Regarding Enumeration of Molecular Isomers

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In this paper, a simple theoretical approach to counting of substitution isomers is described. It is based on Pólya's theorem and on point groups as recently described by us [Baraldi, I.; Fiori, C.; Vanossi, D. *J. Math. Chem.* **1999**, *25*, 23−30] and extended in this paper. Several applications are developed that range from molecules without symmetry to molecules with icosahedral symmetry ($\mathbf{I}_h$). The problem of the appearance of stereoisomers is also analyzed.

INTRODUCTION

In a recent work[1] we were able to express the cycle index of all point groups as a function of a limited number of initial geometrical parameters. Such parameters are the number m of elements composing the domain D of substitution sites (points, elements) of the molecule having **G** symmetry and the numbers ($n(C_n)$, $n(\sigma)$, ...) that identify how many points of set D lie on symmetry elements (C_n, σ, ...) of the molecule. One of the primary utilities of the results of this work resides in the fact that the chemical applications of the Pólya−Redfield theorem, such as the counting of isomers, for which several methods have been developed,[2−11] can be made much more understandable to the chemical community.

In this paper, the logical development of the previous work is presented. Precisely, after introducing the cycle index of a domain D given by the union of substitution domains corresponding to the different molecular orbits determined by **G** symmetry on D, significant molecular applications are discussed. Such applications include the development of some series counting isomers, the corresponding formulas for the total number of isomers, and examples of enumeration of molecular isomers. In particular, where possible, we pay attention to the problem of stereoisomerism, and the counting of the isomers is made both with the extended molecular point group (achiral point group) and with the proper rotational group (chiral point group). The problem of the substitutions in the fullerene C_{60}, a topic of recent interest,[12] is also analyzed.

MATHEMATICAL DEVELOPMENT

We consider a molecule (M) having m atoms with n distinct elements and molecular formula

$$A_{m_1}^{(1)} A_{m_2}^{(2)} \ldots A_{m_n}^{(n)}$$

where m_i is the number of atoms of the ith element $A^{(i)}$ of M. It is evident that

$$m = \sum_{i=1}^{n} m_i \qquad (2)$$

$\mathbf{G} = \{\hat{g}_i, i = 1, 2, ..., g\}$ denotes the molecular point group of finite order g of M. By action of **G** on M, the m atoms are split up in $n_o(\mathbf{G})$ distinct orbits, or better **G**-orbits, and such a number is given by the formula

$$n_o = n_o(\mathbf{G}) = n_o(\mathbf{G},\mathrm{M}) = \frac{1}{g} \sum_{\hat{g}_i \in \mathbf{G}} n(\hat{g}_i) \qquad (3)$$

where $n(\hat{g}_i)$ is the number of atoms of the molecule that are stationary during the molecular motion connected to the symmetry operation $\hat{g}_i$. Equation 3 expresses the Cauchy−Frobenius lemma also called Burnside's lemma.

Each **G**-orbit is formed of a certain number of equivalent atoms or equivalent molecular groups. With n_i we indicate such number, which is a divisor of g, and we have

$$m = \sum_{i=1}^{n_o} n_i \qquad (4)$$

As a consequence, the number of equivalent atoms is a divisor of g.

We now develop the procedure to obtain the enumeration of molecular isomers. Because the elements (points) of each **G**-orbit are disjoint to the elements of other **G**-orbits, the **G**-orbits can be considered independent of each other. Evidently such a procedure can be used also in the case in which two or more **G**-orbits are considered as a whole.

The domain D of substitution sites of M, which include m points, is given by the union of the domains D_i ($i = 1, 2, ..., n_o$) of the elements of different **G**-orbits,

$$D = \bigcup_{i=1}^{n_o} D_i \qquad (5)$$

where D_i indicates the domain of the ith **G**-orbit of length n_i; i.e. $D_i = \{d_{ij}, j = 1, 2, ..., n_i\}$ contains $n_i = |D_i|$ elements. It is known that if $|\mathrm{St}(d_{ij})|$ indicates the dimension of the stabilizer of the jth element of subset D_i, then

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$$n_i|\mathrm{St}(d_{ij})| = g \tag{6}$$

To each subset D_i we combine a group of distinct permutations given by the permutations of the n_i elements of D_i, when D_i undergoes the symmetry operations belonging to **G**. Let $\mathbf{P}_i = \mathbf{P}_i(\mathbf{H}_i) = \mathbf{P}(\mathbf{H}_i,D_i)$ be such a permutation group, where $\mathbf{H}_i$ is one of the subgroups of **G** ($\mathbf{H}_i \leq \mathbf{G}$), including the banal subgroups $\mathbf{C}_1$ and **G**, and such that $\mathbf{P}_i$ is isomorphic to $\mathbf{H}_i$. ($\mathbf{P}_i$ is a transitive permutation group on D_i.) The cycle index of such a permutation group is

$$Z(\mathbf{P}_i,n_i) = Z(\mathbf{P}_i(\mathbf{H}_i),n_i) = Z(x_{i1},x_{i2}, ..., x_{in_i}) = \frac{1}{h_i}\sum_{P\in\mathbf{P}_i} x_{i1}^{e_{1P}} x_{i2}^{e_{2P}}...x_{in_i}^{e_{n_iP}} \tag{7}$$

where the symbols have the common meaning (h_i is the order of $\mathbf{H}_i$, x_{ij} the jth indeterminate of Z_i, e_{jP} the number of cycles of degree j in the permutation $P \in \mathbf{P}_i$).

With each **G**-orbit being treated in an independent way with respect to the substitution, the cycle index of the total permutation group

$$\mathbf{P}(\mathbf{G}) = \mathbf{P}(\mathbf{G},D) = \sum_{i=1}^{n_o}\mathbf{P}_i \tag{8}$$

is

$$Z(\mathbf{P}(\mathbf{G}),m) = \prod_{i=1}^{n_o} Z(\mathbf{P}_i,n_i) = \prod_{i=1}^{n_o} Z(x_{i1},x_{i2}, ..., x_{in_i}) = \prod_{i=1}^{n_o}\frac{1}{h_i}\sum_{P\in\mathbf{P}_i} x_{i1}^{e_{1P}} x_{i2}^{e_{2P}}...x_{in_i}^{e_{n_iP}} \tag{9}$$

With each $Z(\mathbf{P}_i,n_i)$ being written as a function of the initial parameters according to ref 1, also $Z(\mathbf{P}(\mathbf{G}),m)$ will be a function of such parameters.

The counting series of molecular isomers is obtained from eq 9, making the substitution

$$x_{ik} \rightarrow w_{i1}^k + w_{i2}^k + ... + w_{i\alpha_i}^k \tag{10}$$

where α_i indicates the number of different elements or molecular groups, i.e., the distinct substitutes, that can be attached to the n_i points of subset D_i and w_{ij} is the weight function of the jth substitute of subset D_i. The formula for the series counting isomers is then

$$\mathrm{CI}(\mathbf{P}(\mathbf{G})m) = \prod_{i=1}^{n_o} Z(w_{i1} + w_{i2} + ... + w_{i\alpha_i}, {w_{i1}}^2 + {w_{i2}}^2 + ... + {w_{i\alpha_i}}^2, ..., w_{i1}^{n_i} + w_{i2}^{n_i} + ... + w_{i\alpha_i}^{n_i}) \tag{11}$$

and that for the total number of isomers is

$$\mathrm{NI}(\mathbf{P}(\mathbf{G}),m) = \prod_{i=1}^{n_o} Z_i(\alpha_i,\alpha_i,...,\alpha_i) \tag{12}$$

Expanding eq 11, we obtain a combination of terms of the general form

$$\prod_{i=1}^{n_o}\prod_{j=1}^{\alpha_i} w_{ij}^{k_{ij}} \tag{13}$$

with

$$n_i = \sum_{j=1}^{\alpha_j} k_{ij} \tag{14}$$

and then

$$m = \sum_{i=1}^{n_o}\sum_{j=1}^{\alpha_j} k_{ij} \tag{15}$$

The coefficient of this term, in the expanded form, is the number of isomers of molecular formula

$$A_{k_{11}}^{(11)} A_{k_{12}}^{(12)}...A_{k1\alpha_1}^{(1\alpha_1)} A_{k_{21}}^{(21)}...A_{k_{ij}}^{(ij)}...A_{k_{n_o\alpha_i}}^{(n_o\alpha_i)} \tag{16}$$

where the correspondence $A_{k_{ij}}^{(ij)} = w_{ij}^{k_{ij}}$ has been made, and each element has been identified by two indices, i and j. k_{ij} gives the numbers of elements of j type in the ith **G**-orbit. To simplify the notation, in what follows the molecular formula of isomers will be indicated as $...W_iX_jY_k...$.

APPLICATIONS

The application of the previously developed theory begins with molecules without geometrical symmetry, $\mathbf{C}_1$ point group, and then continues with molecules of increasing symmetry, to conclude with molecules of icosahedral symmetry. To be more exact, the molecular systems considered are as follows: oxiran ($\mathbf{C}_{2v}$), molecules with molecular formula AB_3 ($\mathbf{C}_{3v}$), adamantane-2,6-dione ($\mathbf{D}_{2d}$), dibenzodioxine ($\mathbf{D}_{2h}$), coronene ($\mathbf{D}_{6h}$), molecules with molecular formula AB_4 ($\mathbf{T}_d$), molecules with molecular formula AB_6 ($\mathbf{O}_h$), cubane ($\mathbf{O}_h$), borane anion ($B_{12}H_{12}^{2-}$, $\mathbf{I}_h$), and fullerene C_{60} ($\mathbf{I}_h$). Use also of the molecular rotational subgroups (chiral groups) to see when stereoisomers appear completes the analysis of molecular isomers.

(1) Molecules without Symmetry. The molecular point group is $\mathbf{G} \equiv \mathbf{C}_1 = \{\hat{E}\}$, and the number of **G**-orbits is equal to the number of atoms of M, $n_o(\mathbf{C}_1) = m$. We have

$$Z(\mathbf{P}(\mathbf{C}_1),m) = \prod_{i=1}^{m} x_{i1}^1 \tag{17}$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{C}_1),m) = \prod_{i=1}^{m}(w_{i1} + w_{i2} + ... + w_{i\alpha_i}) \tag{18}$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{C}_1),m) = \prod_{i=1}^{m}\alpha_i \tag{19}$$

In the case in which $\alpha_1 = \alpha_2 = ... = \alpha_m = \alpha$ and $w_{ij} = w_j$ ($j = 1, 2, ..., \alpha$), then

$$\mathrm{CI}(\mathbf{P}(\mathbf{C}_1),m) = (w_1 + w_2 + ... + w_\alpha)^m = \sum\frac{m!}{r_1!r_2!...r_\alpha!} w_1^{r_1}w_2^{r_2}...w_\alpha^{r_\alpha} \tag{20}$$

where the sum is taken over all α-tuples of nonnegative

Table 1

			X_iY_j		
α	*m*	NI	*i*	*j*	isomer no.
2	4	16	4	0	2
			3	1	8
			2	2	6
			$X_iY_jZ_k$		
			i	*j*	*k*	isomer no.
3	3	27	3	0	0	3
			2	1	0	18
			1	1	1	6

integers (r_1, r_2, ..., r_α) such that $r_1 + r_2 + ... + r_\alpha = m$, and

$$\mathrm{NI}(\mathbf{P}(\mathbf{C}_1),m) = \alpha^m \tag{21}$$

For $\alpha = 2$, the last two formulas are reduced to

$$\mathrm{CI}(\mathbf{P}(\mathbf{C}_1),m) = (w_1 + w_2)^m = \sum_{k=0}^{m}\binom{m}{k} w_1^{\,k} w_2^{\,m-k} \tag{22}$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{C}_1),m) = 2^m = \sum_{k=0}^{m}\binom{m}{k} \tag{23}$$

Equation 20 expresses a generalization of the *binomial theorem* given by eq 22 and is known as the *multinomial theorem*.

Table 1 gives some examples of isomer counting and their enumeration within $\mathbf{C}_1$ symmetry.

(2) Molecule with C_{2v} Symmetry.

$$\mathbf{C}_{2v} = \{\hat{E},\hat{C}_2,\hat{\sigma}_{xz},\hat{\sigma}_{yz}\}$$
$$\mathbf{C}_2 = \{\hat{E},\hat{C}_2\}$$

Oxiran (C_2H_4O). The spatial distribution of the atoms in this molecule and the $\mathbf{C}_{2v}$ symmetry generates three distinct **G**-orbits, $n_o(\mathbf{C}_{2v}) = 3$, of dimensions one, two, and four, respectively. The domain *D* is thus decomposed:

$$D = \underbrace{D_1}_{\text{one-dimensional}} \cup \underbrace{D_2}_{\text{two-dimensional}} \cup \underbrace{D_3}_{\text{four-dimensional}}$$
$$(n_1 = |D_1| = 1, \quad n_2 = |D_2| = 2, \quad n_3 = |D_3| = 4) \tag{24}$$

The permutation group of different domains is

$$\mathbf{P}_1 = \mathbf{P}(\mathbf{C}_{2v},D_1) = \mathbf{P}(\mathbf{C}_1,D_1) \tag{25}$$

$$\mathbf{P}_2 = \mathbf{P}(\mathbf{C}_{2v},D_2) = \mathbf{P}(\mathbf{C}_2,D_2) \tag{26}$$

$$\mathbf{P}_3 = \mathbf{P}(\mathbf{C}_{2v},D_3) \tag{27}$$

and the cycle index is

$$Z(\mathbf{P}_1,1) = x_{11}^1 \tag{28}$$

$$Z(\mathbf{P}_2,2) = {}^1/_2(x_{21}^2 + x_{22}^1) \tag{29}$$

$$Z(\mathbf{P}_3,4) = {}^1/_4(x_{31}^4 + 3x_{32}^2) \tag{30}$$

In all, we have

$$Z(\mathbf{P}(\mathbf{C}_{2v}),7) = {}^1/_8 x_{11}^1(x_{21}^2 + x_{22}^1)(x_{31}^4 + 3x_{32}^2) \tag{31}$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{C}_{2v}),7) = {}^1/_8\alpha_1(\alpha_2^2 + \alpha_2)(\alpha_3^4 + 3\alpha_3^2) \tag{32}$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{C}_{2v}),7) = {}^1/_8(w_{11}^1 + w_{12}^1 + ... + w_{1\alpha_1}^1)[(w_{21}^1 + w_{22}^1 + ... + w_{2\alpha_2}^1)^2 + (w_{21}^2 + w_{22}^2 + ... + w_{2\alpha_2}^2)][(w_{31}^1 + w_{32}^1 + ... + w_{3\alpha_3}^1)^4 + 3(w_{31}^2 + w_{32}^2 + ... + w_{3\alpha_3}^2)^2] \tag{33}$$

In Table 2 we report some results of the total number of isomers (NI) calculated from eq 32.

In the case of $\alpha_1 = \alpha_2 = \alpha_3 = 2$ eq 33 is reduced to

$$\mathrm{CI}(\mathbf{P}(\mathbf{C}_{2v}),7) = {}^1/_8(w_{11}^1 + w_{12}^1)[(w_{21}^1 + w_{22}^1)^2 + (w_{21}^2 + w_{22}^2)][(w_{31}^1 + w_{32}^1)^4 + 3(w_{31}^2 + w_{32}^2)^2] \tag{33′}$$

and the enumeration of different isomers is given in Table 3. Using $\mathbf{C}_2$ symmetry, $n_o(\mathbf{C}_2) = 4$, and the domain is thus decomposed

$$D = \underbrace{D_1}_{\text{one-dimensional}} \cup \underbrace{D_2 \cup D_3 \cup D_4}_{\text{two-dimensionals}}$$
$$(n_1 = |D_1| = 1, \quad n_2 = |D_2| = n_3 = |D_3| = n_4 = |D_4| = 2) \tag{34}$$

The permutation group of different domains is

$$\mathbf{P}_1 = \mathbf{P}(\mathbf{C}_2,D_1) = \mathbf{P}(\mathbf{C}_1,D_1) \tag{35}$$

$$\mathbf{P}_i = \mathbf{P}(\mathbf{C}_2,D_2) \qquad i = 2, 3, 4 \tag{36}$$

and the corresponding cycle index

$$Z(\mathbf{P}_1,1) = x_{11}^1 \tag{37}$$

$$Z(\mathbf{P}_i,2) = {}^1/_2(x_{i1}^2 + x_{i2}^1) \qquad i = 2, 3, 4 \tag{38}$$

In all we have

$$Z(\mathbf{P}(\mathbf{C}_2),7) = {}^1/_8 x_{11}^1 \prod_{i=2}^{4}(x_{i1}^2 + x_{i2}^2) \tag{39}$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{C}_2),7) = {}^1/_8\alpha_1 \prod_{i=2}^{4}(\alpha_i^2 + \alpha_i^1) \tag{40}$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{C}_2),7) = {}^1/_8(w_{11}^1 + w_{12}^1 + ... + w_{1\alpha_1}^1)\prod_{i=2}^{4}[(w_{i1}^1 + w_{i2}^1 + ... + w_{i\alpha_i}^1)^2 + (w_{i1}^2 + w_{i2}^2 + ... + w_{i\alpha_i}^2)] \tag{41}$$

Table 4 reports some values of the total number of isomers (NI) obtained with eq 40. In the particular case of $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 2$, the cycle index is

$$\mathrm{CI}(\mathbf{P}(\mathbf{C}_2),7) = {}^1/_8(w_{11}^1 + w_{12}^1)\prod_{i=2}^{4}[(w_{i1}^1 + w_{i2}^1)^2 + (w_{i1}^2 + w_{i2}^2)] \tag{41′}$$

and the repartition of different isomers is given in Table 5.

Table 2

α_1	α_2	α_3	NI($\mathbf{P}(\mathbf{C}_{2v})$,7)
1	1	1	1
2	1	1	2
1	2	1	3
1	1	2	7
2	2	1	6
1	2	2	21
2	1	2	14
2	2	2	42
3	1	1	3
1	3	1	6
1	1	3	27
3	2	1	9
...	...	...	...
3	2	2	63
...	...	...	...
3	3	3	486
...	...	...	...

Table 3[a]

$V_iW_jX_kY_lZ_m$					
i	*j*	*k*	*l*	*m*	isomer no.
0	0	1	2	4	8
0	1	1	1	4	4
0	1	1	2	3	8
0	1	2	2	2	12
1	1	1	1	3	4
1	1	1	2	2	6

[a] $\alpha_1 = \alpha_2 = \alpha_3 = 2$.

Table 4

α_1	α_2	α_3	α_4	NI($\mathbf{P}(\mathbf{C}_2)$,7)
1	1	1	1	1
2	1	1	1	2
1	2	1	1	3
1	1	2	1	3
1	1	1	2	3
1	1	2	2	9
2	2	1	1	6
2	1	2	1	6
2	1	1	2	6
...	...	...	...	
2	2	2	1	18
...	...	...	...	...
2	2	2	2	54
3	1	1	1	3
1	3	1	1	6
...	...	...	...	...
3	2	2	1	27
...	...	...	...	...
3	2	2	2	81
...	...	...	...	...
3	3	3	3	648
...	...	...	...	...

The 12 stereoisomers present are eight of TV_2XY_3 type and four of $TUVXY_3$ type.

(3) Molecules with C_{3v} Symmetry.

$$\mathbf{C}_{3v} = \{\hat{E}, 2\hat{C}_3, 3\hat{\sigma}_v\}$$

$$\mathbf{C}_3 = \{\hat{E}, 2\hat{C}_3\}$$

The Case of a Trigonal Pyramid (AB_3). The symmetry of this type of molecule is $\mathbf{C}_{3v}$ and its chiral group is $\mathbf{C}_3$. For both symmetries, the atoms of the molecule are decomposed in two **G**-orbits, $n_o(\mathbf{C}_{3v}) = n_o(\mathbf{C}_3) = 2$. One

Table 5[a]

$T_iU_jV_kW_lX_mY_nZ_o$							
i	*j*	*k*	*l*	*m*	*n*	*o*	isomer no.
0	0	0	1	2	2	2	16
0	0	1	1	1	2	2	24
0	1	1	1	1	1	2	12
1	1	1	1	1	1	1	2

[a] $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 2$.

G-orbit has one element and the other three elements. The decomposition of the domain *D* is

$$D = \underset{\text{one-dimensional}}{D_1} \cup \underset{\text{three-dimensional}}{D_2} \qquad (n_1 = |D_1| = 1, \quad n_2 = |D_2| = 3) \quad (42)$$

The permutation groups of both point groups are

$$\mathbf{P}_1 = \mathbf{P}(\mathbf{C}_{3v}, D_1) = \mathbf{P}(\mathbf{C}_3, D_1) = \mathbf{P}(\mathbf{C}_1, D_1) \quad (43)$$

$$\mathbf{P}_2(\mathbf{C}_{3v}) = \mathbf{P}(\mathbf{C}_{3v}, D_2) \quad (44)$$

$$\mathbf{P}_2(\mathbf{C}_3) = \mathbf{P}(\mathbf{C}_3, D_2) \quad (44')$$

From ref 1, the general expressions of the cycle index for a domain *D* of *m* elements submitted to symmetries $\mathbf{C}_{3v}$ and $\mathbf{C}_3$ are, respectively,

$$Z(\mathbf{C}_{3v}, m) = {}^1/_6(x_1^m + 2x_1^{n(C_3)} x_3^{(m-n(C_3))/3} + 3x_1^{n(\sigma_v)} x_2^{(m-n(\sigma_v))/2}) \quad (45)$$

$$Z(\mathbf{C}_3, m) = {}^1/_3(x_1^m + 2x_1^{n(C_3)} x_3^{(m-n(C_3))/3}) \quad (45')$$

from which

$$Z(\mathbf{P}_2(\mathbf{C}_{3v}), 3) = {}^1/_6(x_{21}^3 + 2x_{23}^1 + 3x_{21}^1 x_{22}^1) \quad (46)$$

$$Z(\mathbf{P}_2(\mathbf{C}_3), 3) = {}^1/_3(x_{21}^3 + 2x_{23}^1) \quad (46')$$

Obviously,

$$Z(\mathbf{P}_1, 1) = x_{11}^1 \quad (47)$$

and then the total cycle index is

$$Z(\mathbf{P}(\mathbf{C}_{3v}), 4) = {}^1/_6 x_{11}^1 (x_{21}^3 + 2x_{23}^1 + 3x_{21}^1 x_{22}^1) \quad (48)$$

$$Z(\mathbf{P}(\mathbf{C}_3), 4) = {}^1/_3 x_{11}^1 (x_{21}^3 + 2x_{23}^1) \quad (48')$$

As a consequence

$$\mathrm{CI}(\mathbf{P}(\mathbf{C}_{3v}), 4) = {}^1/_6(w_{11}^1 + w_{12}^1 + \ldots + w_{1\alpha_1}^1)\{(w_{21}^1 + w_{22}^1 + \ldots + w_{2\alpha_2}^1)^3 + 2(w_{21}^3 + w_{22}^3 + \ldots + w_{2\alpha_2}^3) + 3(w_{21}^1 + w_{22}^1 + \ldots + w_{2\alpha_2}^1)(w_{21}^2 + w_{22}^2 + \ldots + w_{2\alpha_2}^2)\} \quad (49)$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{C}_3), 4) = {}^1/_3(w_{11}^1 + w_{12}^1 + \ldots + w_{1\alpha_1}^1)\{(w_{21}^1 + w_{22}^1 + \ldots + w_{2\alpha_2}^1)^3 + 2(w_{21}^3 + w_{22}^3 + \ldots + w_{2\alpha_2}^3)\} \quad (50)$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{C}_{3v}), 4) = {}^1/_6 \alpha_1 \alpha_2 (2 + 3\alpha_2 + \alpha_2^2) \quad (51)$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{C}_3), 4) = {}^1/_3 \alpha_1 \alpha_2 (2 + \alpha_2^2) \quad (52)$$

Table 6

α_1	α_2	NI($\mathbf{P}(\mathbf{C}_3)$,4)	NI($\mathbf{P}(\mathbf{C}_{3v})$,4)
1	1	1	1
1	2	4	4
2	1	2	2
2	2	8	8
2	3	22	20
3	2	12	12
3	3	33	30
3	4	72	60
4	3	44	40
4	4	96	80
...	...	...	...

Table 7[a]

$W_iX_jY_kZ_l$				isomer no.	
i	*j*	*k*	*l*	$\mathbf{C}_{3v}$	$\mathbf{C}_3$
1	0	0	3	12	12
1	0	1	2	36	36
1	1	1	1	12	24

[a] $\alpha_1 = 3$, $\alpha_2 = 4$.

Table 8

α_1	α_2	α_3	α_4	α_5	α_6	NI($\mathbf{P}(\mathbf{D}_{2d})$,24)
1	1	1	1	1	1	1
2	1	1	1	1	1	3
1	1	2	1	1	1	6
1	1	1	1	1	2	43
2	2	1	1	1	1	9
2	1	2	1	1	1	18
2	1	1	1	1	2	129
1	1	1	1	2	2	258
2	2	2	1	1	1	54
2	2	2	1	1	2	2322
...	...	...	...	...	...	...

In Table 6 we have compared some NI values of both symmetries. The ratio

$$\frac{\mathrm{NI}(\mathbf{P}(\mathbf{C}_{3v}),4)}{\mathrm{NI}(\mathbf{P}(\mathbf{C}),4)} = \frac{1}{2} + \frac{3}{2}\frac{\alpha_2^2}{(2\alpha_2 + \alpha_2^3)}$$

and Table 6 indicate that there are stereoisomers for $\alpha_2 \geq 3$. In Table 7, the enumeration of different isomers in the case of $\alpha_1 = 3$, $\alpha_2 = 4$ is reported. The table shows that the 12 stereoisomers are all of WXYZ type.

4. Molecule with D_{2d} Symmetry.

$$\mathbf{D}_{2d} = \{\hat{E}, 2\hat{S}_4, \hat{C}_2, 2\hat{C}'_2, 2\sigma_d\}$$

$$\mathbf{D}_2 = \{\hat{E}, \hat{C}_{2x}, \hat{C}_{2y}, \hat{C}_{2z}\}$$

Adamantane-2,6-dione ($C_{10}H_{12}O_2$). The $\mathbf{D}_{2d}$ symmetry of this molecule gives six **G**-orbits, $n_o(\mathbf{D}_{2d}) = 6$, two two-dimensional generated by the carbonyl groups, three four-dimensional, and the other eight-dimensional. The last is due to eight equivalent hydrogen atoms. The molecular domain D is then decomposed in such a way

$$D = \underbrace{D_1 \cup D_2}_{\text{two-dimensionals}} \cup \underbrace{D_3 \cup D_4 \cup D_5}_{\text{four-dimensionals}} \cup \underbrace{D_6}_{\text{eight-dimensional}}$$

$$(n_i = |D_i| = 2\ (i = 1, 2),\quad n_j = |D_j| = 4\ (j = 3, 4, 5),\ n_6 = |D_6| = 8) \quad (53)$$

Table 9[a]

$T_iU_jV_kW_lX_mY_nZ_o$							
i	*j*	*k*	*l*	*m*	*n*	*o*	isomer no.
2	2	4	4	4	0	8	2
2	2	4	4	4	1	7	2
2	2	4	4	4	2	6	12
2	2	4	4	4	3	5	14
2	2	4	4	4	4	4	13

[a] $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = \alpha_5 = 1$, $\alpha_6 = 2$.

The permutation groups are

$$\mathbf{P}_i = \mathbf{P}(\mathbf{D}_{2d}, D_i) = \mathbf{P}(\mathbf{C}_2, D_i) \qquad i = 1, 2 \quad (54)$$

$$\mathbf{P}_j = \mathbf{P}(\mathbf{D}_{2d}, D_j) \qquad j = 3,4,5 \quad (55)$$

$$\mathbf{P}_6 = \mathbf{P}(\mathbf{D}_{2d}, D_6) \quad (56)$$

The cycle index of these permutation groups is obtained from Tables 1 and 2 of ref 1 and is

$$Z(\mathbf{P}_i, 2) = {}^1/_2(x_{i1}^2 + x_{i2}^1) \qquad i = 1, 2 \quad (57)$$

$$Z(\mathbf{P}_j, 4) = {}^1/_8(x_{j1}^4 + 3x_{j2}^2 + 2x_{j4}^1 + 2x_{j1}^2\, x_{j2}^1) \qquad j = 3, 4, 5 \quad (58)$$

$$Z(\mathbf{P}_6, 8) = {}^1/_8(x_{61}^8 + 5x_{62}^4 + 2x_{64}^2) \quad (59)$$

The total cycle index is

$$Z(\mathbf{P}(\mathbf{D}_{2d}),24) = \frac{1}{2^2 8^4}[\prod_{i=1}^{2}(x_{i1}^2 + x_{i2}^1)][\prod_{j=3}^{5}(x_{j1}^4 + 3x_{j2}^2 + 2x_{j4}^1 + 2x_{j1}^2\, x_{j2}^1)][x_{61}^8 + 5x_{62}^4 + 2x_{64}^2] \quad (60)$$

and the series counting isomers and the numbers of isomers have the expressions

$$\mathrm{CI}(\mathbf{P}(\mathbf{D}_{2d}),24) = \frac{1}{2^2 8^4}\{\prod_{i=1}^{2}[(w_{i1}^1 + w_{i2}^1 + \ldots + w_{i\alpha_i}^1)^2 + (w_{i1}^2 + w_{i2}^2 + \ldots + w_{i\alpha_i}^2)]\}\{\prod_{j=3}^{5}[(w_{j1}^1 + w_{j2}^1 + \ldots + w_{j\alpha_j}^1)^4 + 3(w_{j1}^2 + w_{j2}^2 + \ldots + w_{j\alpha_j}^2)^2 + 2(w_{j1}^4 + w_{j2}^4 + \ldots + w_{j\alpha_j}^4) + 2(w_{j1}^1 + w_{j2}^1 + \ldots + w_{j\alpha_j}^1)^2(w_{j1}^2 + w_{j2}^2 + \ldots + w_{j\alpha_j}^2)]\}\{(w_{61}^1 + w_{62}^1 + \ldots + w_{6\alpha_6}^1)^8 + 5(w_{61}^2 + w_{62}^2 + \ldots + w_{6\alpha_6}^2)^4 + 2(w_{61}^4 + w_{62}^4 + \ldots + w_{6\alpha_6}^4)^2\} \quad (61)$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{D}_{2d}),24) = \frac{1}{2^2 8^4}\{\prod_{i=1}^{2}(\alpha_i^2 + \alpha_i)\prod_{j=3}^{5}(\alpha_j^4 + 3\alpha_j^2 + 2\alpha_j^1 + 2\alpha_j^3)(\alpha_6^8 + 5\alpha_6^4 + 2\alpha_6^2)\} \quad (62)$$

In Table 8 selected total numbers of isomers (NI) are reported, while in Table 9 the explicit enumeration of isomers for $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = \alpha_5 = 1$ and $\alpha_6 = 2$ is presented. With the $\mathbf{D}_2$ point group we obtain $n_o(\mathbf{D}_2) = 8$, and the total domain is thus decomposed,

$$D = \underbrace{D_1 \cup D_2 \cup D_3 \cup D_4}_{\text{two-dimensionals}} \cup \underbrace{D_5 \cup D_6 \cup D_7 \cup D_8}_{\text{four-dimensionals}}$$

$$(n_i = |D_i| = 2\ (i = 1, ..., 4),\quad n_j = |D_j| = 4\ (j = 5, ..., 8)) \quad (63)$$

The permutation groups are

$$\mathbf{P}_i = \mathbf{P}(\mathbf{D}_2,D_i) = \mathbf{P}(\mathbf{C}_2,D_i) \qquad i = 1, 2, 3, 4$$

$$\mathbf{P}_j = \mathbf{P}(\mathbf{D}_2,D_j) \qquad j = 5, 6, 7, 8$$

and using the formula

$$Z(\mathbf{D}_2,m) = {}^1/_4(x_1^m + \sum_{k=x,y,z} x_1^{n(C_{2k})}\, x_2^{(m-n(C_{2k}))/2}) \quad (64)$$

one obtain

$$Z(\mathbf{P}(\mathbf{D}_2,D_j),4) = {}^1/_4(x_{j1}^4 + 2x_{j1}^2\, x_{j2}^1 + x_{j2}^2) \qquad j = 5, ..., 8 \quad (65)$$

Because

$$Z(\mathbf{P}(\mathbf{D}_2,D_i),2) = {}^1/_2(x_{i1}^2 + x_{i2}^1) \qquad i = 1, ..., 4 \quad (66)$$

we have

$$Z(\mathbf{P}(\mathbf{D}_2),24) = \frac{1}{2^4}\frac{1}{4^4}\prod_{i=1}^{4}(x_{i1}^2 + x_{i2}^1)\prod_{j=5}^{8}(x_{j1}^4 + 2x_{j1}^2\, x_{j2}^1 + x_{j2}^2) \quad (67)$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{D}_2),24) = \frac{1}{2^4}\frac{1}{4^4}\prod_{i=1}^{4}(\alpha_i^2 + \alpha_i)\prod_{j=5}^{8}(\alpha_j^4 + 2\alpha_j^3 + \alpha_j^2) \quad (68)$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{D}_2),24) = \frac{1}{2^4 4^4}\prod_{i=1}^{4}[(w_{i1}^1 + w_{i2}^1 + ... + w_{i\alpha_i}^1)^2 + (w_{i1}^2 + w_{i2}^2 + ... + w_{i\alpha_i}^2)]\prod_{j=5}^{8}[(w_{j1}^1 + w_{j2}^1 + ... + w_{j\alpha_j}^1)^4 + 2(w_{j1}^1 + w_{j2}^1 + ... + w_{j\alpha_j}^1)^2 (w_{j1}^2 + w_{j2}^2 + ... + w_{j\alpha_j}^2) + (w_{j1}^2 + w_{j2}^2 + ... + w_{j\alpha_j}^2)^2] \quad (69)$$

Table 10 shows some NI values calculated with eq 68, while Table 11 reports the enumeration of different isomers in the case of $\alpha_i = 1$ ($i = 1, 2, ..., 6$) and $\alpha_7 = \alpha_8 = 2$, where we have 38 stereoisomers.

(5) Molecule with D_{2h} Symmetry.

$$\mathbf{D}_{2h} = \{\hat{E},\hat{C}_{2x},\hat{C}_{2y},\hat{C}_{2z},\hat{\imath},\hat{\sigma}_{xy},\hat{\sigma}_{xz},\hat{\sigma}_{yz}\}$$

$$\mathbf{D}_2 = \{\hat{E},\hat{C}_{2x},\hat{C}_{2y},\hat{C}_{2z}\}$$

Dibenzodioxin ($C_{12}H_8O_2$). Using eq 3 and the $\mathbf{D}_{2h}$ point group, for this compound we obtain six **G**-orbits, $n_o(D_{2h}) = 6$, thus composed: the two oxygens form one **G**-orbit, the twelve carbon atoms three **G**-orbits of length four, and the eight hydrogen two **G**-orbits of four elements. The total molecular domain is thus decomposed

Table 10

α_1	α_2	α_3	α_4	α_5	α_6	α_7	α_8	NI($\mathbf{P}(\mathbf{D}_2)$,24)
1	1	1	1	1	1	1	1	1
2	1	1	1	1	1	1	1	3
1	1	1	1	1	1	2	1	9
3	1	1	1	1	1	1	1	6
1	1	1	1	1	1	3	1	36
4	1	1	1	1	1	1	1	10
1	1	1	1	1	1	4	1	100
2	2	1	1	1	1	1	1	9
2	1	1	1	1	1	2	1	27
1	1	1	1	1	1	2	2	81
...	...	...	...	...	...	...	...	...
2	2	2	1	1	1	1	1	27
2	2	1	1	1	2	1	1	81
...	...	...	...	...	...	...	...	...
2	2	2	1	1	1	2	2	2187
...	...	...	...	...	...	...	...	...

Table 11[a]

$Q_hR_iSjT_kU_lV_mW_nX_oY_pZ_q$										
h	*i*	*j*	*k*	*l*	*m*	*n*	*o*	*p*	*q*	isomer no.
2	2	2	2	4	4	4	0	4	0	4
2	2	2	2	4	4	4	0	3	1	16
2	2	2	2	4	4	4	0	2	2	12
2	2	2	2	4	4	3	1	3	1	16
2	2	2	2	4	4	3	1	2	2	24
2	2	2	2	4	4	2	2	2	2	9

[a] $\alpha_i = 1$ ($i = 1, 2, ..., 6$); $\alpha_7 = \alpha_8 = 2$.

$$D = \underbrace{D_1}_{\text{two-dimensional}} \cup \underbrace{D_2 \cup D_3 \cup D_4 \cup D_5 \cup D_6}_{\text{four-dimensionals}}$$

$$(n_1 = |D_1| = 2, \qquad n_j = |D_j| = 4\ (j = 2, 3, ..., 6)) \quad (70)$$

From Table 1 and 2 of ref 1, the cycle index of the permutation groups

$$\mathbf{P}_1 = \mathbf{P}(\mathbf{D}_{2h},D_1) = \mathbf{P}(\mathbf{C}_2,D_1) \quad (71)$$

$$\mathbf{P}_j = \mathbf{P}(\mathbf{D}_{2h},D_j) \qquad (j = 2, 3, ..., 6) \quad (72)$$

are

$$Z(\mathbf{P}_1,2) = {}^1/_2(x_{11}^2 + x_{12}^1) \quad (73)$$

$$Z(\mathbf{P}_j,4) = {}^1/_4(x_{j1}^4 + 3x_{j2}^2) \qquad j = 2, 3, ..., 6 \quad (74)$$

Then

$$Z(\mathbf{P}(\mathbf{D}_{2h}),22) = \frac{1}{2}\frac{1}{4^5}(x_{11}^2 + x_{12}^1)\prod_{j=2}^{6}(x_{j1}^4 + 3x_{j2}^2) \quad (75)$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{D}_{2h}),22) = \frac{1}{2}\frac{1}{4^5}[(w_{11}^1 + w_{12}^1 + ... + w_{1\alpha_1}^1)^2 + (w_{11}^2 + w_{12}^2 + ... + w_{1\alpha_1}^2)]\prod_{j=2}^{6}[(w_{j1}^1 + w_{j2}^1 + ... + w_{j\alpha_j}^1)^4 + 3(w_{j1}^2 + w_{j2}^2 + ... + w_{j\alpha_j}^2)^2] \quad (76)$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{D}_{2h}),22) = \frac{1}{2}\frac{1}{4^5}[(\alpha_1^2 + \alpha_1^1)\prod_{j=2}^{6}(\alpha_j^4 + 3\alpha_j^2)] \quad (77)$$

Table 12

α_1	α_2	α_3	α_4	α_5	α_6	NI($\mathbf{P}(\mathbf{D}_{2h})$,22)
1	1	1	1	1	1	1
2	1	1	1	1	1	2
1	2	1	1	1	1	7
2	2	1	1	1	1	21
1	2	2	1	1	1	49
2	2	2	1	1	1	147
1	2	2	2	1	1	343
2	2	2	2	1	1	1029
1	2	2	2	2	1	2401
2	2	2	2	2	1	7203
1	2	2	2	2	2	16807
2	2	2	2	2	2	50421
3	1	1	1	1	1	6
1	3	1	1	1	1	27
4	1	1	1	1	1	10
1	4	1	1	1	1	76
...	...	...	...	...	...	...

Table 13[a]

$S_iT_jU_kV_lW_mX_nY_oZ_p$								
i	*j*	*k*	*l*	*m*	*n*	*o*	*p*	isomer no.
2	4	4	4	0	4	0	4	4
2	4	4	4	0	4	1	3	8
2	4	4	4	0	4	2	2	12
2	4	4	4	1	3	1	3	4
2	4	4	4	1	3	2	2	12
2	4	4	4	2	2	2	2	9

[a] $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 1$; $\alpha_5 = \alpha_6 = 2$.

Table 14

α_1	α_2	α_3	α_4	NI($\mathbf{P}(\mathbf{D}_{6h})$,36)
1	1	1	1	1
2	1	1	1	13
1	1	2	1	382
3	1	1	1	92
1	1	3	1	44727
4	1	1	1	430
1	1	4	1	1400536
2	2	1	1	169
2	1	2	1	4966
1	1	2	2	145924
2	2	2	1	64558
1	2	2	2	1897012
2	2	2	2	24661156
...	...	...	...	...

Some total numbers of isomers, computed using eq 77, are reported in Table 12, while Table 13 gives the enumeration of the different isomers when $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 1$ and $\alpha_5 = \alpha_6 = 2$.

With respect to previous results obtained with $\mathbf{D}_{2h}$ symmetry on dibenzodioxin, no change is obtained with $\mathbf{D}_2$ symmetry. There are no stereoisomers in this structure as is evident from planar geometry.

(6) Molecule with D_{6h} Symmetry.

$$\mathbf{D}_{6h} = \{\hat{E},2\hat{C}_6,2\hat{C}_3,\hat{C}_2,3\hat{C}'_2,3\hat{C}''_2,\hat{\imath},2\hat{S}_3,2\hat{S}_6,\hat{\sigma}_h,3\hat{\sigma}_d,3\hat{\sigma}_v\}$$

$$\mathbf{D}_6 = \{\hat{E},2\hat{C}_6,2\hat{C}_3,\hat{C}_2,3\hat{C}'_2,3\hat{C}''_2\}$$

Coronene ($C_{24}H_{12}$). The $\mathbf{D}_{6h}$ symmetry of this molecule gives four **G**-orbits, $n_o(\mathbf{D}_{6h}) = 4$. The twelve hydrogen atoms give one **G**-orbit, while the twenty-four carbon atoms give two **G**-orbits of six elements and one of twelve elements. The molecular domain *D* is then decomposed in such a way

$$D = \underbrace{D_1 \cup D_2}_{\text{six-dimensionals}} \cup \underbrace{D_3 \cup D_4}_{\text{twelve-dimensionals}}$$

$$(n_i = |D_i| = 6\ (i = 1, 2), \quad n_j = |D_j| = 12\ (j = 3, 4)) \quad (78)$$

From Table 2 of ref 1, the cycle index of the permutation groups

$$\mathbf{P}_i = \mathbf{P}(\mathbf{D}_{6h},D_i) \qquad i = 1, 2 \quad (79)$$

$$\mathbf{P}_j = \mathbf{P}(\mathbf{D}_{6h},D_j) \qquad j = 3, 4 \quad (80)$$

are

$$Z(\mathbf{P}_i,6) = {}^1/_{12}(x_{i1}^6 + 4x_{i2}^3 + 2x_{i3}^2 + 2x_{i6}^1 + 3x_{i1}^2 x_{i2}^2) \qquad i = 1, 2 \quad (81)$$

$$Z(\mathbf{P}_j,12) = {}^1/_{12}(x_{j1}^{12} + 7x_{j2}^6 + 2x_{j3}^4 + 2x_{j6}^2) \qquad j = 3, 4 \quad (82)$$

The expression for the total cycle index, the series counting isomers, and the number of isomers is

$$Z(\mathbf{P}(\mathbf{D}_{6h}),36) = {}^1/_{12^4}\prod_{i=1}^{2}(x_{i1}^6 + 4x_{i2}^3 + 2x_{i3}^2 + 2x_{i6}^1 + 3x_{i1}^2 x_{i2}^2)\prod_{j=3}^{4}(x_{j1}^{12} + 7x_{j2}^6 + 2x_{j3}^4 + 2x_{j6}^2) \quad (83)$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{D}_{6h}),36) = {}^1/_{12^4}\prod_{i=1}^{2}[(w_{i1}^1 + w_{i2}^1 + \ldots + w_{i\alpha_i}^1)^6 + 4(w_{i1}^2 + w_{i2}^2 + \ldots + w_{i\alpha_i}^2)^3 + 2(w_{i1}^3 + w_{i2}^3 + \ldots + w_{i\alpha_1}^3)^2 + 2(w_{i1}^6 + w_{i2}^6 + \ldots + w_{i\alpha_i}^6) + 3(w_{i1}^1 + w_{i2}^1 + \ldots + w_{i\alpha_i}^1)^2 (w_{i1}^2 + w_{i2}^2 + \ldots + w_{i\alpha_i}^2)^2]\prod_{j=3}^{4}[(w_{j1}^1 + w_{j2}^1 + \ldots + w_{j\alpha_j}^1)^{12} + 7(w_{j1}^2 + w_{j2}^2 + \ldots + w_{j\alpha_j}^2)^6 + 2(w_{j1}^3 + w_{j2}^3 + \ldots + w_{j\alpha_j}^3)^4 + 2(w_{j1}^6 + w_{j2}^6 + \ldots + w_{j\alpha_j}^6)^2] \quad (84)$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{D}_{6h}),36) = {}^1/_{12^4}\prod_{i=1}^{2}(\alpha_i^6 + 4\alpha_i^3 + 2\alpha_i^2 + 2\alpha_i^1 + 3\alpha_i^4)\prod_{j=3}^{4}(\alpha_j^{12} + 7\alpha_j^6 + 2\alpha_j^4 + 2\alpha_j^2) \quad (85)$$

In Table 14 are reported examples of total numbers of isomers (NI) calculated with eq 85, while Table 15 reports the number of different isomers obtained using eq 84 with $\alpha_k = 1$ ($k = 1, 2, 3$) and $\alpha_4 = 4$.

With respect to previous results obtained with $\mathbf{D}_{6h}$ symmetry on coronene, no change is obtained with $\mathbf{D}_6$ symmetry. There are no stereoisomers in this structure as is evident from planar geometry.

(7) Molecules Having Tetrahedral Symmetry.

$$\mathbf{T}_d = \{\hat{E},3\hat{C}_2,8\hat{C}_3,6\hat{S}_4,6\hat{\sigma}\}$$

$$\mathbf{T} = \{\hat{E},3\hat{C}_2,4\hat{C}_3,4\hat{C}_3^2\}$$

Molecules with Molecular Formula AB_4 (CH_4, SiF_4, MnO_4^-, ...). Using both symmetries one obtains $n_o(\mathbf{T}_d) =$

Table 15[a]

$V_iW_jX_kY_lZ_m$					
i	*j*	*k*	*l*	*m*	isomer no.
6	6	6	0	12	2
6	6	6	1	11	2
6	6	6	2	10	18
6	6	6	3	9	38
6	6	6	4	8	100
6	6	6	5	7	132
6	6	6	6	6	90

[a] $\alpha_k = 1$ ($k = 1, 2, 3$); $\alpha_4 = 4$.

Table 16

α_1	α_2	NI(**P**(**T**),5)	NI(**P**($\mathbf{T}_d$),5)
1	1	1	1
2	1	2	2
1	2	5	5
2	2	10	10
3	1	3	3
1	3	15	15
3	2	15	15
2	3	30	30
3	3	45	45
4	1	4	4
1	4	36	35
4	2	20	20
2	4	72	70
4	3	60	60
3	4	108	105
4	4	144	140
...	...	...	...
5	5	375	350
...	...	...	...

$n_o(\mathbf{T}) = 2$, and thus

$$D = \underbrace{D_1}_{\text{one-dimensional}} \cup \underbrace{D_2}_{\text{four-dimensional}}$$
$$(n_1 = |D_1| = 1, \quad n_2 = |D_2| = 4) \tag{86}$$

From Tables 1 and 2 of ref 1, the cycle index of the permutation groups

$$\mathbf{P}_1 = \mathbf{P}(\mathbf{T}_d,D_1) = \mathbf{P}(\mathbf{T},D_1) = \mathbf{P}(\mathbf{C}_1,D_1) \tag{87}$$
$$\mathbf{P}_2(\mathbf{T}_d) = \mathbf{P}(\mathbf{T}_d,D_2) \tag{88}$$
$$\mathbf{P}_2(\mathbf{T}) = \mathbf{P}(\mathbf{T},D_2) \tag{88'}$$

are

$$Z(\mathbf{P}_1,1) = x_{11}^1 \tag{89}$$
$$Z(\mathbf{P}_2(\mathbf{T}_d),4) = {}^1/_{24}(x_{21}^4 + 3x_{22}^2 + 6x_{24}^1 + 8x_{21}^1 x_{23}^1 + 6x_{21}^2 x_{22}^1) \tag{90}$$
$$Z(\mathbf{P}_2(\mathbf{T}),4) = {}^1/_{12}(x_{21}^4 + 8x_{21}^1 x_{23}^1 + 3x_{22}^2) \tag{90'}$$

The cycle indices of the total permutation groups are

$$Z(\mathbf{P}(\mathbf{T}_d),5) = {}^1/_{24}x_{11}^1(x_{21}^4 + 3x_{22}^2 + 6x_{24}^1 + 8x_{21}^1 x_{23}^1 + 6x_{21}^2 x_{22}^1) \tag{91}$$
$$Z(\mathbf{P}(\mathbf{T}),5) = x_{11}^1({}^1/_{12})(x_{21}^4 + 8x_{21}^1 x_{23}^1 + 3x_{22}^2) \tag{91'}$$

Table 17[a]

$V_iW_jX_kY_lZ_m$					isomer no.	
i	*j*	*k*	*l*	*m*	**T**	$\mathbf{T}_d$
1	4	0	0	0	4	4
1	3	1	0	0	12	12
1	2	2	0	0	6	6
1	2	1	1	0	12	12
1	1	1	1	1	2	1

[a] $\alpha_1 = 1$; $\alpha_2 = 4$.

and the formulas for the total number of isomers and the series counting isomers are

$$\mathrm{NI}(\mathbf{P}(\mathbf{T}_d),5) = {}^1/_{24}\alpha_1(\alpha_2^4 + 6\alpha_2^3 + 11\alpha_2^2 + 6\alpha_2) \tag{92}$$
$$\mathrm{NI}(\mathbf{P}(\mathbf{T}),5) = {}^1/_{12}\alpha_1(\alpha_2^4 + 11\alpha_2^2) \tag{92'}$$
$$\mathrm{CI}(\mathbf{P}(\mathbf{T}_d),5) = {}^1/_{24}(w_{11}^1 + w_{12}^1 + ... + w_{1\alpha_1}^1)[(w_{21}^1 + w_{22}^1 + ... + w_{2\alpha_2}^1)^4 + 3(w_{21}^2 + w_{22}^2 + ... + w_{2\alpha_2}^2)^2 + 6(w_{21}^4 + w_{22}^4 + ... + w_{2\alpha_2}^4) + 8(w_{21}^1 + w_{22}^1 + ... + w_{2\alpha_2}^1) \times (w_{21}^3 + w_{22}^3 + ... + w_{2\alpha_2}^3) + 6(w_{21}^1 + w_{22}^1 + ... + w_{2\alpha_2}^1)^2 \times (w_{21}^2 + w_{22}^2 + ... + w_{2\alpha_2}^2)] \tag{93}$$
$$\mathrm{CI}(\mathbf{P}(\mathbf{T}),5) = {}^1/_{12}(w_{11}^1 + w_{12}^1 + ... + w_{1\alpha_1}^1)[(w_{21}^1 + w_{22}^1 + ... + w_{2\alpha_2}^1)^4 + 3(w_{21}^2 + w_{22}^2 + ... + w_{2\alpha_2}^2)^2 + 8(w_{21}^1 + w_{22}^1 + ... + w_{2\alpha_2}^1)(w_{21}^3 + w_{22}^3 + ... + w_{2\alpha_2}^3)] \tag{93'}$$

The comparison of some total numbers of isomers (NI) obtained using eqs 92 and 92′ is reported in Table 16. This table and the ratio NI(**P**($\mathbf{T}_d$),5)/NI(**P**(**T**),5) show that stereoisomers begin to appear for $\alpha_2 \geq 4$.

The enumeration of different isomers for $\alpha_1 = 1$ and $\alpha_2 = 4$ is given in Table 17 for both symmetries. There is one stereoisomer of VWXYZ type.

8. Molecules Having Octahedral Symmetry.

$$\mathbf{O}_h = \{\hat{E},8\hat{C}_3,6\hat{C}_4,3\hat{C}_4^2,6\hat{C}_2,\hat{\imath},8\hat{S}_6,6\hat{S}_4,3\hat{\sigma}_h,6\hat{\sigma}_d\}$$
$$\mathbf{O} = \{\hat{E},8\hat{C}_3,6\hat{C}_4,3\hat{C}_4^2,6\hat{C}_2\}$$

(8.a) Molecules with Molecular Formula AB_6 (SF_6, ...). Using eq 3, we obtain $n_o(\mathbf{O}_h) = n_o(\mathbf{O}) = 2$, the atom A gives one **G**-orbit, and the atoms B the other **G**-orbit of length six. The molecular domain *D* is thus decomposed

$$D = \underbrace{D_1}_{\text{one-dimensional}} \cup \underbrace{D_2}_{\text{six-dimensional}}$$
$$(n_1 = |D_1| = 1, \quad n_2 = |D_2| = 6) \tag{94}$$

Because

$$\mathbf{P}_1 = \mathbf{P}(\mathbf{O}_h,D_1) = \mathbf{P}(\mathbf{O},D_1) = \mathbf{P}(\mathbf{C}_1,D_1) \tag{95}$$

then

$$Z(\mathbf{P}_1,1) = x_{11}^1 \tag{96}$$

On the other hand,

$$\mathbf{P}_2(\mathbf{O}_h) = \mathbf{P}(\mathbf{O}_h, D_2) \tag{97}$$

$$\mathbf{P}_2(\mathbf{O}) = \mathbf{P}(\mathbf{O}, D_2) \tag{98}$$

and from Tables 1 and 2 of ref 1, it follows

$$Z(\mathbf{P}_2(\mathbf{O}),6) = {}^1/_{24}(x_{21}^6 + 6x_{21}^2 x_{24}^1 + 3x_{21}^2 x_{22}^2 + 8x_{23}^2 + 6x_{22}^3) \tag{99}$$

$$Z(\mathbf{P}_2(\mathbf{O}_h),6) = {}^1/_{48}[x_{21}^6 + 7x_{22}^3 + 8(x_{26}^1 + x_{23}^2) + 6(x_{21}^2 x_{24}^1 + x_{22}^1 x_{24}^1) + 9x_{21}^2 x_{22}^2 + 3x_{21}^4 x_{22}^1] \tag{100}$$

then

$$Z(\mathbf{P}(\mathbf{O}),7) = {}^1/_{24}x_{11}^1(x_{21}^6 + 6x_{21}^2 x_{24}^1 + 3x_{21}^2 x_{22}^2 + 8x_{23}^2 + 6x_{22}^3) \tag{101}$$

$$Z(\mathbf{P}(\mathbf{O}_h),7) = {}^1/_{48}x_{11}^1[x_{21}^6 + 7x_{22}^3 + 8(x_{26}^1 + x_{23}^2) + 6(x_{21}^2 x_{24}^1 + x_{22}^1 x_{24}^1) + 9x_{21}^2 x_{22}^2 + 3x_{21}^4 x_{22}^1] \tag{102}$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{O}),7) = {}^1/_{24}(w_{11}^1 + w_{12}^1 + \ldots + w_{1\alpha_1}^1)[(w_{21}^1 + w_{22}^1 + \ldots + w_{2\alpha_2}^1)^6 + 6(w_{21}^2 + w_{22}^2 + \ldots + w_{2\alpha_2}^2)^3 + 8(w_{21}^3 + w_{22}^3 + \ldots + w_{2\alpha_2}^3)^2 + 6(w_{21}^1 + w_{22}^1 + \ldots + w_{2\alpha_2}^1)^2(w_{21}^4 + w_{22}^4 + \ldots + w_{2\alpha_2}^4) + 3(w_{21}^1 + w_{22}^1 + \ldots + w_{2\alpha_2}^1)^2(w_{21}^2 + w_{22}^2 + \ldots + w_{2\alpha_2}^2)^2] \tag{103}$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{O}_h),7 = {}^1/_{48}(w_{11}^1 + w_{12}^1 + \ldots + w_{1\alpha_1}^1)[(w_{21}^1 + w_{22}^1 + \ldots + w_{2\alpha_2}^1)^6 + 7(w_{21}^2 + w_{22}^2 + \ldots + w_{2\alpha_2}^2)^3 + 8((w_{21}^6 + w_{22}^6 + \ldots + w_{2\alpha_2}^6) + (w_{21}^3 + w_{22}^3 + \ldots + w_{2\alpha_2}^3)^2) + 6((w_{21}^1 + w_{22}^1 + \ldots + w_{2\alpha_2}^1)^2(w_{21}^4 + w_{22}^4 + \ldots + w_{2\alpha_2}^4) + (w_{21}^2 + w_{22}^2 + \ldots + w_{2\alpha_2}^2)(w_{21}^4 + w_{22}^4 + \ldots + w_{2\alpha_2}^4)) + 9(w_{21}^1 + w_{22}^1 + \ldots + w_{2\alpha_2}^1)^2(w_{21}^2 + w_{22}^2 + \ldots + w_{2\alpha_2}^2)^2 + 3(w_{21}^1 + w_{22}^1 + \ldots + w_{2\alpha_2}^1)^4(w_{21}^2 + w_{22}^2 + \ldots + w_{2\alpha_2}^2)] \tag{104}$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{O}),7) = {}^1/_{24}\alpha_1\alpha_2^2[\alpha_2^4 + 3\alpha_2^2 + 12\alpha_2^1 + 8] \tag{105}$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{O}_h),7) = {}^1/_{48}\alpha_1[\alpha_2^6 + 3\alpha_2^5 + 9\alpha_2^4 + 13\alpha_2^3 + 14\alpha_2^2 + 8\alpha_2^1] \tag{106}$$

From eqs 105 and 106 one obtains the data reported in Table 18 for selected total numbers of isomer (NI). The table and the ratio NI($\mathbf{P}(\mathbf{O}_h)$,7)/NI($\mathbf{P}(\mathbf{O})$,7) show that the stereoisomers appear for $\alpha_2 \geq 3$. Table 19 gives the enumeration of different isomers in the case of $\alpha_1 = 1$ and $\alpha_2 = 4$. The table shows that of twenty stereoisomers four are of $VWXYZ_3$ type, four of $VX_2Y_2Z_2$ type, and twelve of $VWXY_2Z_2$ type.

(8.b) Cubane (C_8H_8). An interesting molecule with $\mathbf{O}_h$ symmetry is cubane. From eq 2 we obtain two **G**-orbits of length six for both point groups, $n_o(\mathbf{O}_h) = n_o(\mathbf{O}) = 2$, the eight hydrogen atoms give one **G**-orbit, and the eight carbon atoms the other **G**-orbit. The molecular domain is

Table 18

α_1	α_2	NI($\mathbf{P}(\mathbf{O})$,7)	NI($\mathbf{P}(\mathbf{O}_h)$,7)
1	1	1	1
1	2	10	10
2	1	2	2
2	2	20	20
3	1	3	3
1	3	57	56
3	2	30	30
2	3	114	112
3	3	171	168
4	1	4	4
1	4	240	220
4	2	40	40
2	4	480	440
4	3	228	224
3	4	720	660
4	4	960	880
...	...	...	...
4	6	8904	7084
...	...	...	...

Table 19[a]

$V_iW_jX_kY_lZ_m$					isomer no.	
i	j	k	l	m	**O**	$\mathbf{O}_h$
1	0	0	0	6	4	4
1	0	0	1	5	12	12
1	0	0	2	4	24	24
1	0	0	3	3	12	12
1	0	1	1	4	24	24
1	0	1	2	3	72	72
1	1	1	1	3	20	16
1	0	2	2	2	24	20
1	1	1	2	2	48	36

[a] $\alpha_1 = 1$; $\alpha_2 = 4$.

Table 20

α_1	α_2	NI($\mathbf{P}(\mathbf{O}_h)$,16)	NI($\mathbf{P}(\mathbf{O})$,16)
1	1	1	1
1	2	22	23
1	3	267	333
1	4	1996	2916
1	5	10375	16725
1	6	41406	70911
...	...	...	...
2	2	484	529
2	3	5874	7659
2	4	43912	67068
2	5	228250	384675
...	...	...	...

$$D = \underbrace{D_1 \cup D_2}_{\text{eight-dimensionals}} \qquad (n_1 = |D_1| = n_2 = |D_2| = 8) \tag{107}$$

Because

$$\mathbf{P}_i(\mathbf{O}_h) = \mathbf{P}(\mathbf{O}_h, D_i) \qquad i = 1, 2 \tag{108}$$

$$\mathbf{P}_i(\mathbf{O}) = \mathbf{P}(\mathbf{O}, D_i) \qquad i = 1, 2 \tag{108'}$$

from Tables 1 and 2 of ref 1, it follows

$$Z(\mathbf{P}_i(\mathbf{O}_h),8) = {}^1/_{48}[x_{i1}^8 + 13x_{i2}^4 + 8(x_{i2}^1 x_{i6}^1 + x_{i1}^2 x_{i3}^2) + 12x_{i4}^2 + 6x_{i1}^4 x_{i2}^2] \qquad i = 1, 2 \tag{109}$$

$$Z(\mathbf{P}_i(\mathbf{O}),8) = {}^1/_{24}[x_{i1}^8 + 9x_{i2}^4 + 8x_{i1}^2 x_{i3}^2 + 6x_{i4}^2] \qquad i = 1, 2 \tag{109'}$$

The formulas for the total cycle index, the counting isomers,

Table 21[a]

$W_iX_jY_kZ_l$				isomer no.	
i	*j*	*k*	*l*	$\mathbf{O}_h$	**O**
8	8	0	0	3	3
8	7	1	0	6	6
8	6	2	0	18	18
8	6	1	1	9	9
8	5	3	0	18	18
8	5	2	1	36	42
8	4	4	0	18	21
8	4	3	1	60	78
8	4	2	2	48	66
8	3	3	2	51	72

[a] $\alpha_1 = 1$; $\alpha_2 = 3$.

Table 22

α_1	α_2	NI(**P**(**I**),7)	NI(**P**($\mathbf{I}_h$),7)
1	1	1	1
1	2	96	82
2	2	9216	6724
2	3	873504	441078
3	3	82791801	28933641
...	...	...	...

and the number of isomers are

$$Z(\mathbf{P}(\mathbf{O}_h),16) = {}^1/_{48^2}\prod_{i=1}^{2}[x_{i1}^8 + 13x_{i2}^4 + 8(x_{i2}^1 x_{i6}^1 + x_{i1}^2 x_{i3}^2) + 12x_{i4}^2 + 6x_{i1}^4 x_{i2}^2] \quad (110)$$

$$Z(\mathbf{P}(\mathbf{O}),16) = {}^1/_{24^2}\prod_{i=1}^{2}[x_{i1}^8 + 9x_{i2}^4 + 8x_{i1}^2 x_{i3}^2 + 6x_{i4}^2] \quad (111)$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{O}_h),16) = {}^1/_{48^2}\prod_{i=1}^{2}[(w_{i1}^1 + w_{i2}^1 + ... + w_{i\alpha_i}^1)^8 + 13(w_{i1}^2 + w_{i2}^2 + ... + w_{i\alpha_i}^2)^4 + 8((w_{i1}^2 + w_{i2}^2 + ... + w_{i\alpha_i}^2)(w_{i1}^6 + w_{i2}^6 + ... + w_{i\alpha_i}^6) + (w_{i1}^1 + w_{i2}^1 + ... + w_{i\alpha_i}^1)^2(w_{i1}^3 + w_{i2}^3 + ... + w_{i\alpha_i}^3)^2) + 12(w_{i1}^4 + w_{i2}^4 + ... + w_{i\alpha_i}^4)^2 + 6(w_{i1}^1 + w_{i2}^1 + ... + w_{i\alpha_i}^1)^4(w_{i1}^2 + w_{i2}^2 + ... + w_{i\alpha_i}^2)^2] \quad (112)$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{O}),16) = {}^1/_{24^2}\prod_{i=1}^{2}[(w_{i1}^1 + w_{i2}^1 + ... + w_{i\alpha_i}^1)^8 + 9(w_{i1}^2 + w_{i2}^2 + ... + w_{i\alpha_i}^2)^4 + 8(w_{i1}^1 + w_{i2}^1 + ... + w_{i\alpha_i}^1)^2(w_{i1}^3 + w_{i2}^3 + ... + w_{i\alpha_i}^3)^2 + 6(w_{i1}^4 + w_{i2}^4 + ... + w_{i\alpha_i}^4)^2] \quad (113)$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{O}_h),16) = {}^1/_{48^2}\prod_{i=1}^{2}[\alpha_i^8 + 20\alpha_i^2 + 21\alpha_i^4 + 6\alpha_i^6] \quad (114)$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{O}),16) = {}^1/_{24^2}\prod_{i=1}^{2}[\alpha_i^8 + 6\alpha_i^2 + 17\alpha_i^4] \quad (115)$$

Some results obtained using eqs 114 and 115 are presented in Table 20. The table and the ratio NI(**P**($\mathbf{O}_h$),16)/NI(**P**(**O**),16) show that stereoisomers already begin to appear from α_1 or α_2 equal to 2. Table 21 indicates the enumeration of isomers of cubane for $\alpha_1 = 2$ and $\alpha_2 = 3$. The number and the type of stereoisomers indicated in Table 21 are as follows: 6 $W_8X_5Y_2Z$, 3 $W_8X_4Y_4$, 18 $W_8X_4Y_3Z$, 18 $W_8X_4Y_2Z_2$, 21 $W_8X_3Y_3Z_2$.

Table 23[a]

$W_iX_jY_kZ_l$				isomer no.	
i	*j*	*k*	*l*	$\mathbf{I}_h$	**I**
12	0	12	0	2	2
12	0	11	1	2	2
12	0	10	2	6	6
12	0	3	9	10	10
12	0	4	8	20	24
12	0	5	7	24	28
12	0	6	6	18	24

[a] $\alpha_1 = 1$; $\alpha_2 = 2'$.

Table 24

α	NI(**P**,60)
1($\mathbf{I}_h$)	1
2($\mathbf{I}_h$)	9 607 679 885 269 312
3($\mathbf{I}_h$)	353 259 652 293 727 442 874 919 719
...	...
1(**I**)	1
2(**I**)	19 215 358 678 900 736
3(**I**)	706 519 304 586 988 199 183 738 259
...	...

Table 25

$C_{60-n}Y_n$		isomer no.	
$60-n$	*n*	$\mathbf{I}_h$	**I**
60	0	1	1
59	1	1	1
58	2	23	37
57	3	303	577
56	4	4 190	8 236
55	5	45 718	91 030
54	6	418 470	835 476
53	7	3 220 218	6 436 782
52	8	21 330 558	42 650 532
51	9	123 204 921	246 386 091
50	10	628 330 629	1 256 602 779
49	11	2 855 893 755	5 711 668 755
48	12	11 661 527 055	23 322 797 475
47	13	43 057 432 740	86 114 390 460
46	14	144 549 869 700	289 098 819 780
45	15	443 284 859 624	886 568 158 468
44	16	1 246 738 569 480	2 493 474 394 140
43	17	3 226 849 468 425	6 453 694 644 705
42	18	7 708 584 971 055	15 417 163 018 725
41	19	17 040 023 323 785	34 080 036 632 565
40	20	34 932 048 763 560	69 864 082 608 210
39	21	66 537 224 405 790	133 074 428 781 570
38	22	117 952 355 252 550	235 904 682 814 710
37	23	194 877 787 472 550	389 755 540 347 810
36	24	300 436 595 453 640	600 873 146 368 170
35	15	432 628 675 734 195	865 257 299 572 455
34	26	582 384 767 014 701	1 164 769 471 671 687
33	27	733 373 386 161 407	1 466 746 704 458 899
32	28	864 332 935 668 892	1 728 665 795 116 244
31	29	953 746 664 302 456	1 907 493 251 046 152
30	30	985 538 239 868 528	1 971 076 398 255 692

Table 26

$C_{60-j-k}Y_jZ_k$			isomer no.	
$60-j-k$	j	k	$\mathbf{I}_h$	$\mathbf{I}$
60	0	0	1	1
58	1	1	31	59
57	2	1	871	1711
56	3	1	16 297	32 509
56	2	2	24 635	48 981
55	4	1	227 794	455 126
55	3	2	455 560	910 252
54	5	1	2 503 774	5 006 386
54	4	2	6 261 710	12 519 010
54	3	3	8 345 202	16 688 080
53	6	1	22 530 942	45 057 474
53	5	2	67 592 070	135 172 422
53	4	3	112 649 922	225 287 370
52	7	1	170 579 826	341 149 446
52	6	2	597 046 590	1 194 050 466
52	5	3	1 194 038 370	2 388 046 122
52	4	4	1 492 581 510	2 985 098 760
51	8	1	1 108 750 851	2 217 471 399
51	7	2	4 434 993 576	8 869 885 596
51	6	3	10 348 257 762	20 696 400 864
51	5	4	15 522 380 874	31 044 599 586
50	9	1	6 282 867 981	12 565 671 261
50	8	2	28 272 997 233	56 545 698 807
50	7	3	75 394 156 968	150 788 055 132
50	6	4	131 940 023 670	263 879 452 746
50	5	5	158 327 652 018	316 654 915 830
49	10	1	31 414 258 005	62 828 356 305
49	9	2	157 071 208 125	314 141 781 525
49	8	3	471 213 051 075	942 425 344 575
49	7	4	942 426 020 250	1 884 850 689 150
49	6	5	1 319 396 199 030	2 638 790 964 810
48	11	1	139 936 042 155	279 871 768 995
48	10	2	769 648 590 165	1 539 295 620 135
48	9	3	2 565 492 007 305	5 130 982 438 035
48	8	4	5 772 358 314 450	11 544 712 697 700
48	7	5	9 235 769 953 410	18 471 536 753 670
...	...	...	...	...
47	12	1	559 743 873 780	1 119 487 075 980
47	11	2	3 358 462 751 280	6 716 922 455 880
47	10	3	12 314 359 752 240	24 628 715 671 560
47	9	4	30 785 898 643 500	61 571 789 178 900
47	8	5	55 414 514 806 460	110 829 220 522 020
...	...	...	...	...
46	13	1	2 023 688 790 060	4 047 376 351 620
46	12	2	13 153 978 191 900	26 307 949 848 180
46	11	3	52 615 896 256 560	105 231 785 142 120
46	10	4	144 693 719 816 100	289 387 419 828 780
46	9	5	289 387 418 354 580	578 774 818 281 660
...	...	...	...	...
45	14	1	6 649 262 306 220	13 298 522 298 180
45	13	2	46 544 833 883 100	93 089 656 087 260
45	12	3	201 694 262 591 820	403 388 509 737 300
45	11	4	605 082 783 215 820	1 210 165 529 134 380
45	10	5	1 331 182 104 087 240	2 662 364 164 095 900
...	...	...	...	...
44	15	1	19 947 785 411 700	39 895 566 894 540
44	14	2	149 608 392 875 100	299 216 763 414 900
44	13	3	698 172 434 405 460	1 396 344 841 308 900
44	12	4	2 269 060 427 169 900	4 538 120 775 224 400
44	11	5	5 445 744 922 357 740	10 891 489 762 209 420
...	...	...	...	...
43	16	1	54 856 407 810 105	109 712 808 959 985
43	15	2	438 851 254 192 560	877 702 471 679 880
43	14	3	2 194 256 204 656 560	4 388 512 356 399 400
43	13	4	7 679 896 695 577 260	15 359 793 254 397 900
43	12	5	19 967 731 315 672 140	39 935 462 461 434 540
...	...	...	...	...
42	17	1	138 754 440 115 335	277 508 869 722 315
42	16	2	1 179 412 744 162 455	2 358 825 424 830 765
42	15	3	6 290 201 089 111 320	12 580 402 094 155 800
42	14	4	23 588 254 119 543 300	47 176 507 981 557 900
42	13	5	66 047 111 141 027 940	132 094 221 987 821 940
...	...	...	...	...

Table 26. Continued

$C_{60-j-k}Y_jZ_k$			isomer no.	
$60-j-k$	j	k	$\mathbf{I}_h$	$\mathbf{I}$
41	18	1	323 760 356 124 975	647 520 696 018 735
41	17	2	2 913 843 180 259 935	5 827 686 264 168 615
41	16	3	16 511 777 818 410 105	33 023 555 496 955 485
41	15	4	66 047 111 199 045 900	132 094 221 987 821 940
41	14	5	198 141 333 249 029 940	396 282 665 963 465 820
...	...	...	...	...
40	19	1	698 640 762 881 985	1 397 281 501 935 165
40	18	2	6 637 087 247 896 875	13 274 174 343 496 605
40	17	3	39 822 522 912 381 825	79 645 045 610 304 405
40	16	4	169 245 722 439 007 830	338 491 444 181 800 140
40	15	5	541 586 310 578 988 840	1 083 172 620 300 140 700
...	...	...	...	...
35	24	1	10 815 716 292 073 875	21 631 432 489 303 455
35	23	2	129 788 595 268 670 520	259 577 189 871 641 460
35	22	3	995 045 895 055 550 520	1 990 091 789 015 917 860
35	21	4	5 472 752 421 742 555 950	10 945 504 839 587 548 230
35	20	5	22 985 560 166 027 497 830	45 971 120 326 267 704 150
...	...	...	...	...
30	29	1	29 566 145 470 111 336	59 132 290 782 430 712
30	28	2	428 709 109 093 298 632	857 418 216 926 936 024
30	27	3	4 001 285 010 715 996 492	8 002 570 019 222 905 544
30	26	4	27 008 673 821 432 285 976	54 017 347 633 822 290 312
30	25	5	140 445 103 844 530 719 360	280 890 207 674 702 370 360
...	...	...	...	...

9. Molecules with Icosahedral Symmetry.

$$\mathbf{I}_h = \{\hat{E},12\hat{C}_5,12\hat{C}_5^2,20\hat{C}_3,15\hat{C}_2,\hat{\imath},12\hat{S}_{10},12\hat{S}_{10}^2,20\hat{S}_6,15\hat{\sigma}\}$$

$$\mathbf{I} = \{\hat{E},12\hat{C}_5,12\hat{C}_5^2,20\hat{C}_3,15\hat{C}_2\}$$

(9.a) Borane Anion ($B_{12}H_{12}^{2-}$). The application of symmetry operations of $\mathbf{I}_h$ and $\mathbf{I}$ point group on $B_{12}H_{12}^{2-}$ gives

$$n_o(\mathbf{I}_h) = n_o(\mathbf{I}) = 2$$

and thus

$$D = \underbrace{D_1 \cup D_2}_{\text{twelve-dimensionals}} \qquad (n_1 = |D_1| = n_2 = |D_2| = 12) \tag{116}$$

The permutation groups of two domains

$$\mathbf{P}_i(\mathbf{I}_h) = \mathbf{P}(\mathbf{I}_h,D_i) \qquad i = 1, 2 \tag{117}$$

$$\mathbf{P}_i(\mathbf{I}) = \mathbf{P}(\mathbf{I},D_i) \qquad i = 1, 2 \tag{118}$$

have cycle index

$$Z(\mathbf{P}_i(\mathbf{I}_h),12) = {}^1/_{120}(x_{i1}^{12} + 16x_{i2}^6 + 20x_{i3}^4 + 20x_{i6}^2 + 24x_{i1}^2\,x_{i5}^2 + 24x_{i2}^1\,x_{i10}^1 + 15x_{i1}^4\,x_{i2}^4) \qquad i = 1, 2 \tag{119}$$

$$Z(\mathbf{P}_i(\mathbf{I}),12) = 1/_{60}(x_{i1}^{12} + 24x_{i1}^2\,x_{i5}^2 + 20x_{i3}^4 + 15x_{i2}^6) \qquad i = 1, 2 \tag{120}$$

In all we have

$$Z(\mathbf{P}(\mathbf{I}_h),24) = {}^1/_{120^2}\prod_{i=1}^{2}(x_{i1}^{12} + 16x_{i2}^6 + 20x_{i3}^4 + 20x_{i6}^2 + 24x_{i1}^2\,x_{i5}^2 + 24x_{i2}^1\,x_{i10}^1 + 15x_{i1}^4\,x_{i2}^4) \tag{121}$$

$$Z(\mathbf{P}(\mathbf{I}),24) = 1/_{60^2}\prod_{i=1}^{2}(x_{i1}^{12} + 24x_{i1}^2\,x_{i5}^2 + 20x_{i3}^4 + 15x_{i2}^6) \tag{122}$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{I}_h),24) = {}^1/_{120^2}(\alpha_1^{12} + 15\alpha_1^8 + 16\alpha_1^6 + 44\alpha_1^4 + 44\alpha_1^2)(\alpha_2^{12} + 15\alpha_2^8 + 16\alpha_2^6 + 44\alpha_2^4 + 44\alpha_2^2) \tag{123}$$

$$\mathrm{NI}(\mathbf{P}(\mathbf{I}),24) = {}^1/_{60^2}(\alpha_1^{12} + 15\alpha_1^6 + 44\alpha_1^4)(\alpha_2^{12} + 15\alpha_2^6 + 44\alpha_2^4) \tag{124}$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{I}),24) = {}^1/_{60^2}\prod_{i=1}^{2}[(w_{i1}^1 + w_{i2}^1 + \ldots + w_{i\alpha_i}^1)^{12} + 24(w_{i1}^1 + w_{i2}^1 + \ldots + w_{i\alpha_i}^1)^2(w_{i1}^5 + w_{i2}^5 + \ldots + w_{i\alpha_i}^5)^2 + 20(w_{i1}^3 + w_{i2}^3 + \ldots + w_{i\alpha_i}^3)^4 + 15(w_{i1}^2 + w_{i2}^2 + \ldots + w_{i\alpha_i}^2)^6] \tag{125}$$

$$\mathrm{CI}(\mathbf{P}(\mathbf{I}_h),24) = {}^1/_{120^2}\prod_{i=1}^{2}[(w_{i1}^1 + w_{i2}^1 + \ldots + w_{i\alpha_i}^1)^{12} + 24(w_{i1}^1 + w_{i2}^1 + \ldots + w_{i\alpha_i}^1)^2(w_{i1}^5 + w_{i2}^5 + \ldots + w_{i\alpha_i}^5)^2 + 20(w_{i1}^3 + w_{i2}^3 + \ldots + w_{i\alpha_i}^3)^4 + 16(w_{i1}^2 + w_{i2}^2 + \ldots + w_{i\alpha_i}^2)^6 + 20(w_{i1}^6 + w_{i2}^6 + \ldots + w_{i\alpha_i}^6)^2 + 24(w_{i1}^2 + w_{i2}^2 + \ldots + w_{i\alpha_i}^2)(w_{i1}^{10} + w_{i2}^{10} + \ldots + w_{i\alpha_i}^{10}) + 15(w_{i1}^1 + w_{i2}^1 + \ldots + w_{i\alpha_i}^1)^4(w_{i1}^2 + w_{i2}^2 + \ldots + w_{i\alpha_i}^2)^4] \tag{126}$$

Table 22 shows selected total numbers of isomers (NI) for borane anion obtained using eqs 123 and 124, while Table 23 shows the enumeration of different isomers that appear for $\alpha_1 = 1$ and $\alpha_2 = 2$. The stereoisomers already begin to appear for α_1 or α_2 equal to 2, and in the example of Table

23 we found four stereoisomers of $W_{12}Y_4Z_8$ type, four of $W_{12}Y_5Z_7$ type, and six of $W_{12}Y_6Z_6$ type: in all fourteen stereoisomers.

(9.b) Fullerene (C_{60}). The importance of having an enumeration of possible heterofullerenes is well-documented.[12] Several approaches have been used, and in the case of fullerene C_{60}, to our knowledge, no research has used the cycle index of $\mathbf{I}_h$ group. In this section, a comparison of isomers of fullerene C_{60} using the chiral (**I**) and achiral ($\mathbf{I}_h$) group of icosahedron is reported.

With both symmetries we have only one **G**-orbit, $n_o(\mathbf{I}_h) = n_o(\mathbf{I}) = 1$, thus one domain

$$D = D_1 \qquad (n_1 = |D_1| = 60)$$

and the permutation groups

$$\mathbf{P}(\mathbf{I}_h) = \mathbf{P}(\mathbf{I}_h, D_1)$$

$$\mathbf{P}(\mathbf{I}) = \mathbf{P}(\mathbf{I}, D_1)$$

The usual development gives

$$Z(\mathbf{P}(\mathbf{I}_h),60) = {}^1/_{120}(x_1^{60} + 16x_2^{30} + 20x_3^{20} + 24x_5^{12} + 20x_6^{10} + 24x_{10}^{6} + 15x_1^4 x_2^{28}) \quad (127)$$

$$Z(\mathbf{P}(\mathbf{I}),60) = {}^1/_{60}(x_1^{60} + 15x_2^{30} + 20x_3^{20} + 24x_5^{12}) \quad (128)$$

$$NI(\mathbf{P}(\mathbf{I}_h),60) = {}^1/_{120}(\alpha^{60} + 16\alpha^{30} + 20\alpha^{20} + 24\alpha^{12} + 20\alpha^{10} + 24\alpha^{6} + 15\alpha^{32}) \quad (129)$$

$$NI(\mathbf{P}(\mathbf{I}),60) = {}^1/_{60}(\alpha^{60} + 15\alpha^{30} + 20\alpha^{20} + 24\alpha^{12}) \quad (130)$$

$$CI(\mathbf{P}(\mathbf{I}),60) = {}^1/_{60}[(w_1^1 + w_2^1 + ... + w_\alpha^1)^{60} + 15(w_1^2 + w_2^2 + ... + w_\alpha^2)^{30} + 20(w_1^3 + w_2^3 + ... + w_\alpha^3)^{20} + 24(w_1^5 + w_2^5 + ... + w_\alpha^5)^{12}] \quad (131)$$

$$CI(\mathbf{P}(\mathbf{I}_h),60) = {}^1/_{120}[(w_1^1 + w_2^1 + ... + w_\alpha^1)^{60} + 16(w_1^2 + w_2^2 + ... + w_\alpha^2)^{30} + 20(w_1^3 + w_2^3 + ... + w_\alpha^3)^{20} + 24(w_1^5 + w_2^5 + ... + w_\alpha^5)^{12} + 20(w_1^6 + w_2^6 + ... + w_\alpha^6)^{10} + 24(w_1^{10} + w_2^{10} + ... + w_\alpha^{10})^6 + 15(w_1^1 + w_2^1 + ... + w_\alpha^1)^4 (w_1^2 + w_2^2 + ... + w_\alpha^2)^{28}] \quad (132)$$

In Table 24 we have reported some values of NI calculated using eqs 129 and 130. In passing from the $\mathbf{I}_h$ point group to the **I** point group, for $\alpha \geq 2$ NI almost doubles, because

$$\frac{NI(\mathbf{P}(\mathbf{I}_h),60)}{NI(\mathbf{P}(\mathbf{I}),60)} = \frac{1}{2} + \frac{1}{2}\left(\frac{15\alpha^{32} + \alpha^{30} + 20\alpha^{10} + 24\alpha^{6}}{\alpha^{60} + 15\alpha^{30} + 20\alpha^{20} + 24\alpha^{12}}\right) = \frac{1}{2} + \frac{1}{2}p(\alpha) \quad (133)$$

and the fraction $p(\alpha) = 1$ for $\alpha = 1$ but is negligible with respect to one for $\alpha \geq 2$.

Table 25 shows the enumeration of $C_{60-n}Y_n$ type isomers ($n = 0, ..., 30$), while Table 26 shows a partial list of the enumeration of $C_{60-j-k}Y_jZ_k$ type isomers. The result obtained for $C_{46}Y_{10}Z_4$ can be compared with those reported in ref 12. A small difference is found for the number of isomers corresponding to $\mathbf{I}_h$ symmetry.

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