Journal of Integer Sequences, Vol 5 (2002), Article 02.1.6

Direct Enumeration of Chiral and Achiral Graphs of a Polyheterosubstituted Monocyclic Cycloalkane.

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Abstract

A general pattern inventory is given for a direct enumeration of chiral and achiral graphs of any polyheterosubstituted monocyclic cycloalkane with an empirical formula $C_nX_{m_1}....Y_{m_i}...Z_{m_k}$ *satisfying the condition* $m_1+...+m_i+...+m_k=2n.$ *(1)*

1. INTRODUCTION

The application of different enumeration tools to numerous problems of chemistry is an attractive point for mathematicians and chemists. The abundant chemistry literature on this subject deals with Pólya's counting theorem[1,2] in the series of acyclic organic molecules and among the articles published in this field, one may retain the contribution of Balasubramanian[3,4] who has presented the generalized wreath product method for the enumeration of stereo and position isomers of polysubstituted organic compounds and later explored the applications of combinatorics and graph theory to spectroscopy and quantum chemistry. The idea to calculate the sequences of exact numbers of chiral and achiral skeletons for any molecule of the series of homopolysubstituted monocyclic cycloalkanes $C_nH_{2n-m}X_m$, (X being a non isomerisable substituent), has been discussed by Nemba and Ngouhouo [5], Nemba[6], Nemba and Fah [7], Nemba and Balaban [8].

Our purpose in this study is to present a quick algorithm for direct enumeration of chiral and achiral graphs of stereo and position isomers of any polyheterosubstituted monocyclic cycloalkane with an empirical formula, $C_n X_{m_1} \ldots . Y_{m_i} \ldots Z_{m_k}$ having (k+1)-tuples of positive integers $(n \ , m_1, \ldots, m_i, \ldots, m_k)$ which satisfy equation 1 and denote respectively the ring size and the numbers of non isomerisable substituents of types X…,Y,…and Z. As indicated in a previous study, we assume ring flip to be fast enough to equilibrate conformers [8].

2. FORMULATION OF THE ALGORITHM

Let us note the system $C_n X_{m_1} \ldots . Y_{m_i} \ldots Z_{m_k} = (n \ , m_1, \ldots, m_i, \ldots, m_k)$ and consider as shown in figure-1 the stereograph in D_{nh} symmetry of its parent monocyclic cycloalkane $C_n H_{2n}$. This tridimensional graph contains *2n* substitution sites labelled $1, 2, \ldots, i, \ldots, n$ and $1', 2', \ldots, i', \ldots, n'$. Define the set of divisors D_{2n} or D_n for *2n* and *n* if n odd or even respectively. Then derive the set P of permutations induced by the 4n symmetry operations of D_{nh}. It must be recalled that the chemistry specific notation D_{nh} refers to a point group containing 4n symmetry elements which are for *n* odd :

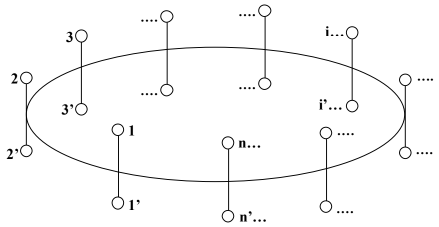
$E,\ nC_2,\ \sigma_h,\ n\sigma_v,\ C_n^r$ with $1 \le r$(odd or even) $\le n$-1, $S_n^{r'}$ with $1 \le r'$(odd) $\le 2n$-1,

and for *n* even :

$E,\ C_2,\ \sigma_h,\ i,\ \frac{n}{2}C_2^{/},\ \frac{n}{2}C_2^{//},\ \frac{n}{2}\sigma_v,\ \frac{n}{2}\sigma_d,\ C_n^r$ with $1 \le r$(odd or even and $\ne \frac{n}{2}$) $\le n$-1,

$S_n^{r'}$ with $1 \le r'$(odd and $\ne \frac{n}{2}$) $\le n$-1.

Figure 1. Stereograph in D_{nh} symmetry of its parent monocyclic cycloalkane $C_n H_{2n}$.



$$P = \left\{ a_1 \left[1^{2n}\right], (n+1)\left[2^n\right], \ldots, a_d \left[d^{\frac{2n}{d}}\right], \ldots, a_n \left[n^2\right], a_{2n}\left[2n\right], n\left[1^2 2^{n-1}\right] \right\} \quad n \ odd, \quad (2)$$

$$P = \left\{ a_1 \left[1^{2n}\right], \frac{3}{2}(n+2)\left[2^n\right], \ldots, a_d \left[d^{\frac{2n}{d}}\right], \ldots, a_n \left[n^2\right], \frac{n}{2}\left[1^4 2^{n-2}\right] \right\} \quad n \ even. \quad (3)$$

Eliminate in P the contributions of reflections and rotoreflections and derive in relations (4)-(5) the set P' of 2n permutations induced by rotation symmetries.

$$P' = \left\{ a_1^{/} \left[1^{2n}\right], n\left[2^{n}\right], \ldots, a_d^{/} \left[d^{\frac{2n}{d}}\right], \ldots, a_n^{/} \left[n^{2}\right] \right\} \text{ } n \text{ odd}, \tag{4}$$

$$P' = \left\{ a_1^{/} \left[1^{2n}\right], (n+1) \cdot \left[2^{n}\right], \ldots, a_d^{/} \left[d^{\frac{2n}{d}}\right], \ldots, a_n^{/} \left[n^{2}\right] \right\} \quad n \text{ even}. \tag{5}$$

The notation $[i^j]$ in expressions (2)-(5) refers to *j* permutation cycles with length *i,* and the coefficients a_d and $a_d^{/}$ are determined from equations (6)-(10) where $\varphi(d)_{rp} = \varphi(d)_{ri}$ and $\varphi(\mu)_{ri}$,

$$a_d = \varphi(d)_{rp} \qquad d(\text{odd}), \tag{6}$$

$$a_{2d} = \varphi(d)_{ri} \qquad d(\text{odd}), \tag{7}$$

$$a_d = \varphi(d)_{rp} + \varphi(d)_{ri} \quad d(\text{even}) \neq 2\mu \ \ (\mu \text{ odd}), \tag{8}$$

$$a_d = \varphi(d)_{rp} + \varphi(d)_{ri} + \varphi(\mu)_{ri} \quad d\ (\text{even}) = 2\mu \ \ (\mu \text{ odd}), \tag{9}$$

$$a_d^{/} = \varphi(d)_{rp} \qquad d \text{ odd or even}. \tag{10}$$

correspond to the Euler totient function for the integer numbers *d* or μ which are the order of proper or improper rotation axes (see indices *rp* or *ri* respectively).

Each permutation resulting from the action of D_{nh} on G induces distinct combinations with repetition (or distinct polyheterosubstitutions) of $(m_1, \ldots, m_i, \ldots, m_k)$ elements of different types X…,Y,… and Z among *2n* substitution sites.

Let $T(a, b, c, \ldots, e, \ldots, f, g) = \dfrac{a!}{b!\,c! \ldots e! \ldots f!\,g!}$ be the multinomial coefficient which corresponds to the number of combinations with repetition of *(b, c,…,e,…,f,g)* objects of kinds X, …,Y,…,Z among $a = 2n$ undistinguishable boxes. Our concern in this step is to derive such numbers resulting from the permutations of types $[d^{\frac{2n}{d}}]$ (with $d \neq 2$), $\left[2^{n}\right]$, $[1^2 2^{n-1}]$ and $[1^4 2^{n-2}]$ listed in P and P'.

a)-If $d_j \in D_c$ is the common divisor of the sequence $(2n \ , m_1, ..., m_i, ..., m_k)$ for *n* odd or even and $D_c = \{1, ..., d_j, ...\}$, therefore the number of distinct combinations with repetition or polyheterosubstitutions of $(m_1, ..., m_i, ..., m_k)$ elements of types X…,Y,… and Z among 2n substitution sites of the stereograph G resulting from the permutation $[d^{\frac{2n}{d}}]$ is given by the multinomial coefficient :

$$T\left(\frac{2n}{d_j}, \frac{m_1}{d_j}, ..., \frac{m_i}{d_j}, ..., \frac{m_k}{d_j}\right).$$

b)-In the case of transpositions (2-cycle permutations) noted $[2^n]$ where $d_j = 2$, the result is:

$$T\left(n, \frac{m_1}{2}, ..., \frac{m_i}{2}, ..., \frac{m_k}{2}\right).$$

c)-For the permutations of types $[1^2 2^{n-1}]$ or $[1^4 2^{n-2}]$: we simultaneously solve the partition eqs (11) and (12)

$$p_1 + p_2 + ... + p_i + ... + p_k = \begin{cases} 2 & n \ \ odd, \\ 4 & n \ \ even. \end{cases} \tag{11}$$

$$m_1^{/} + m_2^{/} + ... + m_i^{/} + ... + m_k^{/} = \begin{cases} n - 1 & n \ \ odd, \\ n - 2 & n \ \ even. \end{cases} \tag{12}$$

to derive the k-tuples of integer numbers $(p_1, p_2 ..., p_i, ..., p_k) \geq 0$ for the choice of the kinds of substituents X,…,Y,… , and Z to be put in 2 or 4 invariant positions and the sequence $(m_1^{/}, m_2^{/}, ..., m_i^{/}, ..., m_k^{/}) \geq 0$ of couples of substituents of the same kind to be placed into n-1 or n-2 boxes. Then check from eq. (13)

$$m_i^{/} = \frac{m_i - p_i}{2} \quad \text{where } 1 \leq i \leq k, \tag{13}$$

the compatibility of each couple $(p_i, m_i^{/})$, in the associated sequences $(p_1, p_2 ..., p_i, ..., p_k) \rightarrow (m_1^{/}, m_2^{/}, ..., m_i^{/}, ..., m_k^{/})$.

Let $T(2; p_1, p_2, ..., p_i, ..., p_k)$ and $T(4; p_1, p_2, ..., p_i, ..., p_k)$ be the number of ways of putting $(p_1, p_2, ..., p_i, ..., p_k)$ substituents of k types into 2 or 4 boxes.

Let $T(n-1; m_1^{/}, m_2^{/}, ..., m_i^{/}, ..., m_k^{/})$ and $T(n-2; m_1^{/}, m_2^{/}, ..., m_i^{/}, ..., m_k^{/})$ denote the numbers of placements of $(m_1^{/}, m_2^{/}, ..., m_i^{/}, ..., m_k^{/})$ elements into *n-1* or *n-2* boxes.

Finally, the numbers of combinations with repetition of $(m_1,...,m_i,...,m_k)$ different substituents among *2n* boxes generated by the permutations $\left[1^2 2^{n-1}\right]$ or $\left[1^4 2^{n-2}\right]$ is the sum over λ of the products of multinomial coefficients as given hereafter:

$$\sum_{\lambda} T\left(2; p_1, p_2,..., p_i,..., p_k\right)\cdot T\left(n-1; m_1^{/}, m_2^{/},..., m_i^{/},..., m_k^{/}\right) \text{ } n \text{ odd,} \qquad (14)$$

$$\sum_{\lambda} T\left(4; p_1, p_2,..., p_i,..., p_k\right)\cdot T\left(n-2; m_1^{/}, m_2^{/},..., m_i^{/},..., m_k^{/}\right) \text{ } n \text{ even,} \qquad (15)$$

and λ indicates the number of compatible solutions $(p_1, p_2..., p_i,..., p_k) \to \left(m_1^{/}, m_2^{/},..., m_i^{/},..., m_k^{/}\right)$ sorted from eqs (11) and (12).

Finally if we set up the differences *P'-P* and *2P-P'* of the averaged contributions of the 4n and 2n permutations of P and P' one may obtain respectively from eqs (16)-(19) the numbers $A_c(n, m_1,...,m_i,...,m_k)$ of chiral graphs (or enantiomer pairs) and $A_{ac}(n, m_1,..., m_i,..., m_k)$ of achiral forms for any polyheterosubstituted monocyclic system $C_nX_{m_1}....Y_{m_i}...Z_{m_k}$.

Hence for *n* odd :

$$A_c(n,m_1,...,m_i,...,m_k) = \frac{1}{4n}\left[\sum_{d_j\neq 2}\left(2a_{d_j}^{/} - a_{d_j}\right)\cdot\begin{pmatrix} \frac{2n}{d_j} \\ \frac{m_1}{d_j},...,\frac{m_i}{d_j},...,\frac{m_k}{d_j}\end{pmatrix} + (n-1)\cdot\begin{pmatrix} n \\ \frac{m_1}{2},...,\frac{m_i}{2},...,\frac{m_k}{2}\end{pmatrix}\right] - \frac{1}{4}\left[\sum_{\lambda}\begin{pmatrix} 2 \\ p_1,...,p_i,...,p_k\end{pmatrix}\cdot\begin{pmatrix} n-1 \\ m_1^{/},...,m_i^{/},...,m_k^{/}\end{pmatrix}\right]. \qquad (16)$$

$$A_{ac}(n,m_1,...,m_i,...,m_k) = \frac{1}{2n}\left[\sum_{d_j\neq 2}\left(a_{d_j} - a_{d_j}^{/}\right)\cdot\begin{pmatrix} \frac{2n}{d_j} \\ \frac{m_1}{d_j},...,\frac{m_i}{d_j},...,\frac{m_k}{d_j}\end{pmatrix} + \begin{pmatrix} n \\ \frac{m_1}{2},...,\frac{m_i}{2},...,\frac{m_k}{2}\end{pmatrix}\right] + \frac{1}{2}\left[\sum_{\lambda}\begin{pmatrix} 2 \\ p_1,...,p_i,...,p_k\end{pmatrix}\cdot\begin{pmatrix} n-1 \\ m_1^{/},...,m_i^{/},...,m_k^{/}\end{pmatrix}\right]. \qquad (17)$$

and for *n* even :

$$A_c(n,m_1,...,m_i,...,m_k) = \frac{1}{4n}\left[\sum_{d_j\neq 2}\left(2a_{d_j}^{/} - a_{d_j}\right)\cdot\begin{pmatrix} \frac{2n}{d_j} \\ \frac{m_1}{d_j},...,\frac{m_i}{d_j},...,\frac{m_k}{d_j}\end{pmatrix} + (\frac{n}{2}-1)\cdot\begin{pmatrix} n \\ \frac{m_1}{2},...,\frac{m_i}{2},...,\frac{m_k}{2}\end{pmatrix}\right] - \frac{1}{8}\left[\sum_{\lambda}\begin{pmatrix} 4 \\ p_1,...,p_i,...,p_k\end{pmatrix}\cdot\begin{pmatrix} n-2 \\ m_1^{/},...,m_i^{/},...,m_k^{/}\end{pmatrix}\right]. \qquad (18)$$

$$A_{ac}(n,m_1,...,m_i,...,m_k) = \frac{1}{2n}\left[\sum_{d_j\neq 2}\left(a_{d_j} - a_{d_j}^{/}\right)\cdot\begin{pmatrix} \frac{2n}{d_j} \\ \frac{m_1}{d_j},...,\frac{m_i}{d_j},...,\frac{m_k}{d_j}\end{pmatrix} + \left(\frac{n}{2}+2\right)\cdot\begin{pmatrix} n \\ \frac{m_1}{2},...,\frac{m_i}{2},...,\frac{m_k}{2}\end{pmatrix}\right] + \frac{1}{4}\left[\sum_{\lambda}\begin{pmatrix} 4 \\ p_1,...,p_i,...,p_k\end{pmatrix}\cdot\begin{pmatrix} n-2 \\ m_1^{/},...,m_i^{/},...,m_k^{/}\end{pmatrix}\right]. \qquad (19)$$

3. APPLICATIONS

Example 1 : Chiral and achiral graphs of $C_9X_9Y_6Z_3$.

Let $n=9, m_1=9, m_2=6, m_3=3$, $D_{18}=\{1,\ 2,\ 3,\ 6,\ 9,\ 18\}$,

P=$\{[1^{18}],\ 10[2^9],\ 2[3^6],\ 2[6^3],\ 6[9^2],\ 6[18],\ 9[1^2 2^8]\}$ and P'=$\{[1^{18}],\ 9[2^9],\ 2[3^6],\ 6[9^2]\}$. The set of common divisors of the sequence (18,9,6,3) is $D_c=\{1,3\}$, $a_1=a_1^/=1$, $a_3=a_3^/=2$. The empirical formula contains *k=3* types of substituents. The solutions of the 2 associated partition equations $p_1+p_2+p_3=2$ and $m_1^/+m_2^/+m_3^/=8$ which verify equation (13) are $(p_1,p_2,p_3)=(1,0,1)\rightarrow(m_1^/,m_2^/,m_3^/)=(4,3,1)$. Therefore λ=1 and from equations (16)-(17) one may obtain respectively :

$$A_c(9,9,6,3)=\frac{1}{36}\left[(2-1)\cdot\begin{pmatrix}18\\9,6,3\end{pmatrix}+(4-2)\cdot\begin{pmatrix}\frac{18}{3}\\\frac{9}{3},\frac{6}{3},\frac{3}{3}\end{pmatrix}\right]-\frac{1}{4}\left[\begin{pmatrix}2\\1,0,1\end{pmatrix}\cdot\begin{pmatrix}8\\4,3,1\end{pmatrix}\right]=113310.$$

$$A_{ac}(9,9,6,3)=\frac{1}{18}\left[(9)\cdot\begin{pmatrix}2\\1,0,1\end{pmatrix}\cdot\begin{pmatrix}8\\4,3,1\end{pmatrix}\right]=280.$$

Example 2 : Chiral and achiral graphs of $C_{12}X_9L_3Y_6Z_6$.

Let $n=12$, $m_1=9$, $m_2=3$, $m_3=6$, $m_4=6$, $D_{12}=\{1,2,3,4,6,12\}$,

$P=\{[1^{24}],\ 21[2^{12}],\ 2[3^8],\ 4[4^6],\ 6[6^4],\ 8[12^2],\ 6[1^4 2^{10}]\}$,

$P'=\{[1^{24}],\ 13[2^{12}],\ 2[3^8],\ 2[4^6],\ 2[6^4],\ 4[12^2]\}$. The set of common divisors of the sequence (24, 9, 3, 6) is $D_c=\{1,3\}$, $a_1=a_1^/=1$, $a_3=a_3^/=2$. The empirical formula contains *k=4* types of substituents. The solutions of the 2 associated partition equations $p_1+p_2+p_3+p_4=4$ and $m_1^/+m_2^/+m_3^/=10$ which verify equation (13) are given in each line of the following matrices :

$$(p_1,p_2,p_3,p_4)=\begin{pmatrix}3&1&0&0\\1&3&0&0\\1&1&2&0\\1&1&0&2\end{pmatrix}\rightarrow(m_1^/,m_2^/,m_3^/,m_4^/)=\begin{pmatrix}3&1&3&3\\4&0&3&3\\4&1&2&3\\4&1&3&2\end{pmatrix}.$$

Therefore λ=4 and from equations (18) -(19) one may obtain respectively :

$$A_c(12,9,3,6,6)=\frac{1}{48}\left[(2-1)\cdot\binom{24}{9,3,6,6}+(4-2)\cdot\binom{\frac{24}{3}}{\frac{9}{3},\frac{3}{3},\frac{6}{3},\frac{6}{3}}\right]$$

$$-\frac{1}{4}\left[\begin{matrix}\binom{4}{3,1,0,0}\cdot\binom{10}{3,1,3,3}+\binom{4}{1,3,0,0}\cdot\binom{10}{4,0,3,3}\\+\binom{4}{1,1,2,0}\cdot\binom{10}{1,1,2,3}+\binom{4}{1,1,0,2}\cdot\binom{10}{4,1,3,2}\end{matrix}\right]=11\,452\,052\,360.$$

$$A_{ac}(12,9,3,6,6)=\frac{1}{4}\left[\begin{matrix}\binom{4}{3,1,0,0}\cdot\binom{10}{3,1,3,3}+\binom{4}{1,3,0,0}\cdot\binom{10}{4,0,3,3}\\+\binom{4}{1,1,2,0}\cdot\binom{10}{1,1,2,3}+\binom{4}{1,1,0,2}\cdot\binom{10}{4,1,3,2}\end{matrix}\right]=96\,600.$$

The problem of counting chiral and achiral forms of molecules is often encountered by organochemists involved in the synthesis of stereo and position isomers in the series of substituted derivatives of monocyclic cycloalkanes where the ring size *n* ranges from *3* to *288* according to the Chemical Abstract Service (CAS) ring System Handbook[9]. Examples 1 and 2 and the sequences $A_c(n,m_1,...,m_i,...,m_k)$ and $A_{ac}(n,m_1,...,m_i,...,m_k)$ given in table 1 for the systems $C_nX_{m_1}Y_{m_2}Z_{m_3}$ illustrate the selectivity and the general application of our pattern inventory. Furthermore, this procedure circumvents the two main steps of Pólya's counting method [1,2] which is largely presented by Pólya,Tarjan and Woods[2], Harary, Palmer, Robinson and Read[10],Tucker[11] and Rouvray[12] and requires first to derive a cycle index according to the parity and the divisibility character of the ring size *n*, and second the transformation of the cycle index into a generating function of order *2n* the coefficients of which are solution of the enumeration problem. Finally the accuracy of our theoretical results is testify by the method of drawing and counting graphs of systems with smaller ring size.

Table 1 : *Number of chiral and achiral graphs of polyheterosubstituted cycloalkane* $C_n X_{m_1} Y_{m_2} Z_{m_3}$,

where n = 3, 4, 5, 6, 8 and $m_1 + m_2 + m_3 = 2n.$

n			**3**		**4**		**5**		**6**		**8**	
m_1	m_2	m_3	A_c	A_{ac}	A_c	A_{ac}	A_c	A_{ac}	A_c	A_{ac}	A_c	A_{ac}
4	1	1	2	1								
3	2	1	4	2								
2	2	2	7	4								
6	1	1			2	3						
5	2	1			8	5						
4	2	2			23	14						
4	3	1			14	7						
3	3	2			30	10						
8	1	1					4	1				
7	2	1					16	4				
6	3	1					40	4				
6	2	2					62	12				
5	4	1					60	6				
5	3	2					120	12				
4	4	2					156	18				
4	3	3					204	12				
10	1	1							4	3		
9	2	1							24	7		
8	3	1							76	13		
8	2	2							118	29		
7	4	1							156	18		
7	3	2							316	28		
6	5	1							220	22		
6	4	2							564	62		
6	3	3							749	44		
5	5	2							672	42		
5	4	3							1128	5 4		
4	4	4							1422	96		
14	1	1									6	3
13	2	1									48	9
12	3	1									333	48
12	2	2									218	19
11	4	1									666	33
11	3	2									1338	54
10	5	1									1476	51
10	4	2									3723	156
10	3	3									4954	102
9	6	1									2470	65
9	5	2									7440	135
9	4	3									12430	165
8	7	1									3180	75
8	6	2									11205	270
8	5	3									22410	225
8	4	4									28065	414
7	7	2									12780	180
7	6	3									29900	260
7	5	4									44880	330
6	6	4									52430	560
6	5	5									62868	390

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