Enumeration of Stereoisomers of Chiral and Achiral Derivatives of Monocyclic Cycloalkanes Having Heteromorphous Alkyl Substituents with Distinct Length k

Alphonse Emadak[1*], Ibrahim Mbouombouo Ndassa[2], Beauregard Thomas Makon[1], Issofa Patouossa[1], Robert Martin Nemba[1]

[1]Laboratory of Applied Physical and Analytical Chemistry, Department of Inorganic Chemistry, Faculty of Sciences, University of Yaounde 1, Yaounde, Cameroon
[2]Laboratory of Chemistry, Department of Chemistry, High Teacher Training College, University of Yaounde 1, Yaounde, Cameroon
Email: *emadak@yahoo.com

Abstract

A combinatorial method based on the determination of the averaged weight of permutations controlling the chirality/achirality fittingness of $2n$ substitution sites of the monocyclic cycloalkane allows to obtain generalized functional equations for direct enumeration of enantiomers pairs and achiral skeletons of any derivatives of monocyclic cycloalkanes having heteromorphic alkyl substituents with the distinct length k with the empirical formula $C_n H_{m_0} \left(R_{k_1} \right)_{m_1} \cdots \left(R_{k_\alpha} \right)_{m_\alpha} \cdots \left(R_{k_\zeta} \right)_{m_\zeta}$, wherein at least two alkyl groups $R_{k_\alpha} = C_{k_\alpha} H_{2k_\alpha + 1}$ of the distinct size $k_{\alpha(1 \le \alpha \le \zeta)}$ each. m_α is the number of alkyl radicals R_{k_α} of the system $C_n H_{m_0} \left(R_{k_1} \right)_{m_1} \cdots \left(R_{k_\alpha} \right)_{m_\alpha} \cdots \left(R_{k_\zeta} \right)_{m_\zeta}$ verifying the relation $\sum_{\alpha=1}^{\zeta} m_\alpha + m_0 = 2n$. The integer sequences of enantiomer pairs and achiral skeletons are given for substituted derivatives of monocyclic cycloalkane for $n = 3$, 4 and $k = 3$, 4, 5. The composite stereoisomerism of this particular compound is also highlighted.

Keywords

Enumeration, Stereoisomer, Chirality, Achirality, Monocyclic Cycloalkane, Order of Alkyl Trees, Polyalkylation

1. Introduction

From the 1800s to 1870, the enumeration of isomers in chemistry consisted of a manual enumeration based on the so-called "draw and count" method which consists of drawing and counting all the possible molecular structures of a given organic compound in two dimensions or a plan. This exhausting exercise used to expose certain risks of repetition and/or omission of structures, especially for large molecules [1].

Chemists sorted out these difficulties of enumeration of chemical structures by developing methods and models of enumeration using not only mathematical theories (group theory, graph theory, etc.) but also more and more information technology tools (computers, softwares, etc.). This allowed to first generate several methods of enumeration of the isomers of constitution or function [2] [3] [4] [5] [6] and in a second step of the enumeration of isomers of substitution then the elaboration of the direct formulas of quantitative determination stereoisomers [7]-[16]. Concretely, the computation of the number of stereoisomers of the homopolysubstituted and heteropolysubstituted monocyclic cycloalkane has been the subject of several studies [17]-[22]. Nemba *et al.* have dealt in this dynamic with the problem of enumeration of substituted monocycloalkanes with homomorphic alkyl substituents [23] and Emadak *et al.* have enumerated the enumeration of substituted monocyclic cycloalkanes having sterically heteromorphic alkyl substituents of identical k order [24].

In this work, we are interested in determining the number of enantiomeric pairs and achiral skeletons of cycloalkanes with heteromorphic alkyl substituents of distinct order k. To simplify the language, we will speak of heteropolyalkylation of monocyclic cycloalkane with alkyl radicals of distinct k size. Beyond the direct formulas of computation established, this work highlights, on the one hand, a composite stereoisomerism due to the intrinsic chirality of the alkyl trees and to the extrinsic chirality induced by their positioning or placement on the monocycloalkane, on the other hand, the total number of different stereoisomers increases correlatively with the number of chiral centers present in the molecular graph and finally the concepts of pseudochirality, pseudosymmetry and enantiomeric mirror in the molecules of this family of saturated hydrocarbon compounds is also elucidated.

2. Definitions and Mathematical Formulation

2.1. Stereograph Composition of G_k^γ

Let us consider the system $C_n H_{m_0} \left(R_{k_1} \right)_{m_1} \cdots \left(R_{k_\alpha} \right)_{m_\alpha} \cdots \left(R_{k_\zeta} \right)_{m_\zeta}$, the empirical formula of the heteropolyalkylated monocyclic cycloalkane having heteromorphous alkyl substituents including at least two alkyl groups noted $R_{k_\alpha} = C_{k_\alpha} H_{2k_\alpha+1}$, having the distinct order, size or length k_α, with $(1 \le \alpha \le \zeta)$. m_α is the number of alkyl radicals R_{k_α} of the system $C_n H_{m_0} \left(R_{k_1} \right)_{m_1} \cdots \left(R_{k_\alpha} \right)_{m_\alpha} \cdots \left(R_{k_\zeta} \right)_{m_\zeta}$ where

$$\sum_{\alpha=1}^{\zeta} m_{\alpha} + m_0 = 2n .$$

The molecular composite stereograph $G_{k_{\alpha}}$ of the system

$$C_n H_{m_0} \left(R_{k_1} \right)_{m_1} \cdots \left(R_{k_{\alpha}} \right)_{m_{\alpha}} \cdots \left(R_{k_{\zeta}} \right)_{m_{\zeta}}$$
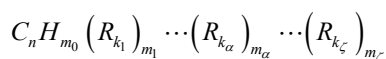
is obtained by connecting the roots of the graphs of the distinct planted steric trees $R_{k_{\alpha}}$ to the sites or positions of substitution of the stereograph G of the parent molecule of the monocyclic cycloalkane $C_n H_{2n}$ described in our previous work [24]. The mathematical and graphical interpretations of this composition of the graph G and the graphs $R_{k_{\alpha}}$ to obtain $G_{k_{\alpha}}$ are given respectively by the relation (1) and **Figure 1**.

$$G_{k_{\alpha}} = G \circ R_{k_{\alpha}(1 \le \alpha \le \zeta)} = C_n H_{m_0} \left(R_{k_1} \right)_{m_1} \cdots \left(R_{k_{\alpha}} \right)_{m_{\alpha}} \cdots \left(R_{k_{\zeta}} \right)_{m_{\zeta}} \qquad (1)$$

$G_{k_{\alpha}}$ is the stereograph of a monocyclic cycloalkane heteropolyalkylated having alkyl radicals $R_{k_{\alpha}}$ of distinct size k. The approach used to enumerate stereoisomers of the system $C_n H_{m_0} \left(R_{k_1} \right)_{m_1} \cdots \left(R_{k_{\alpha}} \right)_{m_{\alpha}} \cdots \left(R_{k_{\zeta}} \right)_{m_{\zeta}}$ is to first determine the number of heteromorphic combinations of distinct alkyl radicals of orders k_{α}, with ($1 \le \alpha \le \zeta$), and then to carry out the product of the latter by the results of the enumeration of the stereoisomers of the homopolysubstituted and/or heteropolysubstituted monocyclic cycloalkane obtained in our previous work [21] [22] [25].

2.2. Calculation of the Number of Combinations of Heteromorphous Alkyl Radicals of Distinct Size *k*

According to graph theory, any alkyl radical $C_k H_{2k+1}$ is equivalent to a planted steric tree which may have one or more isomers or stereoisomers including the chiral and achiral forms. s_k and p_k respectively give the total number and the number of steric trees planted of order *k*. We recall that the generating functions which give these numbers were established by Robinson *et al.* [26] in polynomials' series: $s(x) = \sum_k s_k x^k$ and $p(x) = \sum_k p_k x^k$ for $0 \le k \le 14$. Values of s_k, p_k and s_k-p_k for $0 \le k \le 18$ are computed and compiled in **Table 1**.

Graphs of planted steric trees ($C_k H_{2k+1}$) can be combined in three sets whose
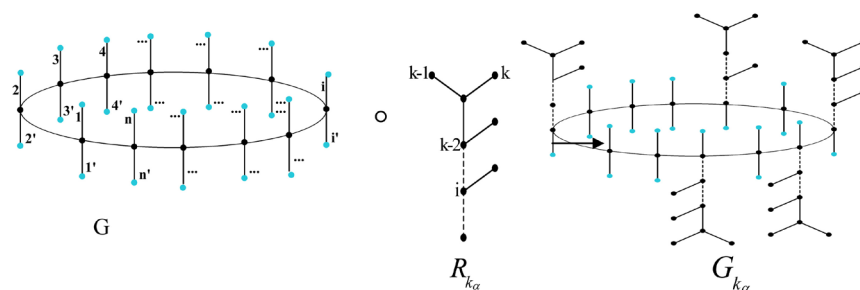
Figure 1. Composition of graph *G* with distinct planted heteromorphous trees.

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Table 1. Value of s_k, p_k, and s_k-p_k for $k \le 18$.

k	s_k	p_k	s_k-p_k
0	1	1	0
1	1	1	0
2	1	1	0
3	2	2	0
4	5	3	2
5	11	5	6
6	28	8	20
7	74	14	60
8	199	23	176
9	551	41	510
10	1533	69	1464
11	4436	122	4314
12	12,832	208	12,624
13	37,496	370	37,126
14	110,500	636	109,864
15	327,420	1134	326,286
16	979,819	1963	977,856
17	2,944,873	3505	2,941,368
18	8,896,515	6099	8,890,416

elements are equivalent to stereoisomers of sterically distinct alkyl radicals, namely:

- E_{a+c} is the set of chiral and achiral trees of cardinality s_k. Elements of E_{a+c} are pairs of enantiomers and achiral skeletons.
- E_a is *the* set of achiral trees of cardinality p_k. Elements of E_a are achiral skeletons.
- E_c is the set pairs enantiomers of cardinality s_k-p_k.

From these definitions, we can write the following relations:

$$\left| E_{c+a} \right| = s_k, \left| E_a \right| = p_k \Rightarrow \begin{cases} E_{c+a} = E_c \cup E_a \\ E_c \cap E_a = \phi \end{cases} \tag{2}$$

Considering (2), we have:
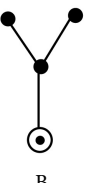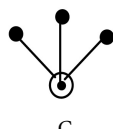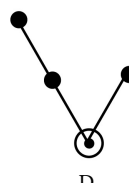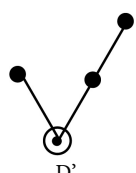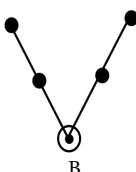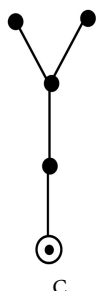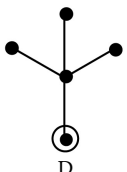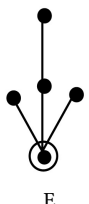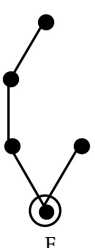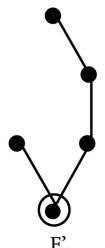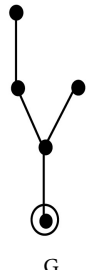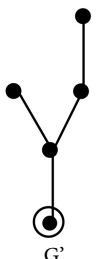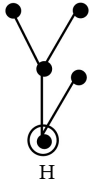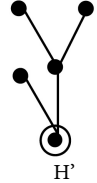
$$\left| E_{c+a} \right| = \left| E_c \right| + \left| E_a \right| \Rightarrow \left| E_c \right| = \left| E_{c+a} \right| - \left| E_a \right| \tag{3}$$

$$\text{And consequently } \left| E_c \right| = s_k - p_k \tag{4}$$

Table 2 gives us the graphic representation of some distinct sterical trees of size k identified by letters, $1 \le k \le 5$.

Note that a pair of enantiomers is represented by the same letter whose two stereoisomers are differentiated by the apostrophe.

Table 2. Graphical representation of some planted trees identified by letters of the alphabet.

Size k	Alkyl radicals or planted trees
1	
2	
3	
4	
5	

Before calculating the numbers of heteromorphic combinations of distinct alkyl radicals of different order *k*, we first define the different sets of alkyl radicals

of distinct orders k_α, with ($1 \le \alpha \le \zeta$). IR_{k_α} is a set constituted of chiral and achiral alkyl radicals having k_α carbons. Considering Table 2 illustrating the alkyl radicals of order 1 to 5 below, and assigning k_α as an index under each letter corresponding to an alkyl radical having k_α carbons, one can set up the following sets:

$$IR_{k_1} = IR_1 = \{A_1\}$$

$$IR_{k_2} = IR_2 = \{A_2\}$$

$$IR_{k_3} = IR_3 = \{A_3, B_3\}$$

$$IR_{k_4} = IR_4 = \{A_4, B_4, C_4, D_4, D_4'\}$$

$$IR_{k_5} = IR_5 = \{A_5, B_5, C_5, D_5, E_5, E_5', F, F_5', G, G_5'\}$$

We can generalize all these sets as follows:

$$IR_{k_\alpha} = \{A_\alpha, B_\alpha, C_\alpha, D_\alpha, D_\alpha', \cdots, Z_\alpha, Z_\alpha'\}.$$

- $IR_{k_\alpha}^a$ designates a set formed of alkyl radicals only achiral and having the same order k_α.

  Example: $IR_1^a = \{A_1\}$, $IR_2^a = \{A_2\}$, $IR_3^a = \{A_3, B_3\}$, $IR_4^a = \{A_4, B_4, C_4\}$, $IR_5^a = \{A_5, B_5, C_5, D_5, E_5\}$, $\cdots$

- $IR_{k_\alpha}^c$ means a group consisting of only chiral alkyl radicals and having the same order k_α.

  Example: $IR_4^c = \{D_5, D_5'\}$, $IR_5^c = \{F_5, F_5', G_5, G_5', H_5, H_5'\}$, $\cdots$

- $Card\, IR_{k_\alpha} = s_{k_\alpha}$, $Card\, IR_{k_\alpha}^a = p_{k_\alpha}$ and $Card\, IR_{k_\alpha}^c = s_{k_\alpha} - p_{k_\alpha}$.

- *A group of substituents or alkyl radicals* refers in this chapter to a combination of at least two different substituent types selected from at least two sets of alkyl radicals of order k_α different and that composes a substitution.

  Example: Heteromorphous substituent groups A_1A_3 and A_1B_3 were formed by combining a radical of IR_1^a and one of IR_3^a.

- *i* is the number of substituent types or alkyl radicals that make up a group of substituents or else *i-uples*. i_α is the number of substituent or alkyl radical of order k_α chosen in IR_{k_α}, $IR_{k_\alpha}^a$ or $IR_{k_\alpha}^c$ such that $i_\alpha \le s_{k_\alpha}$, p_{k_α} or $s_{k_\alpha} - p_{k_\alpha}$ and $\sum_\alpha i_\alpha = i$.

  Example: In the group of heteromorphic substituents $A_1A_3B_3$, $i_3 = 2$, $i_1 = 1$ and $i = 3$; in heteromorphous substituent groups A_1A_3 and A_1B_3 we have $i_3 = 1$, $i_1 = 1$ and $i = 2$.

Following these definitions, we can roll out the algorithm of our method of counting the stereoisomers of the molecular system

$$C_n H_{m_0} \left(R_{k_1}\right)_{m_1} \cdots \left(R_{k_\alpha}\right)_{m_\alpha} \cdots \left(R_{k_\zeta}\right)_{m_\zeta}$$

as follows by first establishing the formula for calculating the number of substituting group or number of *i*-uples of letters identifying the alkyl radicals.

The number of *i-uples* of distinct letters without repetition or groups of subs-

tituents taken in IR_{k_α}, $IR_{k_\alpha}^a$ or $IR_{k_\alpha}^c$ ($1 \le \alpha \le \zeta$) in such a way that we have i types of heteromorphic substituents of different orders k_α and composing a substitution is given respectively by $N_{k_1,k_2,\cdots,k_\alpha} = \prod_\alpha \binom{s_{k_\alpha}}{i_\alpha}$, $N_{k_1,k_2,\cdots,k_\alpha}^a = \prod_\alpha \binom{p_{k_\alpha}}{i_\alpha}$

and $N_{k_1,k_2,\cdots,k_\alpha}^c = \prod_\alpha \binom{s_{k_\alpha} - p_{k_\alpha}}{i_\alpha}$.

The number of i-tuples mixed letter representing heteromorphic combinations of chiral and achiral radicals of distinct orders is given by

$$N_{k_1,k_2,\cdots,k_\alpha}^{a+c} = N_{k_1,k_2,\cdots,k_\alpha} - N_{k_1,k_2,\cdots,k_\alpha}^a - N_{k_1,k_2,\cdots,k_\alpha}^c.$$

Example:

1) Let us determine the number of substituent groups having 2 types of substituents or even 2-ones of letters of which one is taken in IR_3 and in IR_4.

We have $IR_3 = \{A_3, B_3\}$, $IR_4 = \{A_4, B_4, C_4, D_4, D_4'\}$, $s_4 = 5$, $p_4 = 3$, $s_4 - p_4 = 2$, $i_4 = 1$, $s_3 = 2$, $p_3 = 2$, $s_3 - p_3 = 0$, $i_3 = 1$ then

$$N_{3,4} = \binom{2}{1} \cdot \binom{5}{1} = 10$$

which corresponds to the groups of substituents A_3A_4, A_3B_4, A_3C_4, A_3D_4, A_3D_4', B_3A_4, B_3B_4, B_3C_4, B_3D_4, B_3D_4', $N_{3,4}^c = 0$, $N_{3,4}^a = \binom{2}{1} \cdot \binom{3}{1} = 6$ which corresponds

to the groups of substituents A_3A_4, A_3B_4, A_3C_4, B_3A_4, B_3B_4, B_3C_4. $N_{3,4}^{a+c} = 10 - 6 = 4$ which corresponds to the group of substituents A_3D_4, A_3D_4', B_3D_4, B_3D_4'.

2) Let us determine the number of substituent groups having 4 substituent types or even 4-tuples of letters of which one is chosen from IR_1, one in IR_2 and 2 in IR_3.

We have $IR_1 = \{A_1\}$, $IR_2 = \{A_2\}$ and $IR_3 = \{A_3, B_3\}$; $s_1 = 1$, $p_1 = 1$, $s_1 - p_1 = 0$, $i_1 = 1$, $s_2 = 1$, $p_2 = 1$, $s_2 - p_2 = 0$, $i_2 = 1$, $s_3 = 2$, $p_3 = 2$, $s_3 - p_3 = 0$, $i_3 = 2$; $N_{1,2,3} = N_{1,2,3}^a = \binom{1}{1} \cdot \binom{1}{1} \cdot \binom{2}{2} = 1$ which is the group de substituents $A_1A_2A_3B_3$, $N_{1,2,3}^c = 0$, $N_{1,2,3}^{a+c} = 0$.

3) Let us determine the number of substituent groups having 6 substituent types or even 6-tuples of letters, one of which is chosen from IR_1, one in IR_2, two in IR_3 and two in IR_4.

We have $IR_1 = \{A_1\}$, $IR_2 = \{A_2\}$, $IR_3 = \{A_3, B_3\}$ and

$$IR_4 = \{A_4, B_4, C_4, D_4, D_4'\};$$

$s_1 = 1$, $p_1 = 1$, $s_1 - p_1 = 0$, $i_1 = 1$, $s_2 = 1$, $p_2 = 1$, $s_2 - p_2 = 0$, $i_2 = 1$, $s_3 = 2$, $p_3 = 2$, $s_3 - p_3 = 0$, $i_3 = 1$, $s_4 = 5$, $p_4 = 3$, $s_4 - p_4 = 2$, $i_4 = 2$

We obtain $N_{1,2,3,4} = \binom{1}{1} \cdot \binom{1}{1} \cdot \binom{2}{2} \cdot \binom{5}{2} = 10$ which is the following groups of substituents: $A_1A_2A_3B_3A_4B_4$, $A_1A_2A_3B_3A_4C_4$, $A_1A_2A_3B_3A_4D_4$, $A_1A_2A_3B_3A_4D_4'$, $A_1A_2A_3B_3B_4C_4$, $A_1A_2A_3B_3B_4D_4$, $A_1A_2A_3B_3B_4D_4'$, $A_1A_2A_3B_3C_4D_4$, $A_1A_2A_3B_3C_4D_4'$,

$$A_1 A_2 A_3 B_3 D_4 D_4'; \quad N_{1,2,3,4}^a = \binom{1}{1} \cdot \binom{1}{1} \cdot \binom{2}{2} \cdot \binom{3}{2} = 3 \quad \text{is the groups of substituents:}$$

$A_1 A_2 A_3 B_3 A_4 B_4$, $A_1 A_2 A_3 B_3 A_4 C_4$, $A_1 A_2 A_3 B_3 B_4 C_4$; $\quad N_{1,2,3,4}^c = 0$; $\quad N_{1,2,3,4}^{a+c} = 10 - 3 = 7$ which corresponds to the following groups of substituents: $A_1 A_2 A_3 B_3 A_4 D_4$, $A_1 A_2 A_3 B_3 A_4 D_4'$, $A_1 A_2 A_3 B_3 B_4 D_4$, $A_1 A_2 A_3 B_3 B_4 D_4'$, $A_1 A_2 A_3 B_3 C_4 D_4$, $A_1 A_2 A_3 B_3 C_4 D_4'$, $A_1 A_2 A_3 B_3 D_4 D_4'$.

2.3. Calculation of the Number of Chiral and Achiral Skeletons of the System $C_n H_{m_0} \left(R_{k_1} \right)_{m_1} \cdots \left(R_{k_\alpha} \right)_{m_\alpha} \cdots \left(R_{k_\zeta} \right)_{m_\zeta}$

The "stereoisomeric" composition of the system

$$C_n H_{m_0} \left(R_{k_1} \right)_{m_1} \cdots \left(R_{k_\alpha} \right)_{m_\alpha} \cdots \left(R_{k_\zeta} \right)_{m_\zeta}$$
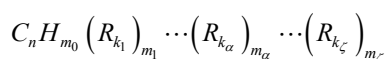
results from 1) the nature of alkyl radicals of distinct k-size (chiral or achiral tree) and 2) the manner of attaching or implanting them to the monocycle (chiral or achiral location on the monocycle).

Unlike the polyalkylation of the monocyclic cycloalkane treated by Nemba *et al.* [23] where we had combinations of alkyl groups of the same order and same steric configuration that is to say homomorphous trees, we perform in this work combinations of heteromorphous alkyl trees having distinct configurations and same order *k*, chiral (c), achiral (a), or mixed (a + c) which will be planted on the monocyclic cycloalkane. In summary and at the risk of repeating ourselves, we observe that once again we have a composite stereoisomerism due to the intrinsic chirality of the alkylated trees and the extrinsic chirality induced by their position or placement on the monocyclic cycloalkane.

The composite stereoisomerism resulting from the present exercise of heteropolyalkylation of the monocyclic cycloalkane is summarized in Table 3 below.

The different entities of Table 3 integrating the stereospecificity of the heteropolyalkylated monocyclic cycloalkane skeletons are defined as follows:

$A_c^c \left(n; m_0, m_1, \cdots, m_\alpha, \cdots, m_\zeta; k_1, \cdots, k_\alpha, \cdots, k_\zeta \right)$: is the number of chiral stereoisomers composed from chiral alkyls (Chiral Radicals—Chiral Placements);

$A_a^c \left(n; m_0, m_1, \cdots, m_\alpha, \cdots, m_\zeta; k_1, \cdots, k_\alpha, \cdots, k_\zeta \right)$: is the number of achiral stereoisomers compounded from chiral alkyls (Chiral Radicals—Achiral Placements);

Table 3. Composite stereoisomerism in heteropolyalkylated monocyclic cycloalkanes [23].

Chirality or achirality of the heteropolyalkylated monocycloalkane	Combinations of steric configurations of alkyl radicals		
Characteristics of placements $m_1, \ldots, m_i, \ldots, m_{sk}$ alkyl trees	*All the radicals combined i to i are chiral*	*All the radicals combined i to i are achiral*	*All the radicals combined i to i are achiral and chiral*
Chiral placements	Chiral radicals—Chiral placement (A_c^c)	Achiral radicals—Chiral placement (A_c^a)	Achiral and chiral radicals—Chiral placement (A_c^{a+c})
Achiral placements	Chiral radicals—Achiral placement (A_a^c)	Achiral radicals—Achiral placement (A_a^a)	Achiral and chiral radicals—Achiral placement (A_a^{a+c})

$A_c^a\left(n;m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta;k_1,\cdots,k_\alpha,\cdots,k_\zeta\right)$: is the number of chiral stereoisomers composed of achiral alkyl trees (Achiral Radicals—Chiral Placements);

$A_a^a\left(n;m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta;k_1,\cdots,k_\alpha,\cdots,k_\zeta\right)$: is the number of achiral stereoisomers compounded from achiral alkyl trees (Achiral Radicals—Achiral Placements);

$A_c^{a-c}\left(n;m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta;k_1,\cdots,k_\alpha,\cdots,k_\zeta\right)$: is the number of chiral stereoisomers composed of achiral and chiral alkyl trees (Achiral and chiral radicals—chiral Placements);

$A_a^{a-c}\left(n;m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta;k_1,\cdots,k_\alpha,\cdots,k_\zeta\right)$: is the number of achiral stereoisomers composed of achiral and chiral alkyl trees (Achiral and chiral radicals—Achiral Placements).

The number of chiral and achiral stereoisomers of a monocyclic cycloalkane heteropolysubstituted by alkyl groups of distinct orders k is directly obtained from the product of the number of groups of substituents $N_{k_1,k_2,\cdots,k_\alpha}^c$, $N_{k_1,k_2,\cdots,k_\alpha}^a$, $N_{k_1,k_2,\cdots,k_\alpha}^{a+c}$ by the number of chiral placements $A_c\left(n,m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta\right)$ and achiral placements $A_a\left(n,m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta\right)$ of alkyl trees on the monocyclic cycloalkane of size n.

For this purpose, we recall the results of our recurrence formulas established in previous papers [21] [22] [25] which gives respectively the numbers of chiral and achiral skeletons $A_c\left(n,m\right)$ and $A_a\left(n,m\right)$ of the system $C_nH_{2n-m}X_m$ and also $A_c\left(n,m_1,m_2,\cdots,m_i,\cdots,m_q\right)$ and $A_a\left(n,m_1,m_2,\cdots,m_i,\cdots,m_q\right)$ of the system $C_nX_{m_1}\cdots Y_{m_i}\cdots Z_{m_q}$. We can therefore generate relations (5)-(10) which give an inventory of the different varieties of stereoisomers resulting from the heteromorphous polyalkylation of the monocyclic cycloalkane with alkyl trees of distinct order k.

$$A_c^c\left(n;m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta;k_1,\cdots,k_\alpha,\cdots,k_\zeta\right) = N_{k_1,k_2,\cdots,k_\alpha}^c \times A_c\left(n,m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta\right) \tag{5}$$

$$A_a^c\left(n;m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta;k_1,\cdots,k_\alpha,\cdots,k_\zeta\right) = N_{k_1,k_2,\cdots,k_\alpha}^c \times A_a\left(n,m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta\right) \tag{6}$$

$$A_c^a\left(n;m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta;k_1,\cdots,k_\alpha,\cdots,k_\zeta\right) = N_{k_1,k_2,\cdots,k_\alpha}^a \times A_c\left(n,m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta\right) \tag{7}$$

$$A_a^a\left(n;m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta;k_1,\cdots,k_\alpha,\cdots,k_\zeta\right) = N_{k_1,k_2,\cdots,k_\alpha}^a \times A_a\left(n,m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta\right) \tag{8}$$

$$A_c^{a+c}\left(n;m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta;k_1,\cdots,k_\alpha,\cdots,k_\zeta\right) = N_{k_1,k_2,\cdots,k_\alpha}^{a+c} \times A_c\left(n,m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta\right) \tag{9}$$

$$A_a^{a+c}\left(n;m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta;k_1,\cdots,k_\alpha,\cdots,k_\zeta\right) = N_{k_1,k_2,\cdots,k_\alpha}^{a+c} \times A_a\left(n,m_0,m_1,\cdots,m_\alpha,\cdots,m_\zeta\right) \tag{10}$$

Therefore, the total number of chiral skeletons of the system

$$C_n H_{m_0} \left(R_{k_1} \right)_{m_1} \cdots \left(R_{k_\alpha} \right)_{m_\alpha} \cdots \left(R_{k_\zeta} \right)_{m_\zeta}$$

is given by:

$$
\begin{aligned}
A_c^{k_1,\cdots,k_\alpha,\cdots,k_\zeta} &\left(n; m_0, m_1, \cdots, m_\alpha, \cdots, m_\zeta; k_1, \cdots, k_\alpha, \cdots, k_\zeta \right) \\
&= A_c^c \left(n; m_0, m_1, \cdots, m_\alpha, \cdots, m_\zeta; k_1, \cdots, k_\alpha, \cdots, k_\zeta \right) \\
&\quad + A_a^c \left(n; m_0, m_1, \cdots, m_\alpha, \cdots, m_\zeta; k_1, \cdots, k_\alpha, \cdots, k_\zeta \right) \\
&\quad + A_c^a \left(n; m_0, m_1, \cdots, m_\alpha, \cdots, m_\zeta; k_1, \cdots, k_\alpha, \cdots, k_\zeta \right) \\
&\quad + A_c^{a+c} \left(n; m_0, m_1, \cdots, m_\alpha, \cdots, m_\zeta; k_1, \cdots, k_\alpha, \cdots, k_\zeta \right) \\
&\quad + A_a^{a+c} \left(n; m_0, m_1, \cdots, m_\alpha, \cdots, m_\zeta; k_1, \cdots, k_\alpha, \cdots, k_\zeta \right)
\end{aligned}
\tag{11}
$$

And the total number of achiral stereoisomers is:

$$
\begin{aligned}
A_a^{k_1,\cdots,k_\alpha,\cdots,k_\zeta} &\left(n; m_0, m_1, \cdots, m_\alpha, \cdots, m_\zeta; k_1, \cdots, k_\alpha, \cdots, k_\zeta \right) \\
&= A_a^a \left(n; m_0, m_1, \cdots, m_\alpha, \cdots, m_\zeta; k_1, \cdots, k_\alpha, \cdots, k_\zeta \right)
\end{aligned}
\tag{12}
$$

3. Some Examples of Application, Results and Graphical Representations

3.1. Number of Stereoisomers of the Heteropolyalkylated Cyclopropane Having Two Heteromorphous Radicals Methyl ($i_1 = 1$) and Ethyl ($i_2 = 1$)

We have $IR_1 = \{A_1\}$, $IR_2 = \{A_2\}$; $s_1 = 1$, $p_1 = 1$, $s_1 - p_1 = 0$, $i_1 = 1$, $s_2 = 1$, $p_2 = 1$, $s_2 - p_2 = 0$, $i_2 = 1$; $N_{1,2} = N_{1,2}^a = \binom{1}{1} \cdot \binom{1}{1} = 1$ which corresponds to the group of substituents $A_1 A_2$, $N_{1,2}^c = 0$, $N_{1,2}^{a+c} = 0$.

The group of substituents $A_1 A_2$ induces heteropolyalkylation of type $C_3 H_{m_0} X_{m_1} Y_{m_2}$ where $X = A_1$, $Y = A_2$ or $X = A_2$ and $Y = A_1$ and $m_0 + m_1 + m_2 = 6$. The numbers of stereoisomers A_a^a, A_c^a, A_a^c, A_c^c, A_a^{a+c} and A_c^{a+c} are respectively obtained from the following formulas:

$$A_a^a = N_{1,2}^a \times A_a, \quad A_c^a = N_{1,2}^a \times A_c, \quad A_a^c = N_{1,2}^c \times A_a, \quad A_c^c = N_{1,2}^c \times A_c,$$
$$A_a^{a+c} = N_{1,2}^{a+c} \times A_a \quad \text{and} \quad A_c^{a+c} = N_{1,2}^{a+c} \times A_c.$$

The numbers of stereoisomers corresponding to placements or positions A_a and A_c of $C_3 H_{m_0} X_{m_1} Y_{m_2}$ having $m_0 \neq 0$, $m_1 \neq 0$, $m_2 \neq 0$ are the same with those of the system $C_n X_{m_1} Y_{m_2} Z_{m_3}$ which have been calculated in our previous paper for $n = 3$ [21] [22] [25]. They are recalled in the present paper.

The numbers of stereoisomers corresponding to placements or positions A_a and A_c of $C_3 H_{m_0} X_{m_1} Y_{m_2}$ having $m_0 = 0$, $m_1 \neq 0$, $m_2 \neq 0$ are equivalent to those of the system $C_n H_{2n-m} X_m$ given in our previous paper for $n = 3$ [21] [22] [25].

Using all these data, the inventory of stereoisomers of the heteropolyalkylated cyclopropane having two distinct alkyl trees methyl ($i_1 = 1$) and ethyl ($i_2 = 1$) is summarized in **Table 4**.

Table 4. Number of stereoisomers of the heteropolyalkylated cyclopropane having two distinct alkyl trees methyl ($i_1 = 1$) and ethyl ($i_2 = 1$).

m_0	m_1	m_2	A_a	A_c	A_a^a	A_c^a	A_a^c	A_c^c	A_a^{a+c}	A_c^{a+c}
1	1	4	1	2	1	2	0	0	0	0
1	2	3	2	4	2	4	0		0	0
2	2	2	4	7	4	7	0	0	0	0
0	1	5	1	0	1	0	0	0	0	0
0	2	4	2	1	2	1	0	0	0	0
0	3	3	2	1	2	1	0	0	0	0

Some graphical representations:

$n = 3$, $m_0 = 4$, $m_1 = 1$, $m_2 = 1$:
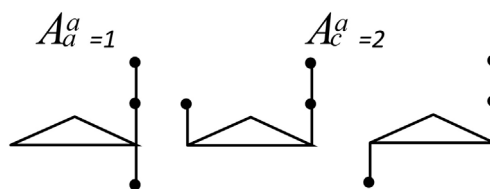
$n = 3$, $m_0 = 3$, $m_1 = 2$, $m_2 = 1$:

3.2. Number of Stereoisomers of Heteropolyalkylated Cyclobutane Having Two Heteromorphous Radicals Methyl ($i_1 = 1$) and Ethyl ($i_2 = 1$)

We have $IR_1 = \{A_1\}$, $IR_2 = \{A_2\}$; $s_1 = 1$, $p_1 = 1$, $s_1 - p_1 = 0$, $i_1 = 1$, $s_2 = 1$, $p_2 = 1$, $s_2 - p_2 = 0$, $i_2 = 1$; $N_{1,2} = N_{1,2}^a = \binom{1}{1} \cdot \binom{1}{1} = 1$ which corresponds to the group of substituents $A_1 A_2$, $N_{1,2}^c = 0$, $N_{1,2}^{a+c} = 0$.

The group of substituents $A_1 A_2$ induces heteropolyalkylation of type $C_4 H_{m_0} X_{m_1} Y_{m_2}$ with $X = A_1$, $Y = A_2$ or $X = A_2$, $Y = A_1$ and $m_0 + m_1 + m_2 = 8$. The numbers of stereoisomers A_a^a A_c^a, A_a^c, A_c^c, A_a^{a+c} and A_c^{a+c} are respectively obtained from the following formulas:

$$A_a^a = N_{1,2}^a \times A_a, \quad A_c^a = N_{1,2}^a \times A_c, \quad A_a^c = N_{1,2}^c \times A_a, \quad A_c^c = N_{1,2}^c \times A_c,$$
$$A_a^{a+c} = N_{1,2}^{a+c} \times A_a \quad \text{and} \quad A_c^{a+c} = N_{1,2}^{a+c} \times A_c.$$

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The numbers of stereoisomers corresponding to placements or positions A_a and A_c of $C_4 H_{m_0} X_{m_1} Y_{m_2}$ having $m_0 \neq 0$, $m_1 \neq 0$, $m_2 \neq 0$ are the same with those of the system $C_n X_{m_1} Y_{m_2} Z_{m_3}$ which have been calculated in our previous paper for $n = 4$ [21] [22] [25]. They are recalled and used in the present paper.

The numbers of stereoisomers corresponding to placements or positions A_a and A_c of $C_4 H_{m_0} X_{m_1} Y_{m_2}$ having $m_0 = 0$, $m_1 \neq 0$, $m_2 \neq 0$ are equivalent to those of the system $C_n H_{2n-m} X_m$ given in our previous paper for $n = 4$ [21] [22] [25].

Using all these data, the inventory of stereoisomers of the heteropolyalkylated cyclobutane having two distinct alkyl trees methyl ($i_1 = 1$) and ethyl ($i_2 = 1$) is summarized in Table 5.
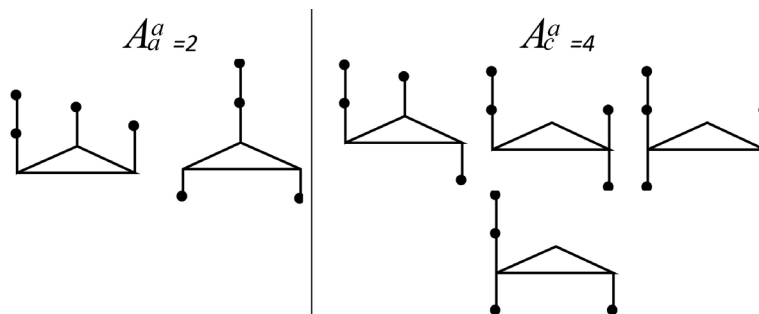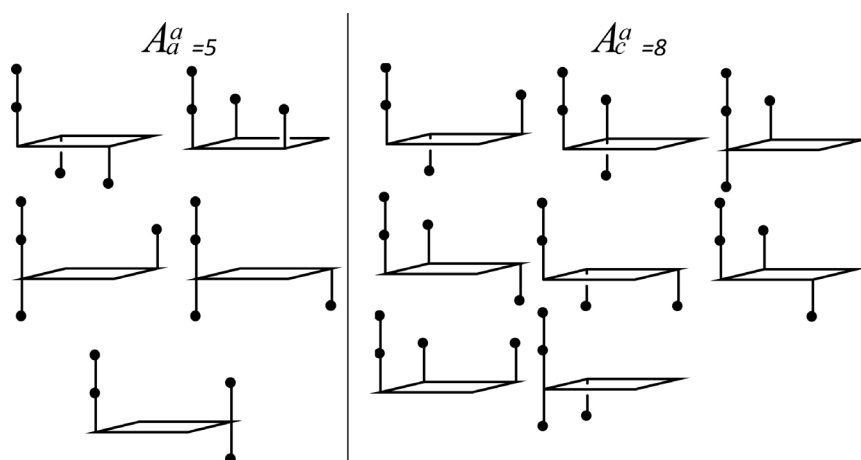
Representation of some graphs:

$n = 4$, $m_0 = 5$, $m_1 = 2$, $m_2 = 1$:

$$A_a^a = 5 \qquad A_c^a = 8$$

3.3. Number of Stereoisomers of Heteropolyalkylated Cyclopropane Having Two Heteromorphous Radicals Propyl (i_3 = 1) and Butyl (i_4 = 1)

We have $IR_3 = \{A_3, B_3\}$, $IR_4 = \{A_4, B_4, C_4, D_4, D_4'\}$, $s_4 = 5$, $p_4 = 3$, $s_4 - p_4 = 2$, $i_4 = 1$, $s_3 = 2$, $p_3 = 2$, $s_3 - p_3 = 0$, $i_3 = 1$ then

$$N_{3,4} = \binom{2}{1} \cdot \binom{5}{1} = 10$$ which corresponds to groups of substituents $A_3 A_4$, $A_3 B_4$, $A_3 C_4$, $A_3 D_4$, $A_3 D_4'$, $B_3 A_4$, $B_3 B_4$, $B_3 C_4$, $B_3 D_4$, $B_3 D_4'$, $N_{3,4}^c = 0$, $N_{3,4}^a = \binom{2}{1} \cdot \binom{3}{1} = 6$

which corresponds to the groups of substituents $A_3 A_4$, $A_3 B_4$, $A_3 C_4$, $B_3 A_4$, $B_3 B_4$, $B_3 C_4$; $N_{3,4}^{a+c} = 10 - 6 = 4$ which corresponds to the group of substituents $A_3 D_4$, $A_3 D_4'$, $B_3 D_4$, $B_3 D_4'$.

All groups of substituents give heteropolyalkylations of type $C_3 H_{m_0} X_{m_1} Y_{m_2}$ such as $m_0 + m_1 + m_2 = 6$; with the group de substituents $A_3 B_4$ for example, we can make the assignment $X = A_3$, $Y = B_4$ or $X = B_4$, $Y = A_3$. Numbers of stereoisomers A_a^a, A_a^c, A_c^a, A_c^c, A_a^{a+c} and A_c^{a+c} are respectively obtained from the following formulas:

Table 5. Number of stereoisomers of heteropolyalkylated cyclobutane having two distinct alkyl trees methyl ($i_1 = 1$) and ethyl ($i_2 = 1$).

m_0	m_1	m_2	A_a	A_c	A_a^a	A_c^a	A_a^c	A_c^c	A_a^{a+c}	A_c^{a+c}
6	1	1	3	2	3	2	0	0	0	0
5	2	1	5	8	5	8	0		0	0
4	2	2	14	23	14	23	0	0	0	0
4	3	1	7	14	7	14	0	0	0	0
3	3	2	10	30	10	30	0	0	0	0
2	3	3	10	30	10	30	0	0	0	0
0	7	1	1	0	1	0	0	0	0	0
0	6	2	4	1	4	1	0	0	0	0
0	5	3	3	2	3	2	0	0	0	0
0	4	4	7	3	7	3	0	0	0	0

$$A_a^a = N_4^a \times A_a, \quad A_c^a = N_4^a \times A_c, \quad A_a^c = N_4^c \times A_a, \quad A_c^c = N_4^c \times A_c, \quad A_a^{a+c} = N_4^{a+c} \times A_a$$

and $A_c^{a+c} = N_4^{a+c} \times A_c$ with $N_{3,4}^a = 6$, $N_{3,4}^c = 0$ and $N_{3,4}^{a+c} = 4$.

The numbers of stereoisomers corresponding to placements or positions A_a and A_c of $C_3 H_{m_0} X_{m_1} Y_{m_2}$ having $m_0 \neq 0$, $m_1 \neq 0$, $m_2 \neq 0$ are the same with those of the system $C_n X_{m_1} Y_{m_2} Z_{m_3}$ which have been calculated in our previous paper for $n = 3$ [21] [22] [25]. They are recalled in the present paper.

The numbers of stereoisomers corresponding to placements or positions A_a and A_c of $C_3 H_{m_0} X_{m_1} Y_{m_2}$ having $m_0 = 0$, $m_1 \neq 0$, $m_2 \neq 0$ are equivalent to those of the system $C_n H_{2n-m} X_m$ given in our previous paper for $n = 3$ [21] [22] [25].

Using all these data, the inventory of stereoisomers of the heteropolyalkylated cyclopropane having two heteromorphous radicals propyl ($i_3 = 1$) and butyl ($i_4 = 1$) is summarized in Table 6.

Some graphical representations:

$n = 3$, $m_0 = 4$, $m_1 = 1$, $m_2 = 1$:
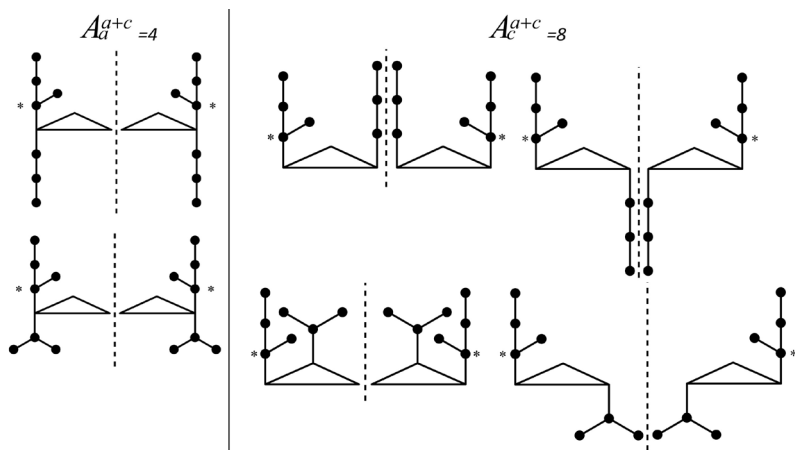
Table 6. Number of stereoisomers of heteropolyalkylated cyclopropane having two heteromorphous radicals propyl ($i_3 = 1$) and butyl ($i_4 = 1$).

m_0	m_1	m_2	A_a	A_c	A_a^a	A_c^a	A_a^c	A_c^c	A_a^{a+c}	A_c^{a+c}
1	1	4	1	2	6	36	0	0	4	8
1	2	3	2	4	12	24	0	0	8	16
2	2	2	4	7	24	42	0	0	16	28
0	1	5	1	0	6	0	0	0	4	0
0	2	4	2	1	12	6	0	0	8	4
0	3	3	2	1	12	6	0	0	8	4

3.4. Number of Stereoisomers of Heteropolyalkylated Cyclobutane Having Two Heteromorphous Radicals Propyl (i_3 = 1) and Butyl (i_4 = 1)

We have $IR_3 = \{A_3, B_3\}$, $IR_4 = \{A_4, B_4, C_4, D_4, D_4'\}$, $s_4 = 5$, $p_4 = 3$, $s_4 - p_4 = 2$, $i_4 = 1$, $s_3 = 2$, $p_3 = 2$, $s_3 - p_3 = 0$, $i_3 = 1$ then

$$N_{3,4} = \binom{2}{1} \cdot \binom{5}{1} = 10$$ which corresponds to groups of substituents A_3A_4, A_3B_4, A_3C_4, A_3D_4, A_3D_4', B_3A_4, B_3B_4, B_3C_4, B_3D_4, B_3D_4', $N_{3,4}^c = 0$, $N_{3,4}^a = \binom{2}{1} \cdot \binom{3}{1} = 6$

which corresponds to the group of substituents A_3A_4, A_3B_4, A_3C_4, B_3A_4, B_3B_4, B_3C_4. $N_{3,4}^{a+c} = 10 - 6 = 4$ which corresponds to groups of substituents A_3D_4, A_3D_4', B_3D_4, B_3D_4'.

The groups of substituents induce heteropolyalkylation of type $C_4H_{m_0}X_{m_1}Y_{m_2}$ such as $m_0 + m_1 + m_2 = 8$, with the group de substituents A_3B_4 for example, we can make the assignment $X = A_3$, $Y = B_4$ or $X = B_4$, $Y = A_3$.

The numbers of stereoisomers A_a^a, A_c^a, A_a^c, A_c^c, A_a^{a+c} and A_c^{a+c} are respectively obtained from the following formulas:

$$A_a^a = N_{3,4}^a \times A_a, \quad A_c^a = N_{3,4}^a \times A_c, \quad A_a^c = N_{3,4}^c \times A_a, \quad A_c^c = N_{3,4}^c \times A_c,$$

$$A_a^{a+c} = N_{3,4}^{a+c} \times A_a \quad \text{and} \quad A_c^{a+c} = N_{3,4}^{a+c} \times A_c,$$

$$\text{with} \quad N_{3,4}^a = 6, \quad N_{3,4}^c = 0 \quad \text{and} \quad N_{3,4}^{a+c} = 4.$$

The numbers of stereoisomers corresponding to placements or positions A_a and A_c of $C_4H_{m_0}X_{m_1}Y_{m_2}$ having $m_0 \neq 0$, $m_1 \neq 0$, $m_2 \neq 0$ are the same with those of the system $C_nX_{m_1}Y_{m_2}Z_{m_3}$ which have been calculated in our previous paper for $n = 4$ [21] [22] [25]. They are recalled and used in the present paper.

The numbers of stereoisomers corresponding to placements or positions A_a and A_c of $C_4H_{m_0}X_{m_1}Y_{m_2}$ having $m_0 = 0$, $m_1 \neq 0$, $m_2 \neq 0$ are equivalent to those of the system $C_nH_{2n-m}X_m$ given in our previous paper for $n = 4$ [21] [22] [25].

Using all these data, the inventory of stereoisomers of the heteropolyalkylated cyclobutane having two heteromorphous radicals propyl ($i_3 = 1$) and butyl ($i_4 = 1$) is summarized in Table 7.

Table 7. Number of stereoisomers of heteropolyalkylated cyclobutane having two heteromorphous radicals propyl ($i_3 = 1$) and butyl ($i_4 = 1$)

m_0	m_1	m_2	A_a	A_c	A_a^a	A_c^a	A_a^c	A_c^c	A_a^{a+c}	A_c^{a+c}
6	1	1	3	2	18	12	0	0	12	8
5	2	1	5	8	30	48	0	0	20	32
4	2	2	14	23	84	138	0	0	56	92
4	3	1	7	14	42	84	0	0	28	56
3	3	2	10	30	60	180	0	0	40	120
0	7	1	1	0	6	0	0	0	4	0
0	6	2	4	1	24	6	0	0	16	4
0	5	3	3	2	18	12	0	0	12	8
0	4	4	7	3	42	18	0	0	28	12

Some graphical representations:

$n = 4$, $m_0 = 6$, $m_1 = 1$, $m_2 = 1$:

$$A_c^{a+c} = 8$$
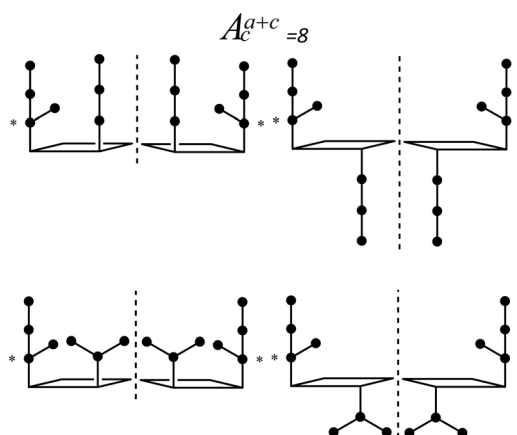
3.5. Number of Stereoisomers of Heteropolyalkylated Cyclopropane Having Heteromorphous Radicals Propyl ($i_3 = 2$) and Butyl ($i_4 = 1$)

We have $IR_3 = \{A_3, B_3\}$, $IR_4 = \{A_4, B_4, C_4, D_4, D'_4\}$, $s_4 = 5$, $p_4 = 3$, $s_4 - p_4 = 2$, $i_4 = 1$, $s_3 = 2$, $p_3 = 2$, $s_3 - p_3 = 0$, $i_3 = 2$ then

$N_{3,4} = \binom{2}{2} \cdot \binom{5}{1} = 5$ which corresponds to groups of substituents $A_3B_3A_4$, $A_3B_3B_4$, $A_3B_3C_4$, $A_3B_3D_4$, $A_3B_3D'_4$; $N_{3,4}^c = 0$, $N_{3,4}^a = \binom{2}{2} \cdot \binom{3}{1} = 3$ which corresponds to groups of substituents $A_3B_3A_4$, $A_3B_3B_4$, $A_3B_3C_4$; $N_{3,4}^{a+c} = 5 - 3 = 2$ which corresponds to groups of substituents $A_3B_3D_4$, $A_3B_3D'_4$.

All those groups of substituents generate heteropolyalkylations of type $C_3H_{m_0}X_{m_1}Y_{m_2}Z_{m_3}$ such as $m_0 + m_1 + m_2 + m_3 = 6$; with the group of substituents $A_3B_3C_4$ for example, we can make the assignment $X = A_3$, $Y = B_3$, $Z = C_4$;

$X = A_3$, $Y = C_4$, $Z = B_3$; $X = B_3$, $Y = A_3$, $Z = C_4$; $X = B_3$, $Y = C_4$, $Z = A_3$; $X = C_4$, $Y = A_3$, $Z = B_3$; $X = C_4$, $Y = B_3$, $Z = A_3$. The numbers of stereoisomers A_a^a, A_c^a, A_a^c, A_c^c, A_a^{a+c} and A_c^{a+c} are respectively obtained from the following formulas:

$$A_a^a = N_{3,4}^a \times A_a, \quad A_c^a = N_{3,4}^a \times A_c, \quad A_a^c = N_{3,4}^c \times A_a, \quad A_c^c = N_{3,4}^c \times A_c,$$

$$A_a^{a+c} = N_{3,4}^{a+c} \times A_a \quad \text{and} \quad A_c^{a+c} = N_{3,4}^{a+c} \times A_c,$$

$$\text{with} \quad N_{3,4}^a = 3, \quad N_{3,4}^c = 0 \quad \text{and} \quad N_{3,4}^{a+c} = 2.$$

The numbers of stereoisomers corresponding to placements or positions A_a and A_c of $C_3H_{m_0}X_{m_1}Y_{m_2}Z_{m_3}$ having $m_0 \neq 0$, $m_1 \neq 0$, $m_2 \neq 0$, $m_3 \neq 0$ are the same with those of the system $C_nX_{m_1}Y_{m_2}Z_{m_3}U_{m_4}$ which have been calculated in our previous paper for $n = 3$ [21] [22] [25]. They are recalled in the present paper.

The numbers of stereoisomers of position A_a and A_c of $C_3H_{m_0}X_{m_1}Y_{m_2}Z_{m_3}$ having $m_0 = 0$, $m_1 \neq 0$, $m_2 \neq 0$, $m_3 \neq 0$ are equivalent to those of the system $C_nX_{m_1}Y_{m_2}Z_{m_3}$ given in our previous paper for $n = 3$ [21] [22] [25].

Using all these data, the inventory of stereoisomers of the heteropolyalkylated cyclopropane having two heteromorphous alkyl trees butyl ($i_4 = 1$) and propyl ($i_3 = 2$) is tabulated in **Table 8**.

Representation of some graphs:

$n = 3$, $m_0 = 0$, $m_1 = 4$, $m_2 = 1$, $m_3 = 1$:

$$A_a^{a+c} = 2$$

$$A_c^{a+c} = 4$$
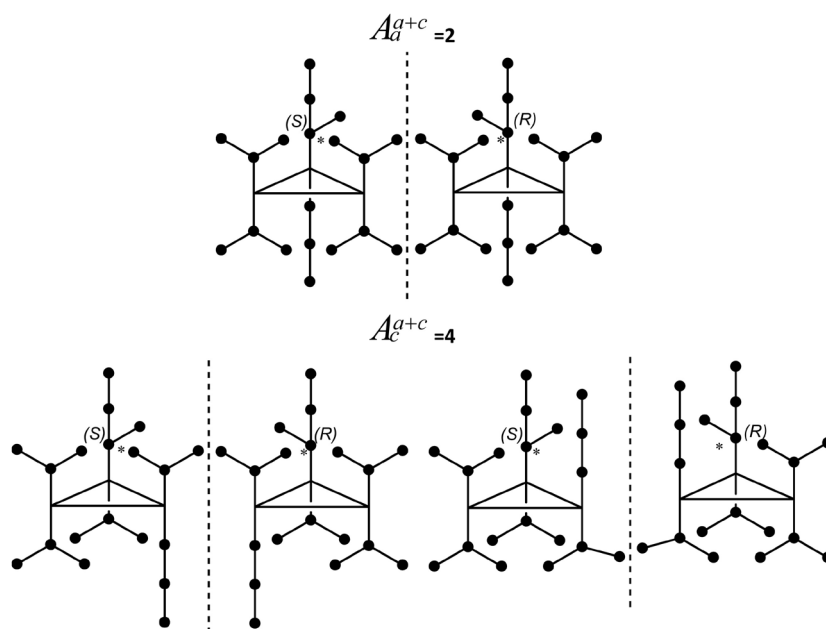
3.6. Number of Stereoisomers of Heteropolyalkylated Cyclobutane Having Heteromorphous Radicals Propyl (i_3 = 2) and Butyl (i_4 = 1)

We have $IR_3 = \{A_3, B_3\}$, $IR_4 = \{A_4, B_4, C_4, D_4, D_4'\}$, $s_4 = 5$, $p_4 = 3$, $s_4 - p_4 = 2$, $i_4 = 1$, $s_3 = 2$, $p_3 = 2$, $s_3 - p_3 = 0$, $i_3 = 2$ then

Table 8. Number of stereoisomers of the heteropolyalkylated cyclopropane having two heteromorphous alkyl trees butyl ($i_4 = 1$) and propyl ($i_3 = 2$).

m_0	m_1	m_2	m_3	A_a	A_c	A_a^a	A_c^a	A_a^c	A_c^c	A_a^{a+c}	A_c^{a+c}
1	1	1	3	0	10	0	30	0	0	0	20
1	1	2	2	2	14	6	42	0	0	4	28
0	1	1	4	1	2	3	6	0	0	2	4
0	1	2	3	2	4	6	12	0	0	4	8
0	2	2	2	4	7	12	21	0	0	8	14

$N_{3,4} = \begin{pmatrix} 2 \\ 2 \end{pmatrix} \cdot \begin{pmatrix} 5 \\ 1 \end{pmatrix} = 5$ which corresponds to groups of substituents $A_3 B_3 A_4$, $A_3 B_3 B_4$,

$A_3 B_3 C_4$, $A_3 B_3 D_4$, $A_3 B_3 D_4'$; $N_{3,4}^c = 0$, $N_{3,4}^a = \begin{pmatrix} 2 \\ 2 \end{pmatrix} \cdot \begin{pmatrix} 3 \\ 1 \end{pmatrix} = 3$ which corresponds to

the groups of substituents $A_3 B_3 A_4$, $A_3 B_3 B_4$, $A_3 B_3 C_4$; $N_{3,4}^{a+c} = 5 - 3 = 2$ which corresponds to groups of substituents $A_3 B_3 D_4$, $A_3 B_3 D_4'$.

All those groups of substituents generate heteropolyalkylations of type $C_4 H_{m_0} X_{m_1} Y_{m_2} Z_{m_3}$ such as $m_0 + m_1 + m_2 + m_3 = 8$; with the group de substituents $A_3 B_3 C_4$ for example, we can make the assignment $X = A_3$, $Y = B_3$, $Z = C_4$; $X = A_3$, $Y = C_4$, $Z = B_3$; $X = B_3$, $Y = A_3$, $Z = C_4$; $Z = B_3$, $Y = C_4$, $Z = A_3$; $X = C_4$, $Y = A_3$, $Z = B_3$; $X = C_4$, $Y = B_3$, $Z = A_3$.

The numbers of stereoisomers A_a^a, A_c^a, A_a^c, A_c^c, A_a^{a+c} and A_c^{a+c} are respectively obtained from the following formulas:

$$A_a^a = N_{3,4}^a \times A_a, \quad A_c^a = N_{3,4}^a \times A_c, \quad A_a^c = N_{3,4}^c \times A_a, \quad A_c^c = N_{3,4}^c \times A_c,$$

$$A_a^{a+c} = N_{3,4}^{a+c} \times A_a \quad \text{and} \quad A_c^{a+c} = N_{3,4}^{a+c} \times A_c$$

$$\text{where} \quad N_{3,4}^a = 3, \quad N_{3,4}^c = 0 \quad \text{and} \quad N_{3,4}^{a+c} = 2.$$

The numbers of stereoisomers corresponding to placements or positions A_a and A_c of $C_4 H_{m_0} X_{m_1} Y_{m_2} Z_{m_3}$ having $m_0 \neq 0$, $m_1 \neq 0$, $m_2 \neq 0$, $m_3 \neq 0$ are equivalent to those of the system $C_n X_{m_1} Y_{m_2} Z_{m_3} U_{m_4}$ which have been calculated in our previous paper for $n = 4$ [21] [22] [25]. They are recalled in the present paper.

The numbers of stereoisomers of position A_a and A_c of $C_4 H_{m_0} X_{m_1} Y_{m_2} Z_{m_3}$ having $m_0 = 0$, $m_1 \neq 0$, $m_2 \neq 0$, $m_3 \neq 0$ are equivalent to those of the system $C_n X_{m_1} Y_{m_2} Z_{m_3}$ calculated in our previous paper for $n = 4$ [21] [22] [25].

Using all these data, the inventory of stereoisomers of the heteropolyalkylated cyclobutane having heteromorphous radicals propyl (i_3 = 2) and butyl (i_4 = 1) is summarized in **Table 9**.

3.7. Number of Stereoisomers of Heteropolyalkylated Cyclopropane Having Heteromorphous Radicals Butyl (i_4 = 2) and Pentyl (i_5 = 2)

We have $IR_4 = \{A_4, B_4, C_4, D_4, D_4'\}$, $IR_5 = \{A_5, B_5, C_5, D_5, E_5, E_5', F, F_5', G, G_5'\}$, $s_4 = 5$, $p_4 = 3$, $s_4 - p_4 = 2$, $i_4 = 2$, $s_5 = 11$, $p_5 = 5$, $s_5 - p_5 = 6$, $i_5 = 2$;

Table 9. Number of stereoisomers of the heteropolyalkylated cyclobutane having heteromorphous radicals propyl ($i_3 = 2$) and butyl ($i_4 = 1$).

m_0	m_1	m_2	m_4	A_a	A_c	A_a^a	A_c^a	A_a^c	A_c^c	A_a^{a+c}	A_c^{a+c}
1	1	1	5	6	18	18	54	0	0	12	36
1	1	2	4	9	48	27	144	0	0	18	56
1	1	3	3	12	64	36	192	0	0	24	128
1	2	2	3	14	98	42	294	0	0	28	196
2	2	2	2	30	150	90	450	0	0	60	300
0	6	1	1	3	2	9	6	0	0	6	4
0	5	1	2	5	8	15	24	0	0	10	16
0	4	2	2	14	23	42	69	0	0	28	46
0	4	3	1	7	14	21	42	0	0	14	28
0	3	3	2	10	30	30	90	0	0	20	60

$$N_{4,5} = \binom{5}{2} \cdot \binom{11}{2} = 550 \,;\quad N_{4,5}^c = \binom{2}{2} \cdot \binom{6}{2} = 15 \quad \text{which corresponds to groups of}$$

substituents $D_4 D_4' F_5 F_5'$, $D_4 D_4' F_5 G_5$, $D_4 D_4' F_5 G_5'$, $D_4 D_4' F_5 H_5$, $D_4 D_4' F_5 H_5'$, $D_4 D_4' F_5' G_5$, $D_4 D_4' F_5' G_5'$, $D_4 D_4' F_5' H_5$, $D_4 D_4' F_5' H_5'$, $D_4 D_4' G_5 G_5'$, $D_4 D_4' G_5 H_5$, $D_4 D_4' G_5 H_5'$, $D_4 D_4' G_5' H_5$, $D_4 D_4' G_5' H_5'$, $D_4 D_4' G_5 H_5'$; $N_{4,5}^a = \binom{3}{2} \cdot \binom{5}{2} = 30$;

$$N_{4,5}^{a+c} = 550 - 30 - 15 = 505 \,.$$

All the groups of substituents generate heteropolyalkylations of type $C_3 H_{m_0} X_{m_1} Y_{m_2} Z_{m_3} U_{m_4}$ such as $m_0 + m_1 + m_2 + m_3 + m_4 = 6$; with the group de substituents $A_4 B_4 C_5 D_5$ for example, we can make the assignment $X = A_4$, $Y = B_4$, $Z = C_5$, $U = D_5$; $X = A_4$, $Y = C_5$, $Z = D_5$, $U = B_4$; $X = B_4$, $Y = A_4$, $Z = D_5$, $U = C_5$ and so on. The numbers of stereoisomers A_a^a, A_c^a, A_a^c, A_c^c, A_a^{a+c} and A_c^{a+c} are respectively obtained from the following formulas:

$$A_a^a = N_{4,5}^a \times A_a \,, \quad A_c^a = N_{4,5}^a \times A_c \,, \quad A_a^c = N_{4,5}^c \times A_a \,, \quad A_c^c = N_{4,5}^c \times A_c \,,$$
$$A_a^{a+c} = N_{4,5}^{a+c} \times A_a \quad \text{and} \quad A_c^{a+c} = N_{4,5}^{a+c} \times A_c \,,$$
$$\text{with} \quad N_{4,5}^a = 30 \,, \quad N_{4,5}^c = 15 \,, \quad N_{4,5}^{a+c} = 505 \,.$$

The numbers of stereoisomers corresponding to placements or positions A_a and A_c of $C_3 H_{m_0} X_{m_1} Y_{m_2} Z_{m_3} U_{m_4}$ having $m_0 \neq 0$, $m_1 \neq 0$, $m_2 \neq 0$, $m_3 \neq 0$; $m_4 \neq 0$ are equivalent to those of the system $C_n X_{m_1} Y_{m_2} Z_{m_3} U_{m_4} V_{m_5}$ determined in our previous paper for $n = 3$ [21] [22] [25].

The numbers of stereoisomers of position A_a and A_c of $C_3 H_{m_0} X_{m_1} Y_{m_2} Z_{m_3} U_{m_4}$ having $m_0 = 0$, $m_1 \neq 0$, $m_2 \neq 0$, $m_3 \neq 0$, $m_4 \neq 0$ are equivalent to those of the system $C_n X_{m_1} Y_{m_2} Z_{m_3} U_{m_4}$ also derived in our previous paper for $n = 3$ [21] [22] [25].

Using all these data, the inventory of stereoisomers of the heteropolyalkylated cyclopropane having heteromorphous alkyl trees butyl ($i_4 = 2$) and pentyl ($i_5 = 2$) is summarized in **Table 10**.

Table 10. Number of stereoisomers of the heteropolyalkylated cyclopropane having heteromorphous alkyl trees butyl ($i_4 = 2$) and pentyl ($i_5 = 2$).

m_0	m_1	m_2	m_3	m_4	A_a	A_c	A_a^a	A_c^a	A_a^c	A_c^c	A_a^{a+c}	A_c^{a+c}
1	1	1	1	2	0	30	0	900	0	450	0	15,150
0	1	1	1	3	0	10	0	300	0	150	0	5050
0	1	1	2	2	2	14	60	420	30	210	1010	7070

3.8. Number of Stereoisomers of Heteropolyalkylated Cyclobutane Having Heteromorphous Radicals Butyl (i_4 = 2) and Pentyl (i_5 = 2)

We have $IR_4 = \{A_4, B_4, C_4, D_4, D_4'\}$, $IR_5 = \{A_5, B_5, C_5, D_5, E_5, E_5', F, F_5', G, G_5'\}$, $s_4 = 5$, $p_4 = 3$, $s_4 - p_4 = 2$, $i_4 = 2$, $s_5 = 11$, $p_5 = 5$, $s_5 - p_5 = 6$, $i_5 = 2$; $N_{4,5} = \binom{5}{2} \cdot \binom{11}{2} = 550$; $N_{4,5}^c = \binom{2}{2} \cdot \binom{6}{2} = 15$ which corresponds to groups of substituents $D_4 D_4' F_5 F_5'$, $D_4 D_4' F_5 G_5$, $D_4 D_4' F_5 G_5'$, $D_4 D_4' F_5 H_5$, $D_4 D_4' F_5 H_5'$, $D_4 D_4' F_5' G_5$, $D_4 D_4' F_5' G_5'$, $D_4 D_4' F_5' H_5$, $D_4 D_4' F_5' H_5'$, $D_4 D_4' G_5 G_5'$, $D_4 D_4' G_5 H_5$, $D_4 D_4' G_5 H_5'$, $D_4 D_4' G_5' H_5$, $D_4 D_4' G_5' H_5'$, $D_4 D_4' H_5 H_5'$; $N_{4,5}^a = \binom{3}{2} \cdot \binom{5}{2} = 30$;

$N_{4,5}^{a+c} = 550 - 30 - 15 = 505$.

All the groups of substituents generate heteropolyalkylations of type $C_4 H_{m_0} X_{m_1} Y_{m_2} Z_{m_3} U_{m_4}$ such as $m_0 + m_1 + m_2 + m_3 + m_4 = 8$; with the group de substituents $A_4 B_4 C_5 D_5$ for example, we can make the assignment $X = A_4$, $Y = B_4$, $Z = C_5$, $U = D_5$; $X = A_4$, $Y = C_5$, $Z = D_5$, $U = B_4$; $X = B_4$, $Y = A_4$, $Z = D_5$, $U = C_5$ and so on. The numbers of stereoisomers A_a^a, A_c^a, A_a^c, A_c^c, A_a^{a+c} and A_c^{a+c} are respectively obtained from the following formulas:

$$A_a^a = N_{4,5}^a \times A_a, \quad A_c^a = N_{4,5}^a \times A_c, \quad A_a^c = N_{4,5}^c \times A_a, \quad A_c^c = N_{4,5}^c \times A_c,$$

$$A_a^{a+c} = N_{4,5}^{a+c} \times A_a \quad \text{and} \quad A_c^{a+c} = N_{4,5}^{a+c} \times A_c,$$

$$\text{with } N_{4,5}^a = 30, \quad N_{4,5}^c = 15, \quad N_{4,5}^{a+c} = 505.$$

The numbers of stereoisomers corresponding to placements or positions A_a and A_c of $C_4 H_{m_0} X_{m_1} Y_{m_2} Z_{m_3} U_{m_4}$ having $m_0 \neq 0$, $m_1 \neq 0$, $m_2 \neq 0$, $m_3 \neq 0$ are equivalent to those of the system $C_n X_{m_1} Y_{m_2} Z_{m_3} U_{m_4} V_{m_5}$ which have been calculated in our previous paper for $n = 4$ [21] [22] [25]. They are recalled in the present paper.

The numbers of stereoisomers of position A_a and A_c of $C_4 H_{m_0} X_{m_1} Y_{m_2} Z_{m_3} U_{m_4}$ having $m_0 = 0$, $m_1 \neq 0$, $m_2 \neq 0$, $m_3 \neq 0$ are equivalent to those of the system $C_n X_{m_1} Y_{m_2} Z_{m_3} U_{m_4}$ calculated in our previous paper for $n = 4$ [21] [22] [25].

Using all these data, the inventory of stereoisomers of the heteropolyalkylated cyclobutane having heteromorphous radicals butyl ($i_4 = 2$) and pentyl ($i_5 = 2$) is summarized in Table 11.

4. Conclusion

The combinatorial method developed in the present paper makes it possible to

Table 11. Number of stereoisomers of heteropolyalkylated cyclobutane having heteromorphous radicals butyl ($i_4 = 2$) and pentyl ($i_5 = 2$).

m_0	m_1	m_2	m_3	m_4	A_a	A_c	A_a^a	A_c^a	A_a^c	A_c^c	A_a^{a+c}	A_c^{a+c}
1	1	1	1	4	6	102	180	3060	90	1530	3030	51,510
1	1	1	2	3	12	204	360	6120	180	3060	6060	103,020
1	1	2	2	2	18	306	540	9180	270	4590	9090	154,530
0	1	1	1	5	6	18	180	540	90	270	3030	9090
0	1	1	2	4	9	48	270	1440	135	720	4545	24,240
0	1	1	3	3	12	64	360	1920	180	960	6060	32,320
0	1	2	2	3	14	98	420	2940	210	1470	7070	49,490
0	2	2	2	2	30	150	900	4500	450	2250	15,150	75,750

directly enumerate enantiomeric pairs and achiral skeletons of the heteropolyalkylated monocyclic cycloalkane $R_{k_\alpha} = C_{k_\alpha} H_{2k_\alpha+1}$ of which at least two noted alkyl groups each has a distinct order $k_\alpha \left(1 \le \alpha \le \zeta\right)$. m_α is the number of alkyl radicals R_{k_α} in the system $C_n H_{m_0} \left(R_{k_1}\right)_{m_1} \cdots \left(R_{k_\alpha}\right)_{m_\alpha} \cdots \left(R_{k_\zeta}\right)_{m_\zeta}$ satisfying the relationship $\sum_{\alpha=1}^{\zeta} m_\alpha + m_0 = 2n$. This procedure has already been successfully applied by Nemba and Balaban for the case of homomorphic heteropolyalkylation [23] and its advantage is to bypass the Polya method [3] which first requires deriving the cycle index in accordance with symmetry and permutation group of the molecular system and then transform the cycle index into a generating function of the order $2n$ before continuing with the composition of the graphs to obtain the results of the system $C_n H_{m_0} \left(R_{k_1}\right)_{m_1} \cdots \left(R_{k_\alpha}\right)_{m_\alpha} \cdots \left(R_{k_\zeta}\right)_{m_\zeta}$. In this work, we have

used the basic concepts of permutation group theory and algebraic combinatorics as tools to highlight the chirality and adequacy of achirality induced by composition of molecular systems through heteromorphic polyalkylation. The number of stereoisomers of this family of compounds evolves exponentially as a function of the number of asymmetric carbons of the molecular system carried not only by the radicals but also by the monocyclic cycloalkane. It is worth remembering that the compounds of this family of hydrocarbons serve as starting materials for extensive kinetic and mechanistic studies, while others are used successfully for important applications such as the manufacture of hydrocarbon resins and other chemicals. Hence the interest of the present scientific contribution.

Acknowledgements

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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