are as follows:

For $q_0, q_1, q_2, q_3 = (5,1,1,1)$ in C_8H_5XYZ

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{5,1,1,1} = 336$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N_{\sigma_1} = 2a_{cs} + a_{c_{2v}} = 0$

$N_{\sigma_{v_2}} = 2a_{c's} + a_{c_{2v}} = 0$

$a_{c_1} = 84, a_{c_2} = a_{cs} = a_{c'_s} = a_{c_{2v}} = 0,$

$PCV(C_8H_5XYZ) = (336, 0, 0, 0) \to IICV(C_8H_5XYZ) = (84, 0, 0, 0, 0)$

For $q_0, q_1, q_2, q_3 = (4,2,1,1)$ in $C_8H_4X_2YZ$

$N_E = 4a_{c_1} + 2a_{c_2} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{4,2,1,1} = 840$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N_{\sigma_1} = 2a_{c_s} + a_{c_{2v}} = \binom{2}{0,0,1,1}\binom{3}{2,1,0,0} = 6$

$N_{\sigma_{v_2}} = 2a_{c'_s} + a_{c_{2v}} = \binom{2}{0,0,1,1}\binom{3}{2,1,0,0} = 6$

$a_{c_1} = 207, a_{c_2} = 0, a_{cs} = a_{c'_s} = 3, a_{c_{2v}} = 0,$

$PCV(C_8H_4X_2YZ) = (840, 0, 6, 6) \to IICV(C_8H_4X_2YZ) = (207, 0, 3, 3, 0)$

For $q_0, q_1, q_2, q_3 = (3,3,1,1)$ in $C_8H_3X_3YZ$

$N_E = 4a_{c_1} + 2a_{cs} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{3,3,1,1} = 1120$

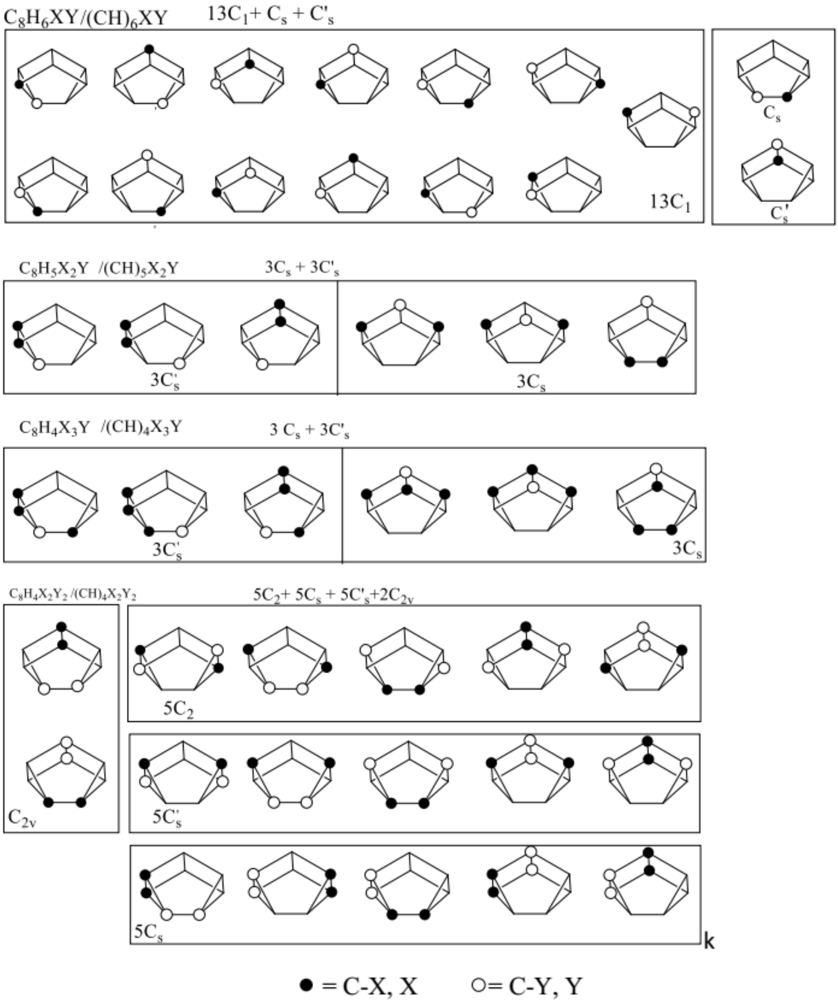

Figure 3. Graphs $13C_1 + C_s + C_s'$, $3C_s + 3C_s'$, $3C_s + 3C_s'$, $5C_2 + 5C_s + 5C_s' + 2C_{2v}$ isomers of heteropolysubstituted cuneanes and cuneane hetero-heteroanalogues of coisomeric series$C_8H_6XY/(CH)_6XY, C_8H_5X_2Y/(CH)_5X_2Y$, $C_8H_4X_3Y/(CH)_4X_3Y$ and $C_8H_4X_2Y_2/(CH)_4X_2Y_2$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N_{\sigma_1} = 2a_{cs} + a_{c_{2v}} = 0$

$N_{\sigma_{v2}} = 2a_{c'_s} + a_{c_{2v}} = 0$

$a_{c_1} = 280, a_{c_2} = 0, a_{cs} = a_{c'_s} = 3, a_{c_{2v}} = 0,$

$PCV(C_8H_4X_2YZ) = (1120, 0, 0, 0) \to IICV(C_8H_4X_2YZ) = (280, 0, 0, 0, 0)$

For $q_0, q_1, q_2, q_3 = (3, 2, 2, 1)$ in $C_8H_3X_2Y_2Z$

$N_E = 4a_{c_1} + 2a_{cs} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{3,2,2,1} = 1680$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N_{\sigma_{v_1}} = 2a_{cs} + a_{c_{2v}} = \binom{2}{1,0,0,1}\binom{3}{1,1,1,0} = 12$

$N_{\sigma_{v2}} = 2a_{c's} + a_{c_{2v}} = \binom{2}{1,0,0,1}\binom{3}{1,1,1,0} = 12$

$a_{c_1} = 414, a_{c_2} = 0, a_{c_s} = a_{c's} = 6, a_{c_{2v}} = 0,$

$PCV(C_8H_3X_2Y_2Z) = (1680, 0, 12, 12) \to IICV(C_8H_3X_2Y2Z) = (414, 0, 6, 6, 0)$

For $q_0, q_1, q_2, q_3 = (2, 2, 2, 2)$ in $C_8H_2X_2Y_2Z_2$

$N_E = 4a_{c_1} + 2a_{cs} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{2,2,2,2} = 2520$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = \binom{4}{1,1,1,1} = 24$

$N_{\sigma_{v_1}} = N_{\sigma_{v_2}} = 2a_{c_s} + a_{c_{2v}} = 2a_{c'_s} + a_{c_{2v}} = [\binom{2}{2,0,0,0}\binom{3}{0,1,1,1} + \binom{2}{0,2,0,0}\binom{3}{1,0,1,1} + \binom{2}{0,0,2,0}\binom{3}{1,1,0,1} + \binom{2}{0,0,0,2}\binom{3}{1,1,1,0}] = 24$

$a_{c_1} = 612, a_{c_2} = a_{cs} = a_{c's} = 6, a_{c_{2v}} = 0,$

$PCV(C_8H_2X_2Y_2Z_2) = (2520, 24, 24, 24) \to IICV(C_8H_2X_2Y2Z_2) = (612, 12, 12, 12, 0)$

The PCM and the IICM composing the V_4 and V_5 associated vector spaces of permutomers and symmetry itemized isomers numbers for these coisomeric series are as follows:

$$PCM\begin{pmatrix} C_8H_{q_0}X_{q_1}Y_{q_2}Z_{q_3} \\ or \\ (CH)_{q_0}X_{q_1}Y_{q_2}Z_{q_3} \end{pmatrix} = \begin{pmatrix} q_0q_1q_2q_3 \\ 5,1,1,1 \\ 4,2,1,1 \\ 3,3,1,1 \\ 3,2,2,1 \\ 2,2,2,2 \end{pmatrix} \underbrace{\begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v1}} & N_{\sigma_{v2}} \\ 336 & 0 & 0 & 0 \\ 840 & 0 & 6 & 6 \\ 1120 & 0 & 0 & 0 \\ 1680 & 0 & 12 & 12 \\ 2520 & 24 & 24 & 24 \end{pmatrix}}_{V_4}$$

$$\downarrow$$

$$IICM\begin{pmatrix} C_8H_{q_0}X_{q_1}Y_{q_2}Z_{q_3} \\ or \\ (CH)_{q_0}X_{q_1}Y_{q_2}Z_{q_3} \end{pmatrix} = \begin{pmatrix} q_0q_1q_2q_3 \\ 5,1,1,1 \\ 4,2,1,1 \\ 3,3,1,1 \\ 3,2,2,1 \\ 2,2,2,2 \end{pmatrix} \underbrace{\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 84 & 0 & 0 & 0 & 0 \\ 207 & 0 & 3 & 3 & 0 \\ 280 & 0 & 0 & 0 & 0 \\ 414 & 0 & 6 & 6 & 0 \\ 612 & 12 & 12 & 12 & 0 \end{pmatrix}}_{V_5}$$

The data of linear mappings between 4 entries $PCV_s$and 5 entries $IICV_s$ for coisomeric series $C_8H_{q_0}X_{q_1}Y_{q_2}Z_{q_3}$ and $(CH)_{q_0}X_{q_1}Y_{q_2}Z_{q_3})$ where $q_0, q_1, q_2, q_3 =$ (5,1,1,1), (4,2,1,1), (3,3,1,1), (3,2,2,1), (2,2,2,2) are : (336, 0, 0,0)→(84,0,0,0,0); (840, 0, 6, 6)→(207,0,3,3,0); (1120,0,0,0)→(280,0,0,0,0); (1680,0,12,12)→(414,0,6,6,0) ;(2520,24,24,24)→(612,12,12,12,0), respectively. These transformations of 4-tuples of permutomers numbers N_E, N_{C_2}, $N_{\sigma_{v1}}, N_{\sigma_{v2}}$ into 5-tuples of symmetry itemized isomers numbers a_{c_1}, a_{c_2}, $a_{cs}, a_{c's}, a_{c_{2v}}$ predict the occurrences of : $(84C_1, 0, 0, 0, 0)$; $(207C_1, 0, 3C_s, 3C'_s, 0)$; $(280C_1, 0, 0, 0, 0)$; $(414C_1, 0, 6C_s, 6C'_s, 0)$; $(612C_1, 12C_2, 12C_s, 12C'_s, 0)$ isomers for $C_8H_5XYZ, C_8H_4X_2YZ, C_8H_3X_3YZ, C_8H_3X_2Y_2Z$, $C_8H_2X_2Y_2Z_2$ and their corresponding heteroanalogues respectively. The graphs depicting reduced numbers of isomers of these series are given in Fig. 4.

In the series $C_8H_{q_0}W_{q_1}X_{q_2}Y_{q_3}Z_{q_4}$ and $(CH)_{q_0}W_{q_1}X_{q_2}Y_{q_3}Z_{q_4})$ where $(q_0, q_1, q_2, q_3, q_4)$ =(4,1,1,1,1), (3,2,1,1,1), (2,2,2,1,1) the denumerants are:

For $(q_0, q_1, q_2, q_3, q_4)$ =(4,1,1,1,1), in C_8H_4WXYZ

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{4,1,1,1} = 1680$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N_{\sigma_{v_1}} = N_{\sigma_{v_2}} = N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 2a_{c_s} + a_{c_{2v}} = 2a_{c'_s} + a_{c_{2v}} = 0$

$a_{c_1} = 420, a_{c_2} = a_{cs} = a_{c's} = a_{c_{2v}} = 0,$

$PCV(C_8H_4WXYZ) = (1680, 0, 0, 0) \rightarrow IICV(C_8H_4WXYZ) = (420, 0, 0, 0, 0)$

For $(q_0, q_1, q_2, q_3, q_4) = (3, 2, 1, 1, 1)$

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{3,2,1,1,1} = 3360$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N_{\sigma_{v_1}} = N_{C_2} = N_{\sigma_{v_2}} = 2a_{c_2} + a_{c_{2v}} = 2a_{c_s} + a_{c_{2_v}} = 2a_{c'_s} + a_{c_{2v}} = 0$

$a_{c_1} = 420, a_{c_2} = a_{c_s} = a_{c'_s} = a_{c_{2v}} = 0,$

$PCV(C_8H_3W_2XYZ) = (3360, 0, 0, 0) \rightarrow IICV(C_8H_3W_2XYZ) = (840, 0, 0, 0, 0)$

For $(q_0, q_1, q_2, q_3, q_4) = (2, 2, 2, 1, 1)$ in $C_8H_2W_2X_2YZ$

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{2,2,2,1,1} = 5040$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N_{\sigma_{v_1}} = N_{\sigma_{v_2}} = 2a_{c_s} + a_{c_{2_v}} = 2a_{c'_s} + a_{c_{2v}} = \binom{2}{0,0,0,1,1}\binom{3}{1,1,1,0,0} = 12$

$a_{c_1} = 1254, a_{c_2} = 0, a_{cs} = a_{c's} = 6, a_{c_{2v}} = 0,$

$PCV(C_8H_2W_2X_2YZ) = (5040, 0, 12, 12) \rightarrow IICV(C_8H_2W_2X_2YZ) = (1260, 0, 6, 6, 0)$

The PCM and the IICM composing the V_4 and V_5 associated vector

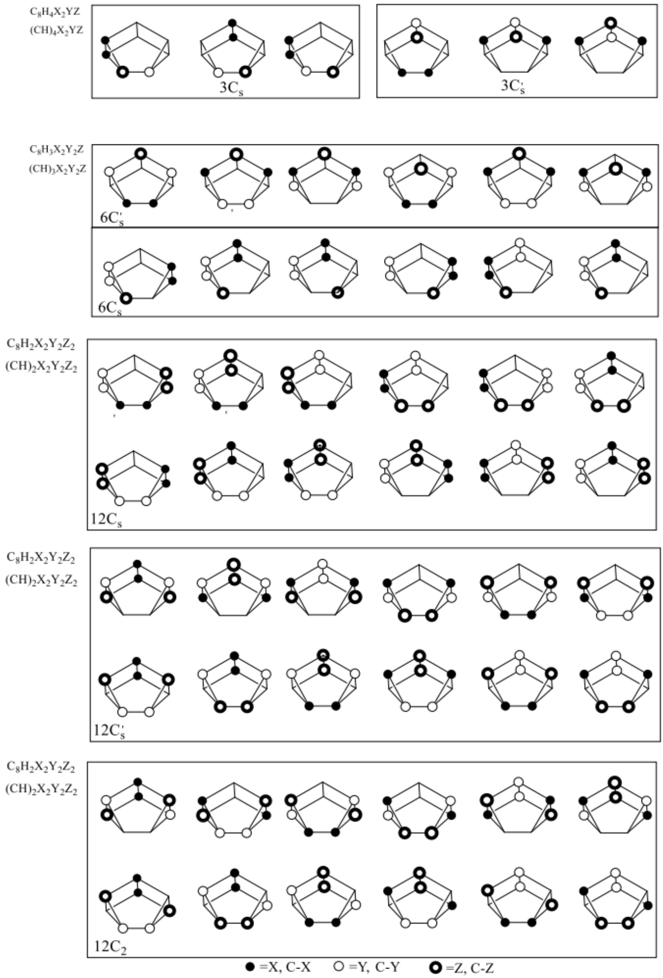

Figure 4. Graphs of $3C_s + 3C_s', 6C_s + 6C_s', 12C_2 + 12C_s + 12C_s'$ coisomeric series of heteropolysubstituted cuneanes and their hetero-heteroanalogues of the series $C_8H_4X_2YZ/(CH)_4X_2YZ, C_8H_3X_2Y_2Z/(CH)_3X_2Y_2Z$ $,C_8H_2X_2Y_2Z_2/(CH)_2X_2Y_2Z_2$.

spaces of permutomers and symmetry itemized isomers numbers for these coisomeric series are as follows:

$$PCM\begin{pmatrix} C_8H_{q_0}W_{q_1}X_{q_2}Y_{q_3}Z_{q_4} \\ or \\ (CH)_{q_0}W_{q_1}X_{q_2}Y_{q_3}Z_{q_4} \end{pmatrix} = \begin{pmatrix} q_0\,q_1\,q_2\,q_3\,q_4 \\ 4\;1\;1\;1\;1 \\ 3\;2\;1\;1\;1 \\ 2\;2\;2\;1\;1 \end{pmatrix} \underbrace{\begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v_1}} & N_{\sigma_{v_2}} \\ 1680 & 0 & 0 & 0 \\ 3360 & 0 & 0 & 0 \\ 5040 & 0 & 12 & 12 \end{pmatrix}}_{V_4}$$

$$\downarrow$$

$$IICM\begin{pmatrix} C_8H_{q_0}W_{q_1}X_{q_2}Y_{q_3}Z_{q_4} \\ or \\ (CH)_{q_0}W_{q_1}X_{q_2}Y_{q_3}Z_{q_4} \end{pmatrix} = \begin{pmatrix} q_0\,q_1\,q_2\,q_3\,q_4 \\ 4\;1\;1\;1\;1 \\ 3\;2\;1\;1\;1 \\ 2\;2\;2\;1\;1 \end{pmatrix} \underbrace{\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 420 & 0 & 0 & 0 & 0 \\ 840 & 0 & 0 & 0 & 0 \\ 1254 & 0 & 6 & 6 & 0 \end{pmatrix}}_{V_5}$$

The data of linear mappings between 4 entries PCV_s and 5 entries $IICV_s$ for coisomeric series $C_8H_{q_0}X_{q_1}Y_{q_2}Zq_3$ and $(CH)_{q_0}X_{q_1}Y_{q_2}Zq_3$) where $(q_0, q_1, q_2, q_3, q_4)$ =(4,1,1,1,1),(3,2,1,1,1), (2,2,2,1.1) are as follows::

(1680, 0, 0, 0)→(420, 0, 0, 0, 0), (3360, 0, 0, 0) →(840, 0, 0, 0, 0) ; (5040,0, 12, 12) → (1254,0, 6, 6,0) These transformations of 4-tuples of permutomers numbers into 5-tuples of symmetry itemized isomers numbers predict the occurrences of 420 C_1, and 840C_1 isomers for $C_8H_4WXYZ/(CH)_4WXYZ$ and $C_8H_3W_2XYZ/(CH)_3W_2XYZ$then $(1254C_1, 0, 6C_s, 6C'_s, 0)$ isomers for $C_8H_2W_2X_2YZ/(CH)_2W_2X_2YZ$. The graphs depicting $6C_s$and $6C'_s$ isomers of the series $C_8H_2W_2X_2YZ/(CH)_2W_2X_2YZ$ are given in Fig. 5.

$C_8H_2W_2X_2YZ$
$(CH)_2W_2X_2YZ$

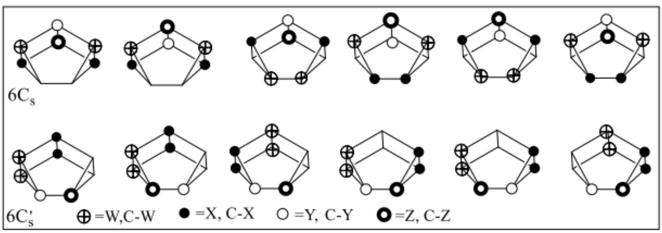

Figure 5. Graphs of $6C_s$ + $6C'_s$ isomers of heteropolysubstituted cuneanes derivatives and their hetero-heteroanalogues of the series $C_8H_2W_2X_2YZ$ and $(CH)_2W_2X_2YZ$.

In the series $C_8H_{q_0}V_{q_1}W_{q_2}X_{q_3}Y_{q_4}Zq_5$ and $(CH)_{q_0}V_{q_1}W_{q_2}X_{q_3}Y_{q_4}Zq_5$) where $(q_0, q_1, q_2, q_3, q_4, q_5)$ =(3,1,1,1,1,1), (2,2,1,1,1,1), the denumerants are:

For $(q_0, q_1, q_2, q_3, q_4, q_5)$ =(3,1,1,1,1,1), in C_8H_3VWXYZ

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{3,1,1,1,1} = 6720$

$N_{C_2} = 2a_{c_2} + a_{c_{2v}} = 0$

$N_{\sigma_{v_1}} = 2a_{c_s} + a_{c_{2v}} = 0$

$N_{\sigma_{v_2}} = 2a_{c'_s} + a_{c_{2v}} = 0$

$a_{c_1} = 6720, a_{c_2} = a_{c_s} = a_{c'_s} = a_{c_{2v}} = 0,$

$PCV(C_8H_3VWXYZ) = (6720, 0, 0, 0) \rightarrow IICV(C_8H_3VWXYZ) = (1680, 0, 0, 0, 0)$

For $(q_0, q_1, q_2, q_3, q_4, q_5)$ =(2,2,1,1,1,1), in $C_8H_2V_2WXYZ$

$N_E = 4a_{c_1} + 2a_{c_2} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{2,2,1,1,1} = 10080$

$N_{C_2} = N_{\sigma_1} = N_{\sigma_{v2}} = 2a_{c_2} + a_{c_{2v}} = 2a_{c'_s} + a_{c_{2v}} = 0$

$a_{c_1} = 2420, a_{c_2} = a_{c_s} = a_{c'_s} = a_{c_{2v}} = 0,$

$PCV(C_8H_2V_2WXYZ) = (10080, 0, 0, 0) \rightarrow IICV(C_8H_2V_2WXYZ) = (1680, 0, 0, 0, 0)$

The collection of PCV_s and $IICV_s$ for these series gives rise to:

$$PCM\begin{pmatrix} C_8H_2V_2WXYZ \\ or\ (CH)_2V_2WXYZ \end{pmatrix} = \begin{pmatrix} q_0 q_1 q_2 q_3 q_4\ q_5 \\ 3, 1, 1, 1, 1, 1 \\ 2, 2, 1, 1, 1, 1 \end{pmatrix} \underbrace{\begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v1}} & N_{\sigma_{v2}} \\ 6720 & 0 & 0 & 0 \\ 10080 & 0 & 0 & 0 \end{pmatrix}}_{\substack{V_4 \\ \downarrow}}$$

$$IICM\begin{pmatrix} C_8H_2V_2WXYZ \\ or\ (CH)_2V_2WXYZ \end{pmatrix} = \begin{pmatrix} q_0 q_1 q_2 q_3 q_4\ q_5 \\ 3, 1, 1, 1, 1, 1 \\ 2, 2, 1, 1, 1, 1 \end{pmatrix} \underbrace{\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 1680 & 0 & 0 & 0 & 0 \\ 2420 & 0 & 0 & 0 & 0 \end{pmatrix}}_{V_5}$$

The linear mappings between 4 entries PCV_s and 5 entries $IICV_s$ are : (6720, 0, 0, 0)→(1680, 0, 0, 0, 0) and (10080, 0, 0, 0) →(2420, 0, 0, 0, 0). These data predict the occurrences of $1680C_1$ and $2420C_1$ isomers for coisomeric series $C_8H_3VWXYZ/(CH)_3VWXYZ$ and $C_8H_2V_2WXYZ/(CH)_2$ V_2WXYZ respectively. In the series $C_8H_{q_0}U_{q_1}V_{q_2}W_{q_3}X_{q_4}Y_{q_5}Z_{q_6}$ and $(CH)_{q_0}U_{q_1}V_{q_2}W_{q_3}X_{q_4}Y_{q_5}Z_{q_6}$ their heteroanalogues where $(q_0, q_1, q_2, q_3, q_4, q_5, q_6)$ =(2,1,1,1,1,1,1)the denumerants are:

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{2,1,1,1,1,1,1} = 20180$

$N_{C_2} = N_{\sigma_{v1}} = N_{\sigma_{v2}} = 2a_{c_2} + a_{c_{2v}} = 2a_{c'_s} + a_{c_{2v}} = 0$

$a_{c_1} = 5040, a_{c_2} = a_{c_s} = a_{c'_s} = a_{c_{2v}} = 0,$

$$PCV\left(C_8H_2UVWXYZ\right) = \begin{pmatrix} q_0 q_1 q_2 q_3 q_4 q_5 q_6 \\ 2,1,1,1,1,1,1 \end{pmatrix} \underbrace{\begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v1}} & N_{\sigma_{v2}} \\ 20160 & 0 & 0 & 0 \end{pmatrix}}_{V4}$$

$$\downarrow$$

$$IICV\left(C_8H_2UVWXYZ\right) = \begin{pmatrix} q_0 q_1 q_2 q_3 q_4 q_5 q_6 \\ 2,1,1,1,1,1,1 \end{pmatrix} \underbrace{\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 5040 & 0 & 0 & 0 & 0 \end{pmatrix}}_{V_5}$$

In the series $C_8H_{q_0}T_{q_1}U_{q_2}V_{q_3}W_{q_4}X_{q_5}Y_{q_6}Z_{q_7}$ and $(CH)_{q_0}T_{q_1}U_{q_2}V_{q_3}W_{q_4}X_{q_5}Y_{q_6}Z_{q_7}$ their heteroanalogues where $(q_0, q_1, q_2, q_3, q_4, q_5, q_6, q_7)$ =(1,1,1, 1,1,1,1,1)the denumerants are :

$N_E = 4a_{c_1} + 2a_{c_s} + 2a_{c'_s} + a_{c_{2v}} = \binom{8}{1,1,1n1,1,1,1,1} = 40320$

$N_{C_2} = N_{\sigma_{v1}} = N_{\sigma_{v_2}} = 2a_{c_2} + a_{c_{2v}} = 2a_{c'_s} + a_{c_{2v}} = 0$

$a_{c_1} = 10080, a_{c_2} = a_{c_s} = a_{c'_s} = a_{c_{2v}} = 0,$

$$PCV\left(C_8HTUVWXYZ\right) = \begin{pmatrix} q_0 q_1 q_2 q_3 q_4 q_5 q_6 q_7 \\ 1,1,1,1,1,1,1,1 \end{pmatrix} \underbrace{\begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v1}} & N_{\sigma_{v2}} \\ 40320 & 0 & 0 & 0 \end{pmatrix}}_{V_4}$$

$$\downarrow$$

$$IICV\left(C_8HTUVWXYZ\right) = \begin{pmatrix} q_0 q_1 q_2 q_3 q_4 q_5 q_6 q_7 \\ 1,1,1,1,1,1,1,1 \end{pmatrix} \underbrace{\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 10080 & 0 & 0 & 0 & 0 \end{pmatrix}}_{V_5}$$

The linear mappings : PCV($C_8H_2UVWXYZ$)→ IICV ($C_8H_2UVWXYZ$) =(20160, 0, 0, 0)→(5040, 0, 0, 0, 0) and PCV ($C_8HTUVWXYZ$)→ IICV ($C_8HTUVWXYZ$) =(40320, 0, 0, 0)→(10080,0,0,0,0) predict the occurrences of 5040C_1 and 10080C_1 isomers for coisomeric series $C_8H_2UVWXYZ/(CH)_2UVWXYZ$ and $C_8HTUVWXYZ/(CH)TUVWXYZ$. Table 3 presents $J_i \times 4$ entries PCMs and $J_i \times 5$ entries $IICM_s$ composing the associated V_4 and V_5 mutidimensional vector spaces of permutomers and symmetry itemized isomers numbers for homo- and heteropolysubstituted cuneane derivatives and cuneane heteroanalogues. For the sake of comparison columns 6 and 7 of table 4 present the numbers of chiral and achiral isomers skeletons $A_c = a_{c_1} + a_{c_2}$, $A_{ac} = a_{c_s} + a_{c'_s} + a_{c_{2v}}$ obtained from bipartite enumeration [12] and the numbers of diastereo isomers $N_p = A_c + A_{ac}$ derived from Polya cycle indices. [13]

5 Concluding remarks

The enumeration leading to the construction of the linear spaces of permutomers and symmetry itemized isomers numbers of C_{2v}-based cuneane derivatives and heteroanalogues presented in this paper includes the following steps:

(1)-the determination of-4-dimensional permutomers count vectors PCV $(N_E, N_{C_2}, N_{\sigma_{v1}}, N_{\sigma_{v2}})$ whose entries are obtained from multinomial or binomial theorems applied in accordance with 4 classes of permutations regulating the arrangements of substituents among 8 substitution sites.

(2)-the determination of 5-dimensional itemized isomers count vector IICV $a_{cs}, a_{c_2}, a_{cs}, a_{c'_s}, a_{c_{2v}}$ whose entries are derived from the resolution of the denumerants of type $N_{g_l} = \sum_{G_j} a_{G_j} w_{G_j}, g_l$ mapping the permutomers numbers $N_E, N_{C_2}, N_{\sigma_{v1}}, N_{\sigma_{v2}}$ as a sum of symmetry adapted isomers numbers a_{G_j} scaled by the weights w_{G_j}, g_l of the subgroups of C_{2v}.

(3)-The construction of the V_4 and V_5 vector spaces of isomers numbers by collecting 4-dimensional PCVs and 5-dimensional IICVs to form the permutomers count matrix (PCM) and the itemized isomers count matrix (IICM) for each series of cuneane derivatives $C_8H_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ or $(CH)_{q_0}X_{q_1}...Y_{q_i}...Z_{q_k}$ cuneane heteroanalogues where $\sum_{i=1}^{k} q_i = 8$ Permutomers and symmetry itemized isomers numbers of substituted C_{2v}-based compounds form 2 associated linear spaces containing 4- and 5-dimensional vectors respectively. Such distribution of isomers populations may open new perspectives of research and teaching in stereochemistry.

Table 2. $(J_i \times 4) - PCM_s$ and $(J_i \times 5) - IICM_s$ composing the structure of the V_4 and V_5 vector spaces of permutomers and symmetry itemized isomers numbers for substituted cuneane derivatives and heteroanalogues. Note for the sake of comparison that $A_c = a_{c_1} + a_{c_2}$, $A_{ac} = a_{c_s} + a_{c'_s} + a_{c_{2v}}$ and $N_p = A_c + A_{ac}$.

$1 \le i \le k$	j_i	Cuneane derivatives	*PCMs* of the V_4 vector space	*IICMs* of the V_5 vector space	Bipartite Enumeration	Polya Numbers
1	5	$C_8H_{q_0}X_{q_1}$ $(CH)_{q_0}X_{q_1}$	$\begin{pmatrix} q_0,q_1 \\ 8,0 \\ 7,1 \\ 6,2 \\ 5,3 \\ 4,4 \end{pmatrix} \begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v_1}} & N_{\sigma_{v_2}} \\ 1 & 1 & 1 & 1 \\ 8 & 0 & 2 & 2 \\ 28 & 4 & 4 & 4 \\ 56 & 0 & 6 & 6 \\ 70 & 6 & 6 & 6 \end{pmatrix}$	$\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 5 & 1 & 1 & 1 & 2 \\ 11 & 0 & 3 & 3 & 0 \\ 14 & 2 & 2 & 2 & 2 \end{pmatrix}$	$\begin{bmatrix} A_c & A_{ac} \\ 0 & 1 \\ 1 & 2 \\ 6 & 4 \\ 11 & 6 \\ 16 & 6 \end{bmatrix}$	$\begin{bmatrix} N_p \\ 1 \\ 3 \\ 10 \\ 17 \\ 22 \end{bmatrix}$
2	5	$C_8H_{q_0}X_{q_1}Y_{q_2}$ $(CH)_{q_0}X_{q_1}Y_{q_2}$	$\begin{pmatrix} q_0q_1q_2 \\ 6,1,1 \\ 5,2,1 \\ 4,3,1 \\ 4,2,2 \\ 3,3,2 \end{pmatrix} \begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v_1}} & N_{\sigma_{v_2}} \\ 56 & 0 & 2 & 2 \\ 168 & 0 & 6 & 6 \\ 280 & 0 & 6 & 6 \\ 420 & 12 & 12 & 12 \\ 560 & 0 & 12 & 12 \end{pmatrix}$	$\begin{pmatrix} q_0q_1q_2 \\ 6,1,1 \\ 5,2,1 \\ 4,3,1 \\ 4,2,2 \\ 3,3,2 \end{pmatrix} \begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 13 & 0 & 1 & 1 & 0 \\ 39 & 0 & 3 & 3 & 0 \\ 67 & 0 & 3 & 3 & 0 \\ 97 & 0 & 5 & 5 & 2 \\ 134 & 0 & 6 & 6 & 0 \end{pmatrix}$	$\begin{bmatrix} A_c & A_{ac} \\ 13 & 2 \\ 39 & 6 \\ 67 & 6 \\ 102 & 12 \\ 134 & 12 \end{bmatrix}$	$\begin{bmatrix} N_p \\ 15 \\ 45 \\ 73 \\ 114 \\ 146 \end{bmatrix}$

Table 2 continued.

i	j_i	Cuneane substituted derivatives and hetero-heteroanaogues	*PCMs* of the V_4 vector space	*IICMs* of the V_5 vector space	Bipartite Enumeration	Polya Numbers
3	5	$C_8H_{q_0}X_{q_1}Y_{q_2}Z_{q_3}$ $(CH)_{q_0}X_{q_1}Y_{q_2}Z_{q_3}$	$\begin{pmatrix} q_0q_1q_2q_3 \\ 5,1,1,1 \\ 4,2,1,1 \\ 3,3,1,1 \\ 3,2,2,1 \\ 2,2,2,2 \end{pmatrix} \begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v_1}} & N_{\sigma_{v_2}} \\ 336 & 0 & 0 & 0 \\ 840 & 0 & 6 & 6 \\ 1120 & 0 & 0 & 0 \\ 1680 & 0 & 12 & 12 \\ 2520 & 24 & 24 & 24 \end{pmatrix}$	$\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 84 & 0 & 0 & 0 & 0 \\ 207 & 0 & 3 & 3 & 0 \\ 280 & 0 & 0 & 0 & 0 \\ 414 & 0 & 6 & 6 & 0 \\ 612 & 12 & 12 & 12 & 0 \end{pmatrix}$	$\begin{pmatrix} A_c & A_{ac} \\ 84 & 0 \\ 207 & 6 \\ 280 & 0 \\ 414 & 12 \\ 624 & 24 \end{pmatrix}$	$\begin{pmatrix} N_p \\ 84 \\ 213 \\ 280 \\ 426 \\ 648 \end{pmatrix}$
4	3	$C_8H_{q_0}W_{q_1}X_{q_2}Y_{q_3}Z_{q_4}$ $(CH)_{q_0}W_{q_1}X_{q_2}Y_{q_3}Z_{q_4}$	$\begin{pmatrix} q_0q_1q_2q_3q_4 \\ 4\ 1\ 1\ 1\ 1 \\ 3\ 2\ 1\ 1\ 1 \\ 2\ 2\ 2\ 1\ 1 \end{pmatrix} \begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v_1}} & N_{\sigma_{v_2}} \\ 1680 & 0 & 0 & 0 \\ 3360 & 0 & 0 & 0 \\ 5040 & 0 & 12 & 12 \end{pmatrix}$	$\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 420 & 0 & 0 & 0 & 0 \\ 840 & 0 & 0 & 0 & 0 \\ 1254 & 0 & 6 & 6 & 0 \end{pmatrix}$	$\begin{pmatrix} A_c & A_{ac} \\ 420 & 0 \\ 840 & 0 \\ 1254 & 12 \end{pmatrix}$	$\begin{pmatrix} N_p \\ 420 \\ 840 \\ 1266 \end{pmatrix}$
5	2	$C_8H_{q_0}V_{q_1}W_{q_2}X_{q_3}Y_{q_4}Z_{q_5}$ $(CH)_{q_0}V_{q_1}W_{q_2}X_{q_3}Y_{q_4}Z_{q_5}$	$\begin{pmatrix} q_0q_1q_2q_3q_4\ q_5 \\ 3,\ 1,\ 1,\ 1,\ 1,\ 1 \\ 2,\ 2,\ 1,\ 1,\ 1,\ 1 \end{pmatrix} \begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v_1}} & N_{\sigma_{v_2}} \\ 6720 & 0 & 0 & 0 \\ 10080 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 1680 & 0 & 0 & 0 & 0 \\ 2520 & 0 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} A_c & A_{ac} \\ 1680 & 0 \\ 2520 & 0 \end{pmatrix}$	$\begin{pmatrix} N_p \\ 1680 \\ 2520 \end{pmatrix}$
6	1	$C_8H_{q_0}U_{q_1}V_{q_2}W_{q_3}X_{q_4}Y_{q_5}Z_{q_6}$ $(CH)_{q_0}U_{q_1}V_{q_2}W_{q_3}X_{q_4}Y_{q_5}Z_{q_6}$	$\begin{pmatrix} q_0q_1q_2q_3q_4q_5q_6 \\ 2,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1 \end{pmatrix} \begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v_1}} & N_{\sigma_{v_2}} \\ 20160 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 5040 & 0 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} A_c & A_{ac} \\ 5040 & 0 \end{pmatrix}$	$\begin{pmatrix} N_p \\ 5040 \end{pmatrix}$
7	1	$C_8H_{q_0}T_{q_1}U_{q_2}V_{q_3}W_{q_4}X_{q_5}Y_{q_6}Z_{q_7}$ $(CH)_{q_0}T_{q_1}U_{q_2}V_{q_3}W_{q_4}X_{q_5}Y_{q_6}Z_{q_7}$	$\begin{pmatrix} q_0q_1q_2q_3q_4q_5q_6q_7 \\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,1,1 \end{pmatrix} \begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v_1}} & N_{\sigma_{v_2}} \\ 40320 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 10080 & 0 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} A_c & A_{ac} \\ 10080 & 0 \end{pmatrix}$	$\begin{pmatrix} N_p \\ 10080 \end{pmatrix}$
8	1	$C_8S_{q_0}T_{q_1}U_{q_2}V_{q_3}W_{q_4}X_{q_5}Y_{q_6}Z_{q_7}$ $STUVWXYZ$	$\begin{pmatrix} q_0q_1q_2q_3q_4q_5q_6q_7 \\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,1,1 \end{pmatrix} \begin{pmatrix} N_E & N_{C_2} & N_{\sigma_{v_1}} & N_{\sigma_{v_2}} \\ 40320 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} a_{C_1} & a_{C_2} & a_{C_s} & a_{C'_s} & a_{C_{2v}} \\ 10080 & 0 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} A_c & A_{ac} \\ 10080 & 0 \end{pmatrix}$	$\begin{pmatrix} N_p \\ 10080 \end{pmatrix}$

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