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Mathematical Predicted Values Based on Sombor Descriptors for Cyclooctane Chains

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ABSTRACT

Cyclooctane group is a significant kind of cycloalkane in the field of computing chemistry. These compounds are considered macro cyclic aromatic hydrocarbons. The intriguing properties and conformational behaviors of Cyclooctane have led to their extensive utilization across various uses in both the alchemical and organic production. In our research, we explore the constructional attributes of Cyclooctane group by examining their primary graph framework. We take into account the unsystematically group with various possibilities and proceed to calculate the mathematical expectation structural value of a particular structure specific to Cyclooctane. These descriptors are derived from a partition based on atom degrees and a more detailed partition called sum-degree partition. Furthermore, we conduct a comparative analysis encompassing various descriptors that are a part of our study. Additionally, we highlight distinctive categories of Cyclooctane chains that exhibit specific values within these descriptors.

1. Introduction

Cyclooctane belongs to the cycloalkane class and consists of an eight-membered cyclic structure with the chemical formula C_8H_{16}. These compounds are saturated hydrocarbons, meaning they contain only single bonds between carbon atoms. Cyclooctane and its derivatives have garnered significant attention within the computational chemistry community in recent decades due to their utility in various fields, including pharmaceutical synthesis, organic chemistry, and the study of combustion kinetics.

Cyclooctane presents a particularly intriguing subject for researchers because it exhibits a multitude of conformations with similar energy levels. Its conformational landscape is complex, featuring numerous energetically equivalent conformers. Additionally, the presence of hydrogen atoms introduces substantial steric effects, further adding to its complexity and interest for scientists.

In modern research, the exploration of cyclooctane's conformational space is a prominent focus for chemists, who employ a range of computational methods for this purpose [1-4]. The study of

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cyclooctane's conformational properties is notably more intricate than that of other cycloalkane due to the presence of a multitude of conformers with comparable energy levels [5].

The molecular motions involving tensional and angular changes, commonly referred to as pseudo rotation, play a crucial role in analyzing torsion angles and quantifying the symmetries inherent in Cyclooctane. Researchers have employed various methods and tools to investigate the energy landscape of Cyclooctane. These studies have revealed that the conformational space of Cyclooctane can be described as a surface rather than a manifold, shedding light on its unique structural characteristics and behavior [6]. Aranda et al. [7] have documented that, in atmospheric conditions, the oxidization procedure of Cyclooctane predominantly happen near the emission origin. This results in a finite degree of climate mass fluctuation. This discovery holds significant value for assessing the primary giver to zonal environmental impacts, like the formation of Los Angeles smog. Additionally, it contributes to our understanding of oceans air aspects and enhances our awareness of lower climate atmosphere precursors through calculation reproduction [3].

In another study by [8], the writer investigated that attaining a high degree of selectivity in the epoxidation reaction is a significant objective in chemical synthesis and catalysis. This involves adding an oxygen atom to a double bond, typically found in alkenes or olefins, and can be enhanced through the careful selection of catalysts, optimizing reaction conditions, and using appropriate reactants exhibited by Cyclooctane within its conformational space. Their findings revealed that Cyclooctane demonstrates superior oxidants.

Selectivity when compared to other cyclic resemblances furthermore under conditions of Spontaneous radical oxidation using O_2 as the oxidant. This selectivity is achieved by employing compressed CO_2 as a versatile platform for the effective and specific oxidation of anticyclones, in conjunction with O_2 and aldehyde. When compared to alternative inert dilution gases under identical conditions, this approach demonstrates superior efficiency. In ideal multiphase scenarios, it can result in the production of up to 20 percent Cyclooctane.

Therefore, cyclooctane emerges as a versatile molecule with substantial potential for industrial and environmental applications, owing to its remarkable properties that are yet to be fully realized. This study primarily aims at the cyclooctane's structural features. In our analysis, we focus on a cyclooctane chain chosen at random, denoted as O, comprising all of its individual atoms. Forming a set of vertexes, which we'll refer to as E(O). Let O_k represent a specific vertex element within V(O). The neighbors of O_k comprise vertex set elements that are directly next to O_k. The number of O_k neighbors indicates the degree of O_k inside the cyclooctane group, and we represent this as d_{ok}. Additionally, we calculate the neighborhood sum degree of O_k, denoted as S_{ok}. By calculating the total degree of connectivity among its adjacent atoms We define two sets:

Let $X_{pr^{(O)}}$={$o_k o_l \in E(O)$: $d_{o_k} =$ p and $d_{o_l} = r$}, and $y_{pr^{(O)}}$={$o_k o_l$ ∈E$(O), s_{o_k}$=p and $s_{o_l} =$ r Let ={$X_{pr^{(O)}}$:$p < r$}, and Y(O)={$y_{pr^{(O)}}$:$p < r$}. Then the following definitions are given for the degree and sum-degree types topological descriptors:

$$x^{d(O)} = \sum_{O_k O_l \in E(O)} x^{d(o_k o_l)}$$

$$= \sum_{x_{pr^{(O)}} \in E(O)} x_{pr^{(O)}} x^{d(p,r)}$$

$$x^{s(O)} = \sum_{O_k O_l \in E(O)} x^{s(o_k o_l)}$$

$$= \sum_{y_{pr^{(O)}} \in E(O)} y_{pr^{(O)}} x^{s(p,r)}$$

Where, we use $x^{d(okol)}$=$x^{d(p,r)}$ such that $d_{(ok)=p}$,$d_{(ol)=r}$ for degree topological indices and such that $x^{S(okol)}$=$x^{S(p,r)}$, $S_{(ok)=p}$,$S_{(ol)=r}$ in the topological indices for neighborhood sum-degree. The functions $x^{d(p,r)}$ and $x^{S(p,r)}$ and are symmetrical, and for our study, we consider the following types of functions.

$$M_1^d(p,r) = \mathrm{p} + \mathrm{r}$$

$$M_2^d(p,r) = \mathrm{pr}$$

$$H^{d(p,r)}=\frac{2}{p+r}$$

$$SC^{d(p,r)} = \frac{1}{\sqrt{p+r}}$$

$$SO^{d(p,r)}=\sqrt{p^2+r^2}$$

The functions defined above are also applicable when considering neighborhood-sum topological indices. These indices are a class of structural descriptors used to analyze molecular structures In the realm of degree-type structural descriptors, the Zagreb indices hold a distinctive historical significance and find common applications in investigating the structural influence on the total p-electron energy within molecules. Moreover, additional indices, notably the harmonic index, sum-connectivity index, and Sombor index, prove to be instrumental in the examination of thermodynamic characteristics inherent to chemical structures. In the realm of the degree-type structural descriptors, the Zagreb indices hold a distinctive historical significant and find common application in investigating the structural influence on the total p-electron energy. They exhibit promising predictive capabilities for properties such as "vaporization enthalpy and entropy in alkenes." [10-12].

In this study, we use a mix of degree and sum-degree considerations for the random Cyclooctane group to estimate the predicted values for these descriptors. Additionally, we furnish precise values for particular categories of chains and carry out a comparative analysis. It is important to highlight that we have corrected inaccuracies associated with the Sombor descriptor, which were found in a very recent publication (to ensure originality and accuracy) [24, 30, 31].

2. Random Cyclooctane Chains

The concept of a linear arrangement for a fixed molecular compound has been a subject of significant interest in the field of computational chemistry. In this context, we examine a random Cyclooctane chain denoted as O_t, which is formed by arranging t octagons in a linear fashion. Each consecutive pair of octagons is connected by an edge, and these connections occur between random vertices. This chain is uniquely represented for t = 1 and t = 2.

For t = 3, there are four distinct feasible Cyclooctane group that originate from O_2, as depicted in Figure 2. We suppose that these relation between octagons occur with possibility ρ_1 , ρ_2, ρ_3, and ρ_4, with the total probability summing to one. In a general sense, a Cyclooctane group O_t, can be build from O_{t-1} "By introducing a terminal octagon with a specific probability through a random process" denoted as ρ_i , where i takes values from 1 to 4. We refer to the resulting Cyclooctane chain corresponding to a probability ρ_i as $(O_t^{\rho i})$, where$1 \leq i \leq 4$.

By iteratively adding terminal octagons according to these probabilities, we can generate random Cyclooctane chains denoted as O_t^{ρ}, where $\rho = \rho_1$, ρ_2, ρ_3, and ρ_4. A Markov process of order zero, also known as a zeroth-order Markov process or a memory-less process, is a stochastic process in which the probability of transitioning from one state to another depends only on the current state and is independent of any. ρ_1 , ρ_2, ρ_3, and ρ_4, remain constant over successive steps, indicating a steady process.

Special classes of the Cyclooctane group can be distinguished by setting specific possibility values to one while setting all others to zero. Consequently, we can categorize these chains into four distinct classes based on these defined possibilities.

$\rho_{1,}\ \rho_{2,}\ \rho_{3,}\ _{and}\ \rho_4$ As shown in fig.3, and we call them asCO_t,ZO_t,,$MO_t$and lO_t. That is CO_t=$O_t^{(1,0,0,0)}$, $ZO_{t,}$=$O_t^{(0,1,0,0)}$, $MO_{t,,}$=$O_t^{(0,0,1,0)}$ and $LO_{t,}$=$O_t^{(0,0,0,1)}$In this manuscript, we have explored the topological properties of without arrangement chemical combination, and for additional details, please refer to the references [13-25].

Throughout this document, we will use the notations $E_{x^d(o_t^\rho)}$ and $E_{x^s(o_t^\rho)}$ to denote the anticipate values associated with the Cyclooctane group O_t^ρ concerning the "topological index considering degree (d) and "neighborhood sum-degree (s)" concerns for random Cyclooctane group in particular. This notation is adopted to prevent any potential confusion regarding the notation of edge sets.

3. Degree Based on Cyclooctane Description

In this section let's talk about the Zagreb harmonic sum-connectivity and the Sombor descriptors for the Cyclooctane group and investigate their precise values for specialized Cyclooctane group scenarios. Additionally, it's important to mention that a recent study [24] has pointed out issues related to the predicted values of Sombor descriptor variation brought on by recurrence relations. For instance, the anticipate value of Sombor was reported as follows in [24]: $E_{so^d}(\mathrm{O}_t^\rho)$= $[11\sqrt{2}+4\sqrt{13}+\rho(5\sqrt{2}-2\sqrt{13})t]-[\rho(5\sqrt{2}-2\sqrt{13})-16\sqrt{2}]$

This expression, although provided in [24], was found to be incorrect, as it yields inaccurate results for Sombor, especially when t=2. We aim to correct such discrepancies and ensure the accuracy of these descriptors.

To compute the topological indices for O_t, which consists of edges with degree pairs (2, 2), (2, 3), and (3, 3), an induction method is applied. This approach takes into account the terminal octagon's edge division of O_t and the degree pairs in the (t-1)-th octagon, and other modifications Calculating the degree pairs of Cyclooctane chains in this situation is made easier by using Figure 4. Theorem 1 for $t \geq 2$, let O_t^ρ berandom cyclooctane chain where $\rho = (\rho_{1,}\rho_{2,}\rho_3,\rho_4)$. Then

(a) $E_{M_1^d}\left(\mathrm{O}_t^\rho\right) = 42\mathrm{t}-10$

(b) $E_{M_2^d}(O_t^\rho)$=49t+ρ_1(t-2)-17

(c) $E_{H^d}(\mathrm{O}_t^\rho)$=$\frac{t}{30}(\rho_1+118)+\frac{1}{15}(1-\rho_1)$

(d) $E_{sc^d}(\mathrm{O}_t^\rho) = \left[2+\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}} \div \rho_1\left(\frac{1}{2}-\frac{2}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)\right]t-\rho_1\left(1-\frac{4}{\sqrt{5}}+\frac{2}{\sqrt{6}}\right)+2-\frac{4}{\sqrt{5}}-\frac{1}{\sqrt{6}}$

(e) $E_{so^d}(\mathrm{O}_t^\rho) = [11\sqrt{2}+4\sqrt{13}+\rho_1(5\sqrt{2})-2\sqrt{13})]t-2\rho_1(5\sqrt{2}-2\sqrt{13})+5\sqrt{2}-4\sqrt{13}$

Proof: Directly computation on O_2^ρ, wehave

$$E_{x^d(O_2^{\rho})} = \begin{cases} 74 & \text{if } x = M_2 \\ 81 & \text{if } x = M_2 \\ \frac{119}{15} & \text{if } x = H \\ 6 + \frac{4}{\sqrt{5}} + \frac{1}{\sqrt{6}} & \text{if } x = SC \\ 27\sqrt{2} + 4\sqrt{13} & \text{if } x = SO \end{cases}$$

Assuming that the theory true for O_{t-1}^{ρ}, we use an induction procedure to categories the edge partition of O_t^{ρ} into four distinct case for $t > 2$.

1. If $O_{t-1}^{\rho} \rightarrow O_t^{\rho_1}$, then

$$x_{22}(O_t^{\rho_1}) = x_{22}(O_{t-1}^{\rho}) + 5,\ x_{23}(O_t^{\rho_1}) = x_{23}(O_{t-1}^{\rho}) + 2,\ \text{and}\ x_{33}(O_t^{\rho_1}) = x_{33}(O_{t-1}^{\rho}) + 2,$$

2. If $O_{t-1}^{\rho} \rightarrow O_t^{\rho_2}$, then

$$x_{22}(O_t^{\rho_2}) = x_{22}(O_{t-1}^{\rho}) + 4,\ x_{23}(O_t^{\rho_2}) = x_{23}(O_{t-1}^{\rho}) + 4,\ \text{and}\ x_{33}(O_t^{\rho_2}) = x_{33}(O_{t-1}^{\rho}) + 1,$$

3. If $O_{t-1}^{\rho} \rightarrow O_t^{\rho_3}$, then

$$x_{22}(O_t^{\rho_3}) = x_{22}(O_{t-1}^{\rho}) + 4,\ x_{23}(O_t^{\rho_3}) = x_{23}(O_{t-1}^{\rho}) + 4,\ \text{and}\ x_{33}(O_t^{\rho_3}) = x_{33}(O_{t-1}^{\rho}) + 1,$$

4. If $O_{t-1}^{\rho} \rightarrow O_t^{4}$, then

$$x_{22}(O_t^{\rho_4}) = x_{22}(O_{t-1}^{\rho}) + 5,\ x_{23}(O_t^{\rho_4}) = x_{23}(O_{t-1}^{\rho}) + 2,\ \text{and}\ x_{33}(O_t^{\rho_4}) = x_{33}(O_{t-1}^{\rho}) + 2.$$

Then, we have

$M_1^d(O_t^{\rho_i}) = M_1^d(O_{t-1}^{\rho}) + 42$ If $i = 1,2,3,4$

$$M_2^d(O_t^{\rho_i}) = M_2^d(O_{t-1}^{\rho}) + \begin{cases} 50 & \text{if } i = 1 \\ 49 & \text{if } i = 2,3,4 \end{cases}$$

$$H^{d}(O_t^{\rho_i}) = H^{d}(O_{t-1}^{\rho}) + \begin{cases} \frac{119}{30} & \text{if } i = 1 \\ \frac{59}{15} & \text{if } i = 2,3,4 \end{cases}$$

$$SC^{d}(O_t^{\rho_i}) = SC^{d}(O_{t-1}^{\rho}) + \begin{cases} \frac{5}{2} + \frac{2}{\sqrt{5}} + \frac{2}{6} & \text{if } i = 1 \\ \frac{5}{2} + \frac{2}{\sqrt{5}} + \frac{2}{\sqrt{6}} & \text{if } i = 2,3,4 \end{cases}$$

$$SO^{d}(O_t^{\rho_i}) = SO^{d}(O_{t-1}^{\rho}) + \begin{cases} 16\sqrt{2} + 2\sqrt{13} & \text{if } i = 1 \\ 11\sqrt{2} + 4\sqrt{13} & \text{if } i = 2,3,4 \end{cases}$$

Hence, the expected values for x are as follows: $\in \{M_1, M_2, H, SC, SO\}$,

$E_{x^d(O_t^{\rho})} = \rho_1 x^{d(O_t^{\rho_1})} + \rho_2 x^{d(O_t^{\rho_1})} + \rho_3 x^{d(O_t^{\rho_1})} + \rho_4 x^{d(O_t^{\rho_1})}$. By substituting the above values for each index, we have $E_{x^d(O_t^{\rho})} = \rho_1 x^{d(O_{t-1}^{\rho_1})} + E_{x^d(O_t^{\rho})} = E_{x^d(O_t^{\rho})}$ and following expressions are derive

$$
\begin{cases}
42 & \text{if } x = M_1 \\
49 & \text{if } x = M_2 \\
\dfrac{59}{15} + \rho_1 & \text{if } x = H \\
2 + \dfrac{4}{\sqrt{5}} + \dfrac{1}{\sqrt{6}} + \rho_1\left(\dfrac{1}{2} - \dfrac{2}{\sqrt{5}} + \dfrac{1}{\sqrt{6}}\right) & \text{if } x = SC \\
2 + \sqrt{2} + \sqrt{13} + \rho_1\left(5\sqrt{2} - \sqrt{2} + \sqrt{13}\right) & if x = SO
\end{cases}
$$

Using and the operation E on both sides of Equation (4), $E_{x^d(O_t^\rho)=}E_{x^d(O_t^\rho)=}$, we get:

$E_{x^d(O_t^\rho)=}E_{x^d(O_{t-1}^\rho)+X}$. Here, X represents the second term on the right-hand side of Eq. (4). We may find "the predicted values of Zagreb, harmonic, sum-connectivity, and Sombor descriptors by solving this recurrence relation while taking into accoun''.

Theorem2. States that for t>2, let CO_t, ZO_t, MO_t, and LO_{t-1} be unique categories of cyclooctane group. Then,

(a) $E_{M_1^d}(CO_t)$=$E_{M_1^d}(ZO_t) = E_{M_1^d}(MO_t)$ =$E_{M_1^d}(LO_t)$=42t-10

(b) $E_{M_1^d}(CO_t)$=50t-19 $E_{M_1^d}(ZO_t)$=$E_{M_1^d}(MO_t)$=$E_{M_1^d}(LO_t)$=49t-17

(c) $E_{H^d}(CO_t)$=$\frac{119}{30}t, E_{H^d}(ZO_t) = E_{H^d}(MO_t) = E_{H^d}(LO_t) = \frac{59}{30}t + \frac{1}{15}$

(d) $E_{SC^{d(CO_t)=}}t\left[\frac{5}{2} + \frac{2}{\sqrt{5}} + \frac{2}{\sqrt{5}}\right] + 1 - \frac{3}{\sqrt{6}}, E_{SC^{d(ZO_t)=}}E_{SC^{d(MO_t)=}}E_{SC^{d(LO_t)=}}t\left[2 + \frac{4}{\sqrt{5}} + \frac{1}{\sqrt{6}}\right] + 2 - \frac{4}{\sqrt{5}} - \frac{1}{\sqrt{6}}$

(e) $E_{SO^{d(CO_t)=}}\left(16\sqrt{2} + 2\sqrt{13}\right)t - 5\sqrt{2}E_{SO^{d(ZO_t)=}}E_{SO^{d(MO_t)=}}E_{SO^{d(LO_t)=}}\left(11\sqrt{2} + 4\sqrt{13}\right)t + 5\sqrt{2} - 4\sqrt{13}$

4. Cyclooctane Neighborhood Sum-Degree Based Descriptors

As in the previous section, we calculate the neighborhood sum-degree-based Zagreb, harmonic, sum-connectivity, and Sombor descriptors for random Cyclooctane. Furthermore, for certain scenarios involving edges with neighborhood-sum pairs, such as (4,4), (4,5), (5,5), (5,7), (5,8), (6,7), (7,7), (8,8), and (8,8), we find the precise values. random Cyclooctane chain descriptions When t=3, we establish the" neighborhood-sum partition" for the analysis.

$O_3^{\rho_1}$ as $y_{44(O)_3^{\rho_1}=11,}$ $y_{45(O)_3^{\rho_1}=6,}$ $y_{57(O)_3^{\rho_1}=4,}$ $y_{58(O)_3^{\rho_1}=2,}$ $y_{78(O)_3^{\rho_1}=2,}$and $y_{88(O)_3^{\rho_1}=11,}$ for $O_3^{\rho_2}$ we have $y_{44(O)_3^{\rho_2}=11,}$ $y_{45(O)_3^{\rho_2}=6,}$ $y_{57(O)_3^{\rho_2}=4,}$ $y_{58(O)_3^{\rho_2}=2,}$ $y_{78(O)_3^{\rho_2}=2,}$ and $y_{77(O)_3^{\rho_2}=2.}$ In the same way ,for $y_{44(O)_3^{\rho_3}=9,}y_{45(O)_3^{\rho_3}=6,}y_{55(O)_3^{\rho_3}=1,}y_{57(O)_3^{\rho_3}=8,}y_{77(O)_3^{\rho_2}=2,}$ and for $O_3^{\rho_4}$ $y_{44(O)_3^{\rho_4}=9,}$ $y_{45(O)_3^{\rho_4}=2,}$ Additionally , it is necessary to establish the transformed edge partition from $O_{t-1}^{\rho_1}$ to $O_t^{\rho_1}(t > 3)$ for cases where t>3. These changes are "based on the neighborhood sum-degree" and are given as follows.

1. If $O_{t-1}^{\rho} \rightarrow O_t^{\rho_1}$, then

$y_{44}(o_t^{\rho_1})$=$x_{44}(o_{t-1}^{\rho})$+5, $y_{45}(o_t^{\rho_1})$=$y_{45}(o_{t-1}^{\rho})$+1, and $y_{57}(o_t^{\rho_1})$=$y_{57}(o_{t-1}^{\rho})$, $y_{58}(o_t^{\rho_1})$=$x_{58}(o_{t-1}^{\rho})$+2, $y_{45}(o_t^{\rho_1})$=$y_{45}(o_{t-1}^{\rho})$−1, and $y_{88}(o_t^{\rho_1})$=$y_{88}(o_{t-1}^{\rho})$+2,

2. If $O_{t-1}^{\rho} \rightarrow O_t^{\rho_2}$, then

$y_{44}(o_t^{\rho_2})$=$x_{44}(o_{t-1}^{\rho})$+2,$y_{45}(o_t^{\rho_2})$=$y_{45}(o_{t-1}^{\rho})$+2, *and*$y_{57}(o_t^{\rho_2})$=$y_{57}(o_{t-1}^{\rho})$+2,$y_{67}(o_t^{\rho_2})$=$x_{67}(o_{t-1}^{\rho})$+2 *and*$y_{77}(o_t^{\rho_2})$=$y_{77}(o_{t-1}^{\rho})$+1,

3. If $O_{t-1}^{\rho} \rightarrow O_t^{\rho_3}$, then

$y_{44}(o_t^{\rho_3})$=$x_{44}(o_{t-1}^{\rho})$+1,$y_{45}(o_t^{\rho_3})$=$y_{45}(o_{t-1}^{\rho})$+2, $and\, y_{55}(o_t^{\rho_3})$=$y_{55}(o_{t-1}^{\rho})$+1 $and\, y_{77}(o_t^{\rho_3})$=$y_{77}(o_{t-1}^{\rho})$+1,

4. If $O_{t-1}^{\rho} \to O_t^4$, then

$y_{44}(o_t^{\rho_4})$=$x_{44}(o_{t-1}^{\rho})$,$y_{45}(o_t^{\rho_4})$=$y_{45}(o_{t-1}^{\rho})$+4, $and\, y_{57}(o_t^{\rho_4})$=$y_{57}(o_{t-1}^{\rho})$+ $and\, y_{77}(o_t^{\rho_4})$=$y_{77}(o_{t-1}^{\rho})$+1,

(a) Theorem3 $t \geq 3$, letO_t^{ρ} be randomcylooctane chain where ρ =($\rho_{1,}\rho_{,2}\rho_{3,}\rho_{4)}.E_{M_1^s}(O_t^{\rho})$=14t($7-\rho_1$)+2($22\rho_1 - 17$)

(b) Proof By considering the four possible chains$O_3^{\rho_i} 1 \leq i \leq 4$ we have$M_1^s(O_3^{\rho_1}) = 262\; and M_1^s(O_3^{\rho_2}) = M_1^s(O_3^{\rho_3}) = M_1^s(O_3^{\rho_4}) = 260 M_1^s(O_3^{\rho}) = 262\rho_1 + 260\rho_2 + 260\rho_3 + 260\rho_4 = 2\rho_1 + 260. t > 3$ we found the $M_1^s(O_t^{\rho_i}) = M_1^s(O_{t-1}^{\rho_3}) + 84\; and\; M_1^s(O_t^{\rho_i}) = M_1^s(O_{t-1}^{\rho_3}) + 98\; i = 2,3,4$ therefore the expected value $E_{M_1^s}\left(0_t^{\rho}\right) = \rho_1 M_1^s(O_t^{\rho_1}) + \rho_2 M_1^s(O_t^{\rho_2}) + \rho_3 M_1^s(O_t^{\rho_3}) + \rho_4 = M_1^s(O_{t-1}^{\rho}) + 98 - 14\rho_1 . t > 3$ solving the recurrence relation we arrive that $E_{M_1^s}(O_t^{\rho})$=14t($7-\rho_1$)+2($22\rho_1 - 17$).

Theorem4. $t \geq 3$, $E_{M_2^s}(O_t^{\rho})$=($236 + 39\rho_2 + 34\rho_3 + 34\rho_4 - 42$).

We have $M_2^s(O_3^{\rho_1}) = 692\; and M_2^s(O_3^{\rho_2}) = 672, M_2^s(O_3^{\rho_3}) = 667\; and M_2^s(O_3^{\rho_4}) = 666. therefore, E_{M_2^s}(O_t^{\rho})$=$(692\rho_1 + 672\rho_2 + 667\rho_3 + 666\rho_4) = 666 + 26\rho_1 + 6\rho_{2+}\rho_3$ for $t > 3$, we obtained the following expression by utilizing the induction process.

$$M_2^s(O_t^{\rho_i}) = M_2^s(O_{t-1}^{\rho}) + \begin{cases} 236 \text{ if } i = 1 \\ 275 \text{ if } i = 2 \\ 270 \text{ if } i = 3 \\ 269 \text{ if } i = 4 \end{cases}$$

Hence $E_{M_2^s}\left(0_t^{\rho}\right) = \rho_1 M_2^s(O_t^{\rho_1}) + \rho_2 M_2^s(O_t^{\rho_2}) + \rho_3 M_2^s(O_t^{\rho_3}) + \rho_4 M_2^s(O_t^{\rho_4}) = M_2^s(O_{t-1}^{\rho}) + 236 + 39\rho_2 + 34\rho_3 + 33\rho_4$. By taking the operator E $E_{M_2^s}(O_t^{\rho}) = E_{M_2^s}(O_{t-1}^{\rho})$ we get $t > 3$. solving the reappearance relation the proof is complete.

Theorem 5. $t \geq 3$, $E_{H^s}(O_t^{\rho}) = (t-3)\left[\frac{3853}{2340}\rho_1 + \frac{2831}{1638}\rho_2 + \frac{2147}{1260}\rho_3 + \frac{107}{63}\rho_4 + \right] + \frac{8501}{1560}\rho_1 + \frac{2963}{546}\rho_2 + \frac{2269}{420}\rho_3 + \frac{340}{63}\rho_4$.

Proof. We first compute the $H^s(O_3^{\rho_1}) = \frac{8501}{1560}$, $H^s(O_3^{\rho_2}) = \frac{2963}{546}$, $H^s(O_3^{\rho_3}) = \frac{2269}{420}$, and $H^s(O_3^{\rho_4}) = \frac{340}{63}$.

Then, $E_{H^s}\left(0_3^{\rho}\right) = \frac{8501}{1560}\rho_1 + \frac{2963}{546}\rho_2 + \frac{2269}{420}\rho_3 + \frac{340}{63}\rho_4$. For $t > 3$, we apply the induction process that

$$H^s(O_t^{\rho_i}) = H^s(O_{t-1}^{\rho_1}) + \begin{cases} \dfrac{119}{30} & \text{if } i = 1 \\ \dfrac{2831}{1638} & \text{if } i = 2 \\ \dfrac{214}{1260} & \text{if } i = 3 \\ \dfrac{107}{63} & \text{if } i = 4 \end{cases}$$

Now $E\left(0_t^{\rho}\right) = \rho_{1_{H^s}}\left(0_3^{\rho}\right) + \rho_{2_{H^s}}\left(0_3^{\rho}\right) + \rho_{3_{H^s}}\left(0_3^{\rho}\right) + \rho_{4_{H^s}}\left(0_3^{\rho}\right) = H^s\left(0_{t-1}^{\;\rho}\right) + X_H$, where $X_H = \frac{3853}{2340}\rho_1 + \frac{2831}{1638}\rho_2 + \frac{2147}{1260}\rho_3 + \frac{107}{63}\rho_4$. By taking the operator E, we get $H^s(O_t^{\rho}) = H^s(O_{t-1}^{\rho}) + X_H$ and we derive solving this recurrence relation.

Proof. By direct computation, we obtained desired result.
$X_{SC} = \frac{1}{390}\left(325 + 290\sqrt{2} + 60\sqrt{13} - 26\sqrt{15}\right)\rho_1 + \frac{1}{546}\left(364 + 273\sqrt{2} + 182\sqrt{3} + 84\sqrt{13} + 39\sqrt{14}\right)\rho_2 + \frac{1}{420}(\rho_3) + \frac{1}{42}\left(56 + 28\sqrt{3} + 3\sqrt{14}\right)\rho_4$.

Theorem 6.
$t > 3, E_{H^s}(O_t^{\rho}) = (t-3)\left[\frac{3853}{2340}\rho_1 + \frac{2831}{1638}\rho_2 + \frac{2147}{1260}\rho_3 + \frac{107}{63}\rho_4 +\right] + \frac{8501}{1560}\rho_1 + \frac{2963}{546}\rho_2 + \frac{2269}{420}\rho_3 + \frac{340}{63}\rho_4$.

Proof. We first compute the $H^s\left(O_3^{\rho_1}\right) = \frac{8501}{1560}$, $H^s\left(O_3^{\rho_2}\right) = \frac{2963}{546}$, $H^s\left(O_3^{\rho_3}\right) = \frac{2269}{420}$, and $H^s\left(O_3^{\rho_4}\right) = \frac{340}{63}$.
Then, $E_{H^s}(O_t^{\rho})$=$\frac{8501}{1560}\rho_1 + \frac{2963}{546}\rho_2 + \frac{2269}{420}\rho_3 + \frac{340}{63}\rho_4$, for $t > 3$, we apply induction process that

$$H^s\left(O_t^{\rho_i}\right) = H^s\left(O_{t-1}^{\rho}\right) + \begin{cases} \dfrac{3853}{2340} \text{ if } i = 1 \\ \dfrac{2831}{1638} \text{ if } i = 2 \\ \dfrac{2147}{1260} \text{ if } i = 3 \\ \dfrac{107}{63} \text{ if } i = 4 \end{cases}$$

$E_{H^s}(O_t^{\rho})$=$\rho_1 H^s\left(O_t^{\rho_1}\right)$+$\rho_2 H^s\left(O_t^{\rho_2}\right) + \rho_3 H^s\left(O_t^{\rho_3}\right) + \rho_4 H^s\left(O_t^{\rho_4}\right) = H^s\left(O_{t-1}^{\rho_1}\right) + X_H$, where,

$$X_H = \frac{3853}{2340}\rho_1 + \frac{2831}{1638}\rho_2 + \frac{2147}{1260}\rho_3 + \frac{107}{63}\rho_4.$$

By taking the operator E, we get $E_{H^s}(O_t^{\rho})$=$E_{H^s}(O_{t-1}^{\rho})$+X_H and by resolving this recurrence relation, we arrive to the outcome.

Theorem 7. For $t > 3$, $E_{SC^s}\left(\mathrm{O}_t^{\rho}\right) = (t-1)\left[\frac{1}{390}\left(325 + 390\sqrt{2} + 60\sqrt{13} - 26\sqrt{15}\right)\rho_1 + \frac{1}{546}\left(364 + 273\sqrt{2} + 182\sqrt{3} + 84\sqrt{13} + 39\sqrt{14}\right)\rho_2 + \frac{1}{420}\left(280 + 105\sqrt{2} + 280\sqrt{3} + 42\sqrt{10} + 30\sqrt{14}\right)\rho_3 + \frac{1}{42}\left(56 + 28\sqrt{3} + 3\sqrt{14}\right)\rho_4\right] + \frac{1}{182}\left(\frac{1}{156}\left(351 + 429\sqrt{2} + 104\sqrt{3} + 24\sqrt{13} + 52\sqrt{15}\right)\rho_1 + 364 + 455\sqrt{2} + 182\sqrt{3} + 28\sqrt{13} + 26\sqrt{14}\right)\rho_2 + \frac{1}{156}\left(351 + 429\sqrt{2} + 104\sqrt{3} + 24\sqrt{13} + 52\sqrt{15}\right)$.

Then, $E_{SC^s}(\mathrm{O}_3^{\rho}) = \frac{1}{156}\left(351 + 429\sqrt{2} + 104\sqrt{3} + 24\sqrt{13} + 52\sqrt{15}\right)\rho_1 + \frac{1}{182}\left(364 + 455\sqrt{2} + 182\sqrt{3} + 28\sqrt{13} + 26\sqrt{14}\right)\rho_2 + \frac{1}{420}\left(840 + 945\sqrt{2} + 560\sqrt{3} + 42\sqrt{10} + 60\sqrt{14}\right)\rho_3 + \frac{1}{21}\left(56 + 42\sqrt{2} + 28\sqrt{3} + 3\sqrt{14}\right)\rho_{4.}$

Proof. By direction computation, we have

$$SC^{s\left(O_t^{\rho_i}\right)} = \begin{cases} \dfrac{1}{156}\left(351 + 429\sqrt{2} + 104\sqrt{3} + 24\sqrt{13} + 52\sqrt{15}\right) \text{ if } i = 1 \\ \dfrac{1}{182}\left(364 + 455\sqrt{2} + 182\sqrt{3} + 28\sqrt{13} + 26\sqrt{14}\right) \text{ if } i = 2 \\ \dfrac{1}{420}\left(840 + 945\sqrt{2} + 560\sqrt{3} + 42\sqrt{10} + 60\sqrt{14}\right) \text{ if } i = 3 \\ \dfrac{1}{21}\left(56 + 42\sqrt{2} + 28\sqrt{3} + 3\sqrt{14}\right) \qquad \text{ if } i = 4 \end{cases}$$

Then, $E_{SC^s}(O_3^{\rho}) = \frac{1}{156}\left(351 + 429\sqrt{2} + 104\sqrt{3} + 24\sqrt{13} + 52\sqrt{15}\right)\rho_1 + \frac{1}{182}\left(364 + 455\sqrt{2} + 182\sqrt{3} + 28\sqrt{13} + 26\sqrt{14}\right)\rho_2 + \frac{1}{420}\left(840 + 945\sqrt{2} + 560\sqrt{3} + 42\sqrt{10} + 60\sqrt{14}\right)\rho_3 + \frac{1}{21}\left(56 + 42\sqrt{2} + 28\sqrt{3} + 3\sqrt{14}\right)\rho_4$. For $t > 3$, by utilizing the induction process

$$SC^{s\left(O_t^{\rho_i}\right)} = \mathrm{SC}^{s\left(O_{t-1}^{\rho}\right)} + \begin{cases} \frac{1}{290}\left(325 + 390\sqrt{2} + 60\sqrt{13} - 26\sqrt{15}\right) & \text{if } i = 1 \\ \frac{1}{546}\left(364 + 273\sqrt{2} + 182\sqrt{3} + 84\sqrt{13} + 39\sqrt{14}\right) & \text{if } i = 2 \\ \frac{1}{420}\left(280 + 105\sqrt{2} + 280\sqrt{3} + 42\sqrt{10} + 30\right) & \text{if } i = 3 \\ \frac{1}{42}\left(56 + 28\sqrt{3} + 3\sqrt{14}\right) & \text{if } i = 4 \end{cases}$$

Therefore, $E_{SC^s}(O_t^{\rho}) = \rho_1 E_{SC^s}(O_t^{\rho_1}) + \rho_2 E_{SC^s}(O_t^{\rho_2}) + \rho_3 E_{SC^s}(O_t^{\rho_3}) + \rho_4 E_{SC^s}(O_t^{\rho_4}) = SC^s(O_t^{\rho_4}) + X_{sc}$, where, $X_{sc} = \frac{1}{390}\left(325 + 390\sqrt{2} + 60\sqrt{13} - 26\sqrt{15}\right)\rho_1 + \frac{1}{546}\left(364 + 273\sqrt{2} + 182\sqrt{3} + 84\sqrt{13} + 39\sqrt{14}\right)\rho_2 + \frac{1}{420}\left(280 + 105\sqrt{2} + 280\sqrt{3} + 42\sqrt{10} + 30\sqrt{14}\right)\rho_3 + \frac{1}{42}\left(56 + 28\sqrt{3} + 5\sqrt{14}\right)\rho_4$. By taking the operator E, we get $E_{SC^s}(O_t^{\rho}) = E_{SC^s}(O_{t-1}^{\rho}) + X_{sc}$, and by solving the preceding recurrence relation, we obtain the expected value of the sum-connectivity index.

Theorem 7. For $t \geq 3$

$E_{SO^s}(O_t^{\rho}) = (t-1)\left[\left(32\sqrt{2} + \sqrt{41} + 2\sqrt{89} - \sqrt{113}\right)\rho_1 + \left(15\sqrt{2} + 2\sqrt{41} + 2\sqrt{74} + 2\sqrt{85}\right)\rho_2 + \left(16\sqrt{2} + 2\sqrt{41} + 4\sqrt{74}\right)\rho_3 + \left(7\sqrt{2} + 4\sqrt{41} + 4\sqrt{74}\right)\rho_4\right] + 2\left(26\sqrt{2} + 3\sqrt{41} + 2\sqrt{74} + \sqrt{89}\right)\rho_1 + 2\left(27\sqrt{2} + 3\sqrt{41} + 3\sqrt{74} + \sqrt{85}\right)\rho_2 + \left(55\sqrt{2} + 6\sqrt{41} + 8\sqrt{74}\right)\rho_3 + \left(46\sqrt{2} + 8\sqrt{41} + 8\sqrt{74}\right)\rho_4$.

Proof. Using the edge partition of $O_3^{\rho_i}$, we find $SC^s(O_3^{\rho_i}) =$

$$\begin{cases} 2\left(26\sqrt{2} + 3\sqrt{41} + 2\sqrt{74} + \sqrt{89} + \sqrt{113}\right) & \text{if } i = 1 \\ 2\left(27\sqrt{2} + 3\sqrt{41} + 3\sqrt{74} + \sqrt{85}\right) & \text{if } i = 2 \\ 55\left(\sqrt{2} + 6\sqrt{41} + 8\sqrt{74}\right) & \text{if } i = 3 \\ \left(46\sqrt{2} + 8\sqrt{41} + 8\sqrt{74}\right) & \text{if } i = 4 \end{cases}$$

Then, $E_{SC^s}(O_3^{\rho}) = 2\left(26 + 3\sqrt{41} + 2\sqrt{3} + \sqrt{89} + \sqrt{113}\right)\rho_1 + 2\left(27 + 3\sqrt{41} + 3\sqrt{74} + \sqrt{85}\right)\rho_2 + \left(55\sqrt{2} + 6\sqrt{41} + 8\sqrt{74}\right)\rho_3 + \left(46\sqrt{2} + 8\sqrt{41} + 8\sqrt{74}\right)\rho_{4.}$ For $t > 3$, we use the induction process to find desired expression,

$$SO^{s\left(O_t^{\rho_i}\right)} = \mathrm{SO}^{s\left(O_{t-1}^{\rho}\right)} + \begin{cases} \left(32\sqrt{2} + \sqrt{41} + 2\sqrt{89} - \sqrt{113}\right) & if\ i = 1 \\ \left(15\sqrt{2} + 2\sqrt{3} + 2\sqrt{74} + 2\sqrt{85}\right) & if\ i = 2 \\ \left(16\sqrt{2} + 2\sqrt{41} + 4\sqrt{74}\right) & if\ i = 3 \\ \left(7\sqrt{2} + 4\sqrt{41} + 4\sqrt{74}\right) & if\ i = 4 \end{cases}$$

Thus $E_{SO^s}(O_t^{\rho}) = \rho_1 E_{SO^s}(O_t^{\rho_1}) + \rho_2 E_{SO^s}(O_t^{\rho_2}) + \rho_3 E_{SO^s}(O_t^{\rho_3}) + \rho_4 E_{SO^s}(O_t^{\rho_4}) = SO^s(O_t^{\rho_4}) + X_{so}$ where $X_{so} = \left(32\sqrt{2} + \sqrt{41} + 2\sqrt{89} - \sqrt{113}\right)\rho_1 + \left(15\sqrt{2} + 2\sqrt{41} + 2\sqrt{74} + 2\sqrt{85}\right)\rho_2 + \left(16\sqrt{2} + 2\sqrt{41} + 4\sqrt{74}\right)\rho_3 + \left(7\sqrt{2} + 4\sqrt{41} + 4\sqrt{74}\right)\rho_{4.}$.By taking the operator E, we get

$E_{SO^s}(O_t^{\rho})=E_{SO^s}(O_{t-1}^{\rho})+X_{SO}$, and We determine Sombor predicted value. We get the anticipated value for the special classes of Cyclooctane chains as a consequence of Theorem 3-7.

Theorem 8 For $t \geq 3$

(a) $E_{M_1^s}(CO_t)$=84t+10, $E_{M_1^s}(ZO_t)E_{M_1^s}(MO_t)$=$E_{M_1^s}(LO_t)$=98t-34

(b) $E_{M_1^s}(CO_t)$=236t-16,$E_{M_1^s}(ZO_t)$= $275t-153$, $E_{M_2^s}(MO_t)$=$270t-143$, $E_{M_1^s}(LO_t)$=269t-141

(c) $E_{H^s}(CO_t)=\frac{3853}{2340}t+\frac{53}{104}, E_{H^s}(ZO_t)=\frac{2831}{1638}t+\frac{22}{9}, E_{H^s}(MO_t)=\frac{2147}{1260}t+\frac{61}{210}, (LO_t)=\frac{107}{63}t+\frac{19}{63}$,

(d) $E_{SC^s(CO_t)}=\frac{1}{390}\left(325+390\sqrt{2}+60\sqrt{13}-26\sqrt{15}\right)(t-1)+\frac{1}{156}\left(351+429\sqrt{2}+104\sqrt{3}+24\sqrt{13}+52\sqrt{15}\right), E_{SC^s(ZO_t)}=\frac{1}{546}\left(364+273\sqrt{2}+182\sqrt{3}+84\sqrt{13}+39\sqrt{14}\right)(t-3)+\frac{1}{182}\left(364+455\sqrt{2}+182\sqrt{3}+28\sqrt{13}+26\sqrt{14}\right)$ $E_{SC^s(MO_t)}=\frac{1}{420}\left(280+105\sqrt{2}+280\sqrt{3}+42\sqrt{10}+30\sqrt{14}\right)(t-3)+\frac{1}{420}\left(840+945\sqrt{2}+560\sqrt{3}+42\sqrt{10}+60\sqrt{14}\right)E_{SC^s(LO_t)}=\frac{1}{42}\left(56+28\sqrt{3}+3\sqrt{14}\right)(t-1)+\frac{1}{21}\left(56+42\sqrt{2}+28\sqrt{3}+3\sqrt{14}\right)$

(e) $E_{SO^s(CO_t)}=\left(32\sqrt{2}+\sqrt{41}+2\sqrt{89}-\sqrt{113}\right)(t-3)+2\left(26\sqrt{2}+3\sqrt{41}+2\sqrt{74}+\sqrt{89}+\sqrt{113}\right), E_{SO^s(ZO_t)}=\left(15\sqrt{2}+2\sqrt{41}+2\sqrt{74}+2\sqrt{85}\right)(t-3)+2\left(27\sqrt{2}+3\sqrt{41}+3\sqrt{74}+2\sqrt{85}\right)E_{SO^s(MO_t)}=\left(16\sqrt{2}+2\sqrt{41}+4\sqrt{74}\right)(t-3)+\left(55\sqrt{2}+6\sqrt{41}+8\sqrt{74}\right), E_{SO^s(LO_t)}=\left(7\sqrt{2}+4\sqrt{41}+2\sqrt{74}\right)(t-3)+\left(46\sqrt{2}+8\sqrt{41}+8\sqrt{74}\right)$

5 Comparative Analysis

A given Cyclooctane chain's harmonic, sum-connectivity, and Sombor indices. The findings of this comparison, which include both degree and sum-degree kinds, are shown in Tables 1 and 2. The numerical data clearly show an ascending sequence in the predicted values of the harmonic, sum-connectivity, Sombor, first, and second Zagreb indices. To present these findings visually, we have included a graphical representation in Figure 5.

Furthermore, as we have experiential that the anticipated standards of Cyclooctane chains under degree-type terminology only depend on ρ_1, we now provide a theoretical comparison for the range $0 \leq \rho_1 \leq 1$

Theorem 9. For $t \geq 3, E_{H^d(O_t)} < E_{SC^d(O_t)} < E_{SO^d(O_t)} < E_{M_1^d(O_t)} < E_{M_2^d(O_t)}$

Proof. We will demonstrate the proof for the first and last inequalities, with the others following in a similar manner. Consider,

$E_{SC^d(O_t)} - E_{H^d(O_t)}$

$$= (t-1)\left[2+\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}+\rho_1\left(\frac{1}{2}-\frac{2}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)\right]+\left(6+\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)-(t-1)\left(\frac{59}{15}+\frac{\rho_1}{30}\right)-\frac{119}{15}$$

$$= (t-1)\left[2+\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}+\rho_1\left(\frac{1}{2}-\frac{2}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)-\frac{59}{15}-\frac{\rho_1}{30}\right]+\left(6s+\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)-\frac{119}{15}$$

$$= (t-1)\left[2+\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}+\rho_1\left(\frac{1}{2}-\frac{2}{\sqrt{5}}+\frac{1}{\sqrt{6}}-\frac{\rho_1}{30}\right)-\frac{59}{15}\right]+\left(6+\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)-\frac{119}{15} >$$

Now consider $E_{M_2^d(O_t)} - E_{M_1^d(O_t)} = 49t + \rho_1(t-2) - 17 - (42t - 10) = 7(t-1) + \rho_1(t-2) > 0$

A result analogous to For the situation of sum-degree-based topological descriptors, Theorem 9 may be proven.

6. Conclusion

In our research, we have conducted a comprehensive investigation into the growth patterns of Cyclooctane group within a probabilistic framework. We have derived the expected values for several topological descriptors in addition to "Zagreb, sum-connectivity, harmonic, and Sombor indices. According to our findings, the harmonic index regularly records the lowest values, while the second Zagreb descriptor consistently displays the greatest values when compared to the other descriptors. Additionally, we investigated a specific program of the Cyclooctane group and calculated the corresponding predicted values. By establishing quantifiable structural correlations, the results of this study offer great potential for improving our capacity to predict the physiochemical properties of Cyclooctane chains.

Conflicts of Interest

The authors declare no conflicts of interest.

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