[Baghdad Science Journal](https://bsj.uobaghdad.edu.iq/home)

Volume 23 | Issue 5 Article 25

5-29-2026

Some Types of Zagreb Indices for General Caterpillar Graph and Their Application in Property Predictions of Molecules

Muayed Mehedi Fathi
Nineveh- Gifted School Directorate of Education in Nineveh, Mosul, Iraq, muoaed1984@gmail.com

Mohammad Shaker Ahmed
Nineveh- Gifted School Directorate of Education in Nineveh, Mosul, Iraq, mohammed.shaker.msa@gmail.com

Muhammad Kamran Jamil
Department of Mathematics, Modern College, Riphah International University, Lahore, Pakistan, m.kamran.sms@gmail.com

Ahmed Mohammed Ali
Department of Mathematics, College of Computer Science and Mathematics, University of Mosul, Mosul, Iraq, ahmedgraph@uomosul.edu.iq

How to Cite this Article

Fathi, Muayed Mehedi; Ahmed, Mohammad Shaker; Jamil, Muhammad Kamran; and Ali, Ahmed Mohammed (2026) "Some Types of Zagreb Indices for General Caterpillar Graph and Their Application in Property Predictions of Molecules," *Baghdad Science Journal*: Vol. 23: Iss. 5, Article 25.
DOI: https://doi.org/10.21123/2411-7986.5309

BAGHDAD SCIENCE JOURNAL 2026;23(5):1895–1912

Scan the QR to view the full-text article on the journal website

RESEARCH ARTICLE

Some Types of Zagreb Indices for General Caterpillar Graph and Their Application in Property Predictions of Molecules

Muayed Mehedi Fathi [1], Mohammad Shaker Ahmed [1], Muhammad Kamran Jamil [2], Ahmed Mohammed Ali [3,*]

[1] Nineveh- Gifted School Directorate of Education in Nineveh, Mosul, Iraq
[2] Department of Mathematics, Modern College, Riphah International University, Lahore, Pakistan
[3] Department of Mathematics, College of Computer Science and Mathematics, University of Mosul, Mosul, Iraq

ABSTRACT

Topological indices in graph theory are considered a very important topic because of its practical importance in some branches of sciences, especially in chemistry, physics and networks, because they are closely related to chemical properties and physical properties, including boiling point, melting point, vapor pressure, molar volume etc. There are several types of topological indices, the most important of which are the indices that depend on the degrees of vertices, especially adjacent or non-adjacent vertices. The Zagreb indices for adjacent vertices and non-adjacent vertices, multiplicative and eccentricity for adjacent vertices in a connected simple graph are considered topological indices that have an impact on knowing many chemical and physical properties. In this paper, we discussed the Zagreb type topological indices of generalized caterpillar graphs, as well as for the molecules alkanes with formula $C_pH_{(2p+2)}$, which is a special case of the statement caterpillar graph and studied some of its properties. In the application section, we presented that the first and second Zagreb coindices (corresponding indices) give high correlation among other Zagreb indices when predicting entropy and ascent factor of alkanes.

Keywords: Caterpillar graph, Chemical compounds, Eccentricity Zagreb indices, Multiplicative Zagreb indices, Zagreb indices and coindices

Introduction

Let G be a finite connected simple graph with vertex set $V = V(G)$ and edge set $E = E(G)$. The cardinality of the vertex set (order) and the edge set (size) are $|V(G)| = p$ and $|E(G)| = q$ respectively. The degree of a vertex v in a graph G is the number of edges incident on v, and is denoted by $deg_G(v)$ or simply $deg(v)$. If a vertex has degree one, then it is called an end vertex, or a pendant of G.[1] The distance between any two distinct vertices u and v, $d(u, v)$ in a connected graph G is the cardinality of edges in a shortest path connecting them. Let v be any vertex in a set of vertices in a connected graph G, the eccentricity of a vertex v, $e(v)$ is the maximum distance between a vertex v to all other vertices in G. Almost 50 years ago, two types of topological indices were found, which are symbolized by M_1 and M_2 and named the first Zagreb index and the second Zagreb index.[2,3] The first Zagreb index was defined in 1972, by Gutman and Trinajstić,[2] while the second Zagreb index was found in 1975, by Randić,[3] where each obtained a formula related to the total energy of electrons and molecules, where the first and second Zagreb indices can be considered to be topological indices based on the degrees of adjacent vertices, as the emergence of these two indices followed the emergence of the Wiener

Received 13 May 2025; revised 26 December 2025; accepted 6 January 2026.
Available online 29 May 2026

* Corresponding author.
E-mail addresses: muoaed1984@gmail.com (M. M. Fathi), mohammed.shaker.msa@gmail.com (M. S. Ahmed), m.kamran.sms@gmail.com (M. K. Jamil), ahmedgraph@uomosul.edu.iq (A. M. Ali).

https://doi.org/10.21123/2411-7986.5309

index,[4] and the Hosoya. $z-$index.[5] Researchers investigated two Zagreb indices for many families of graphs, as well as for graphs that resulted from knowledge operations on the graphs and other indices.[6,7] The species were also used as indices of Zagreb in some chemical structures to determine some of their properties.[8–10] But in 2008, Došlic presented two indices, the first and second Zagreb coindices, since these two topological indices depend on the degrees of non-adjacent vertices.[11] The first and second multiplicative Zagreb indices are presented by Todeschini and others.[12] There are other topological indices that do not depend only on degrees, but rather depend on the distances between two vertices in simply connected graphs, Schultz and Modified Schultz indices.[13] Azari is introducing some other kinds of Zagreb indices for a connected graph G which is called the eccentricity indices.[14]

Topological indices, particularly degree-based ones such as Zagreb indices, are widely used to correlate molecular structure with physicochemical properties, and many studies have demonstrated their effectiveness in *QSPR* analysis. However, the literature still lacks general formulas for Zagreb-type indices of generalized caterpillar graphs and their special case representing alkane molecules, cap C sub p, cap H sub, 2 p plus 2 end subscripts. Moreover, the predictive ability of nonadjacent vertex Zagreb coindices, especially for thermodynamic properties such as entropy and ascent factor, has not been adequately explored. To address these gaps (that is, our aim in this study), this study derives general expressions for several Zagreb indices and coindices for generalized caterpillar graphs and applies them to alkanes. A systematic statistical analysis is then performed to evaluate which indices offer the strongest predictive performance. The novelty of the work lies in demonstrating that the first and second Zagreb coindices provide the lowest prediction errors for entropy and ascent factor, and in presenting general formulas that enable the prediction of the properties of new alkane compounds.

Here are some types of topological indices that will be studied in this article.

Definition 1: The first and second Zagreb indices are defined as follows:

$$M_1(G) = \sum_{vu \in E} \left(deg_G(v) + deg_G(u)\right),$$
$$M_2(G) = \sum_{vu \in E} \left(deg_G(v) \times deg_G(u)\right),$$

where $deg_G(u)$ and $deg_G(v)$ represent the degrees of the adjacent vertices u and v, of a graph G.

Definition 2: The first and second Zagreb coindices are defined as follows:

$$M_1^c(G) = \sum_{vu \notin E} \left(deg_G(v) + deg_G(u)\right),$$
$$M_2^c(G) = \sum_{vu \notin E} \left(deg_G(v) \times deg_G(u)\right),$$

where $deg_G(u)$ and $deg_G(v)$ are represent the degrees of the nonadjacent vertices u and v of a graph G.

Definition 3: The first and second multiplicative Zagreb indices are defined as follows:

$$M_1^m(G) = \prod_{vu \in E} \left(deg_G(v) + deg_G(u)\right),$$
$$M_2^m(G) = \prod_{vu \in E} \left(deg_G(v) \times deg_G(u)\right).$$

Definition 4: The first and second eccentricity Zagreb indices are defined as follows:

$$Ecc_1(G) = \sum_{vu \in E} \left(e(v) + e(u)\right),$$
$$Ecc_2(G) = \sum_{vu \in E} \left(e(v) \times e(u)\right).$$

Definition 5: A general caterpillar graph $GCG(p, \prod_{i=1}^{p} a_i)$ is a tree obtained from a $(v_1 - v_p)-$ path P_p : $v_1, v_2, \ldots, v_p,\ p \geq 3$ by attaching $a_i,\ a_i \geq 1$, for all $i = 1, 2, \ldots, p$, end vertices to each vertex in P_p, as shown in Fig. 1. For simplicity, the general caterpillar graph will be indicated $GCG(p, \prod_{i=1}^{p} a_i)$ with a symbol $\mathcal{H}$.[15]

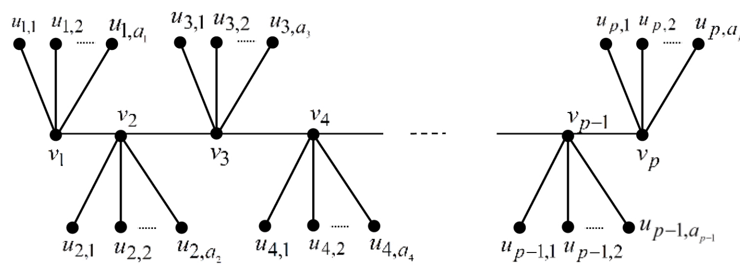


Fig. 1. General Caterpillar Graph $GCG(p, \prod_{i=1}^{p} a_i)$.

Some Properties of General Caterpillar Graph $\mathcal{H} = GCG(p, \prod_{i=1}^{p} a_i)$

1. The vertex set $V(\mathcal{H}) = V(P_p) \cup \{u_{i,j} : 1 \leq j \leq a_i\ for\ all\ i = 1, 2, \ldots, p\}$.
2. The edge set $E(\mathcal{H}) = \{v_i v_{i+1} : i = 1, 2, \ldots, p-1\} \cup \{v_i u_{i,j} : 1 \leq j \leq a_i\ for\ all\ i = 1, 2, \ldots, p\}$.
3. The order and size: $|V(\mathcal{H})| = p + \sum_{i=1}^{p} a_i$ and $|E(\mathcal{H})| = p + \sum_{i=1}^{p} a_i - 1$.
4. The degrees of the vertices in a general caterpillar graph $\mathcal{H}$ are

$$deg_{\mathcal{H}} v_i = a_i + 1,\ i = 1, p.$$

$$deg_{\mathcal{H}} v_i = a_i + 2,\ i = 2, 3, \ldots, p-1.$$

$$deg_{\mathcal{H}} u_{i,j} = 1,\ 1 \leq j \leq a_i \text{ for all } i = 1, 2, \ldots, p.$$

5. From Fig. 1, $e(u_{i,j}) = e(v_i) + 1,\ j = 1, 2, \ldots, a_i$ for all $i = 1, 2, \ldots, p$, such that $e(v_i) = e(v_{p+1-i}) = p + 1 - i$, for all $i = 1, 2, \ldots, \lceil \frac{p}{2} \rceil$.

If $a_i = 2$ for all $i = 2, 3, \ldots, p-1$, and $a_i = 0,\ i = 1, p$, molecules known as alkanes with the chemical formula C_pH_{2p+2}, are obtained, see Fig. 2.

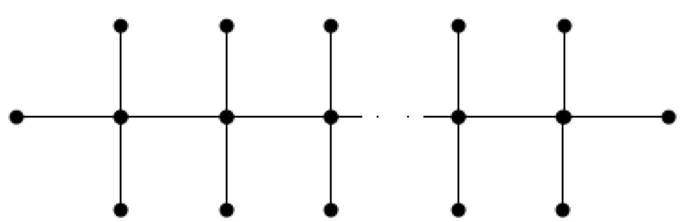


Fig. 2. Alkanes formula C_pH_{2p+2}.

The study was designed to investigate the relationship between selected types of Zagreb indices and the physicochemical properties of a defined set of alkane chemical compounds. $C_pH_{2p+2},\ p \in Z^+$. The dataset was first compiled from reliable literature references, ensuring that all compounds met the inclusion criteria regarding structural clarity and data completeness. The Zagreb indices were used to characterize the molecular structures of compounds by modeling and analyzing these indices using integrative correlation to illustrate the strength of their relationships and to study their physical properties in addition to their chemical properties. These indices were then compared to determine which provided the highest accuracy based on their studied characteristics using statistical functions, such as coefficients of determination and error measures. All analyses were performed using well-established computer and statistical software to ensure methodological accuracy. The overall design provides a methodological framework for assessing the effectiveness of topological indices in predicting the physical and chemical behavior of a set of alkane chemical compounds.

Results and discussion

In this section, the main results are also presented with some important corollaries. In the next theorems, the general formula for the Zagreb indices for a general caterpillar graph is given. $\mathcal{H} = GCG(p, \prod_{i=1}^{p} a_i)$ is obtained.

Theorem 1: *For all $p \geq 3$ and $a_i \geq 1$, $i = 1, 2, \ldots, p$, then:*

1. $M_1(\mathcal{H}) = 4p - 6 - 2(a_1 + a_p) + \sum_{i=1}^{p} a_i(a_i + 5)$.
2. $M_2(\mathcal{H}) = 4p - 3(a_1 + a_p) - (a_2 + a_{p-1}) - 8 + \sum_{i=1}^{p-1} a_i a_{i+1} + \sum_{i=1}^{p} a_i(a_i + 6)$.

Proof: From Definition 1, then:

1. $$M_1(\mathcal{H}) = \sum_{i=1}^{p-1}(degv_i + degv_{i+1}) + \sum_{i=1}^{p}\sum_{j=1}^{a_i}(degv_i + degu_{i,j})$$
$$= (a_1 + 1 + a_2 + 2) + \sum_{i=2}^{p-2}(a_i + a_{i+1} + 4) + \left(a_{p-1} + 2 + a_p + 1\right)$$
$$+ \sum_{j=1}^{a_1}(a_1 + 1 + 1) + \sum_{i=2}^{p-1}\sum_{j=1}^{a_i}(a_i + 2 + 1) + \sum_{j=1}^{a_p}(a_p + 1 + 1)$$
$$= 3 + \sum_{i=1}^{p-1}(a_i + a_{i+1}) + 4\sum_{i=2}^{p-2} 1 + 3 - \sum_{j=1}^{a_1} 1 - \sum_{j=1}^{a_p} 1 + \sum_{i=1}^{p}\sum_{j=1}^{a_i}(a_i + 3)$$
$$= 4p - 6 - 2\left(a_1 + a_p\right) + \sum_{i=1}^{p} a_i\left(a_i + 5\right).$$

2. $$M_2(\mathcal{H}) = \sum_{i=1}^{p-1}(degv_i \times degv_{i+1}) + \sum_{i=1}^{p}\sum_{j=1}^{a_i}(degv_i \times degu_{i,j})$$
$$= (a_1 + 1)(a_2 + 2) + \sum_{i=2}^{p-2}(a_i + 2)(a_{i+1} + 2) + \left(a_{p-1} + 2\right)(a_p + 1)$$
$$+ \sum_{j=1}^{a_1}(a_1 + 1) + \sum_{i=2}^{p-1}\sum_{j=1}^{a_i}(a_i + 2) + \sum_{j=1}^{a_p}(a_p + 1)$$
$$= 4p - 3\left(a_1 + a_p\right) - \left(a_2 + a_{p-1}\right) - 8 + \sum_{i=1}^{p-1} a_i a_{i+1} + \sum_{i=1}^{p} a_i\left(a_i + 6\right). \qquad \blacksquare$$

Corollary 1: *For all $p \geq 3$ and $a_i = a > 0$, $i = 1, 2, \ldots, p$, then:*

1. $M_1(\mathcal{H}) = p(a + 1)(a + 4) - 2(3 + 2a)$.
2. $M_2(\mathcal{H}) = 2p(a + 1)(a + 2) - (a^2 + 8a + 8)$.

Proof: From Theorem 1, then:

1. $M_1(\mathcal{H}) = 4p - 6 - 2(a + a) + \sum_{i=1}^{p} a(a + 5)$
$$= p\,(a + 1)\,(a + 4) - 2\,(3 + 2a).$$

2. $M_2(\mathcal{H}) = 4(p - 2a - 2) + \sum_{i=1}^{p-1} a^2 + \sum_{i=1}^{p} a(a + 6)$
$$= 2p\,(a + 1)\,(a + 2) - \left(a^2 + 8a + 8\right). \qquad \blacksquare$$

Theorem 2: *For all $p \geq 5$ and $a_i \geq 1$, $i = 1, 2, \ldots, p$, then:*

1. $$M_1^c(\mathcal{H}) = 2(p^2 - 4p + 4 + a_1 + a_p) + (4p + a_1 + a_p - 9)\sum_{j=1}^{p} a_j + \sum_{i=2}^{p-1}\sum_{j=1}^{p} a_j a_i + 2\sum_{i=1}^{p-1}\sum_{r=i+1}^{p} a_r a_i \,.$$

2. $$M_2^c(\mathcal{H}) = 2p^2 + 2p(2a_1 - 5) + 13 - 2(a_1^2 + a_p^2) - a_1(6 + a_2 + 2a_p) - a_2 - a_{p-1} - a_p\left(6 + a_{p-1}\right) + 2\left(a_1 + a_p - 1\right)\sum_{j=1}^{p} a_j \ + 2\sum_{i=2}^{p-3}\sum_{j=i+2}^{p-1}(a_i + a_j + a_i a_j) - \frac{1}{2}\sum_{i=1}^{p} a_i(a_i + 1) + \sum_{i=1}^{p}\sum_{j=1}^{p} a_j(a_i + 2) + \sum_{i=2}^{p-2} a_{i+1} a_i.$$

Proof: From Definition 1, then:

1. $$\begin{aligned} M_1^c(\mathcal{H}) &= \sum_{i=1}^{p-2}\sum_{j=i+2}^{p}(degv_i + degv_j) + \sum_{i=1}^{p}\sum\nolimits_{j=1}^{p}\sum_{r=1}^{a_j}(degv_i + degu_{j,r}) \\ &\quad - \sum_{i=1}^{p}\sum_{j=1}^{a_i}(degv_i + degu_{i,j}) \ + \sum_{i=1}^{p}\sum_{j=1}^{a_i-1}\sum_{r=j+1}^{a_i}(degu_{i,j} + degu_{i,r}) \\ &\quad + \sum_{i=1}^{p-1}\sum_{j=1}^{a_i}\sum_{r=i+1}^{p}\sum_{h=1}^{a_r}(degu_{i,j} + degu_{r,h}) \\ &= \sum_{j=3}^{p}(degv_1 + degv_j) + \sum_{i=2}^{p-3}\sum_{j=i+2}^{p-1}(degv_i + degv_j) \\ &\quad + \sum_{i=2}^{p-2}\left(degv_i + degv_p\right) + \sum_{j=1}^{p}\sum_{r=1}^{a_j}(degv_1 + degu_{j,r}) \\ &\quad + \sum_{i=2}^{p-1}\sum_{j=1}^{p}\sum_{r=1}^{a_j}(degv_i + degu_{j,r}) \ + \sum_{j=1}^{p}\sum_{r=1}^{a_j}(degv_p + degu_{j,r}) \\ &\quad - \sum_{j=1}^{a_1}(degv_1 + degu_{1,j}) - \sum_{i=2}^{p-1}\sum_{j=1}^{a_i}(degv_i + degu_{i,j}) \\ &\quad - \sum_{j=1}^{a_p}(degv_p + degu_{p,j}) + \sum_{i=1}^{p}\sum_{j=1}^{a_i-1}\sum_{r=j+1}^{a_i}(degu_{i,j} + degu_{i,r}) \\ &\quad + \sum_{i=1}^{p-1}\sum_{j=1}^{a_i}\sum_{r=i+1}^{p}\sum_{h=1}^{a_r}(degu_{i,j} + degu_{r,h}) \\ &= (a_1 + 3)(p - 3) + \sum_{j=3}^{p-1} a_j + \left(a_1 + a_p + 2\right) + 4\sum_{i=2}^{p-3}(p - i - 2) \\ &\quad + \sum_{i=2}^{p-3}\sum_{j=i+2}^{p-1}(a_i + a_j) + \left(a_p + 3\right)(p - 3) + \sum_{i=2}^{p-2} a_i \\ &\quad + (a_1 + 2)\sum_{j=1}^{p} a_j + \sum_{i=2}^{p-1}\sum_{j=1}^{p} a_j\left(a_i + 3\right) + + \left(a_p + 2\right)\sum_{j=1}^{p} a_j \\ &\quad - (a_1 + 2)\, a_1 - \sum_{i=2}^{p-1} a_i\left(a_i + 3\right) - \left(a_p + 2\right) a_p \end{aligned}$$

$$+2\sum_{i=1}^{p}\sum_{j=1}^{a_i-1}(a_i-\mathrm{j}) \;+2\sum_{i=1}^{p-1}\sum_{j=1}^{a_i}\sum_{r=i+1}^{p}a_r$$
$$=2\left(p^2-4p+4+a_1+a_p\right)+\left(4p+a_1+a_p-9\right)\sum_{j=1}^{p}a_j$$
$$+\sum_{i=2}^{p-1}\sum_{j=1}^{p}a_ja_i+2\sum_{i=1}^{p-1}\sum_{r=i+1}^{p}a_ra_i\ .$$

2. $$M_2^c(\mathcal{H})=\sum_{i=1}^{p-2}\sum_{j=i+2}^{p}(degv_i\times degv_j)+\sum_{i=1}^{p}\sum\nolimits_{j=1}^{p}\sum_{r=1}^{a_j}(degv_i\times degu_{j,r})$$
$$-\sum_{i=1}^{p}\sum_{j=1}^{a_i}(degv_i\times degu_{i,j}) \;+\sum_{i=1}^{p}\sum_{j=1}^{a_i-1}\sum_{r=j+1}^{a_i}(degu_{i,j}\times degu_{i,r})$$
$$+\sum_{i=1}^{p-1}\sum_{j=1}^{a_i}\sum_{r=i+1}^{p}\sum_{h=1}^{a_r}(degu_{i,j}\times degu_{r,h})$$
$$=\sum_{j=3}^{p}(degv_1\times degv_j)+\sum_{i=2}^{p-3}\sum_{j=i+2}^{p-1}(degv_i\times degv_j)$$
$$+\sum_{i=2}^{p-2}\left(degv_i\times degv_p\right)+\sum_{j=1}^{p}\sum_{r=1}^{a_j}(degv_1\times degu_{j,r})$$
$$+\sum_{i=2}^{p-1}\sum_{j=1}^{p}\sum_{r=1}^{a_j}(degv_i\times degu_{j,r}) \;+\sum_{j=1}^{p}\sum_{r=1}^{a_j}(degv_p\times degu_{j,r})$$
$$-\sum_{j=1}^{a_1}(degv_1\times degu_{1,j})-\sum_{i=2}^{p-1}\sum_{j=1}^{a_i}(degv_i\times degu_{i,j})$$
$$-\sum_{j=1}^{a_p}(degv_p\times degu_{p,j})+\sum_{i=1}^{p}\sum_{j=1}^{a_i-1}\sum_{r=j+1}^{a_i}(degu_{i,j}\times degu_{i,r})$$
$$+\sum_{i=1}^{p-1}\sum_{j=1}^{a_i}\sum_{r=i+1}^{p}\sum_{h=1}^{a_r}(degu_{i,j}\times degu_{r,h})$$
$$=(a_1+1)\sum_{j=3}^{p-1}a_j+2(a_1+1)\,(p-3)+\left(a_1+1)(a_p+1\right)$$
$$+\sum_{i=2}^{p-3}\sum_{j=i+2}^{p-1}\left(a_ia_j+2a_i+2a_j+4\right)+\left(a_p+1\right)\sum_{i=2}^{p-2}a_i+2\left(a_p+1\right)(p-3)$$
$$+(a_1+1)\sum_{j=1}^{p}a_j \;+\sum_{i=2}^{p-1}\sum_{j=1}^{p}a_j\,(a_i+2) \;+\left(a_p+1\right)\sum_{j=1}^{p}a_j$$
$$-a_1\,(a_1+1)-\sum_{i=2}^{p-1}a_i\,(a_i+2)-a_p\left(a_p+1\right)$$
$$+\sum_{i=1}^{p}\sum_{j=1}^{a_i-1}(a_i-j) \;+\sum_{i=1}^{p-1}\sum_{j=1}^{a_i}\sum_{r=i+1}^{p}a_r$$
$$=2p^2+2p\,(2a_1-5)+13-2(a_1^2+a_p^2)-a_1\left(6+a_2+2a_p\right)-a_2-a_{p-1}$$
$$-a_p\left(6+a_{p-1}\right)+2\left(a_1+a_p-1\right)\sum_{j=1}^{p}a_j \;+2\sum_{i=2}^{p-3}\sum_{j=i+2}^{p-1}(a_i+a_j+a_ia_j)$$
$$-\frac{1}{2}\sum_{i=1}^{p}a_i\,(a_i+1)+\sum_{i=1}^{p}\sum_{j=1}^{p}a_j\,(a_i+2)+\sum_{i=2}^{p-2}a_{i+1}a_i.$$

■

Corollary 2: *For all $p \geq 3$ and $a_i = a > 0$, $i = 1, 2, \ldots, p$, then:*

1. $M_1^c(\mathcal{H}) = 2p^2(a+1)^2 - p(a+1)(a+8) + 4(a+2)$.
2. $M_2^c(\mathcal{H}) = 2p^2(a+1)^2 - \frac{5p}{2}(a+1)(a+4) + a^2 + 10a + 13$.

Proof: From Theorem 2, then:

1. $M_1^c(\mathcal{H}) = 2(p^2 - 4p + 4 + 2a) + (4p + 2a - 9)ap + a^2p(p-2) + a^2p(p-1)$.

$$= 2p^2(a+1)^2 - p\,(a+1)\,(a+8) + 4\,(a+2)\,.$$

2. $M_2^c(\mathcal{H}) = 2p^2 + 2p(2a-5) + 13 - 4a^2 - a(6+3a) - 2a$

$$-a\,(6+a) + 2\,(2a-1)\sum_{j=1}^{p} a \; + 2\sum_{i=2}^{p-3}\sum_{j=i+2}^{p-1}\left(2a + a^2\right)$$
$$-\frac{1}{2}\sum_{i=1}^{p} a\,(a+1) + \sum_{i=1}^{p}\sum_{j=1}^{p} a\,(a+2) + \sum_{i=2}^{p-2} a^2$$
$$= 2p^2(a+1)^2 - \frac{5p}{2}\,(a+1)\,(a+4) + a^2 + 10a + 13. \qquad \blacksquare$$

Theorem 3: *For all $p \geq 3$ and $a_i \geq 1$, $i = 1, 2, \ldots, p$, then:*

1. $M_1^m(\mathcal{H}) = (a_1 + a_2 + 3)(a_{p-1} + a_p + 3)(a_1 + 2)^{a_1}(a_{p-1} + 3)^{a_{p-1}}(a_p + 2)^{a_p}$

$$\times \prod_{i=2}^{p-2} (a_i + 3)^{a_i}(a_i + a_{i+1} + 4).$$

2. $M_2^m(\mathcal{H}) = (a_1 + 1)^{a_1+1}(a_p + 1)^{a_p+1}(a_{p-1} + 2)^{a_{p-1}}(a_2 + 2)(a_{p-1} + 2) \times \prod_{i=2}^{p-2} (a_i + 2)^{a_i+1}(a_{i+1} + 2)$.

Proof: From Definition 3, then:

1. $M_1^m(\mathcal{H}) = \prod_{vu \in E} (deg_G v + deg_G u)$

$$= \prod_{i=1}^{p-1}(degv_i + degv_{i+1}) \times \prod_{i=1}^{p}\prod_{j=1}^{a_i}(degv_i + degu_{i,j})$$
$$= (a_1 + 1 + a_2 + 2) \times \prod_{i=2}^{p-2}(a_i + a_{i+1} + 4) \times \left(a_{p-1} + 2 + a_p + 1\right)$$
$$\times \prod_{j=1}^{a_1}(a_1 + 1 + 1) \times \prod_{i=2}^{p-1}\prod_{j=1}^{a_i}(a_i + 2 + 1) \times \prod_{j=1}^{a_p}(a_p + 1 + 1)$$
$$= (a_1 + a_2 + 3)\left(a_{p-1} + a_p + 3\right) \times \prod_{i=2}^{p-2}(a_i + a_{i+1} + 4)$$
$$\times \prod_{j=1}^{a_1}(a_1 + 2) \times \prod_{i=2}^{p-1}\prod_{j=1}^{a_i}(a_i + 3) \times \prod_{j=1}^{a_p}(a_p + 2)$$
$$= (a_1 + a_2 + 3)\left(a_{p-1} + a_p + 3\right)(a_1 + 2)^{a_1}\left(a_p + 2\right)^{a_p}$$
$$\times \prod_{i=2}^{p-2}(a_i + a_{i+1} + 4) \times \prod_{i=2}^{p-1}(a_i + 3)^{a_i}$$
$$= (a_1 + a_2 + 3)\left(a_{p-1} + a_p + 3\right)(a_1 + 2)^{a_1}\left(a_{p-1} + 3\right)^{a_{p-1}}\left(a_p + 2\right)^{a_p}$$
$$\times \prod_{i=2}^{p-2}(a_i + 3)^{a_i}(a_i + a_{i+1} + 4).$$

$$
\begin{aligned}
2.\ M_2^m(\mathcal{H}) &= \prod_{vu\in E}(deg_G v \times deg_G u)\\
&= \prod_{i=1}^{p-1}(degv_i \times degv_{i+1}) \times \prod_{i=1}^{p}\prod_{j=1}^{a_i}(degv_i \times degu_{i,j})\\
&= (a_1+1)(a_2+2) \times \prod_{i=2}^{p-2}(a_i+2)(a_{i+1}+2) \times (a_{p-1}+2)(a_p+1)\\
&\quad \times \prod_{j=1}^{a_1}(a_1+1) \times \prod_{i=2}^{p-1}\prod_{j=1}^{a_i}(a_i+2) \times \prod_{j=1}^{a_p}(a_p+1)\\
&= (a_1+1)(a_2+2)(a_{p-1}+2)(a_p+1) \times \prod_{i=2}^{p-2}(a_i+2)(a_{i+1}+2)\\
&\quad \times (a_1+1)^{a_1} \times \prod_{i=2}^{p-1}\prod_{j=1}^{a_i}(a_i+2) \times (a_p+1)^{a_p}\\
&= (a_1+1)^{a_1+1}(a_p+1)^{a_p+1}(a_2+2)(a_{p-1}+2)\\
&\quad \times \prod_{i=2}^{p-2}(a_i+2)(a_{i+1}+2) \times \prod_{i=2}^{p-1}(a_i+2)^{a_i}\\
&= (a_1+1)^{a_1+1}(a_p+1)^{a_p+1}(a_{p-1}+2)^{a_{p-1}}(a_2+2)(a_{p-1}+2) \times \prod_{i=2}^{p-2}(a_i+2)^{a_i+1}(a_{i+1}+2).
\end{aligned}
$$

■

Corollary 3: *For all $p \geq 3$ and $a_i = a$, $i = 1, 2, \ldots, p$, then:*

1. $M_1^m(\mathcal{H}) = (2a+3)^2(a+2)^{2a}(a+3)^{a(p-2)}(2a+4)^{p-3}$.
2. $M_2^m(\mathcal{H}) = (a+1)^{2a+2}(a+2)^{a(p-2)+2p-3}$.

Proof: From Theorem 3, then:

$$
\begin{aligned}
1.\ M_1^m(\mathcal{H}) &= (a+a+3)(a+a+3)(a+2)^a(a+3)^a(a+2)^a \times \prod_{i=2}^{p-2}(a+3)^a(a+a+4)\\
&= (2a+3)^2(a+2)^{2a}(a+3)^{a(p-2)}(2a+4)^{p-3}.
\end{aligned}
$$

$$
\begin{aligned}
2.\ M_2^m(\mathcal{H}) &= (a+1)^{a+1}(a+1)^{a+1}(a+2)^a(a+2)(a+2) \times \textstyle\prod_{i=2}^{p-2}(a+2)^{a+1}(a+2)\\
&= (a+1)^{2a+2}(a+2)^{a+3}(a+2)^{(a+1)(p-3)}(a+2)^{p-3}\\
&= (a+1)^{2a+2}(a+2)^{a(p-2)+2p-3}.
\end{aligned}
$$

■

Theorem 4: *For all ≥ 3, p is an odd and $a_i \geq 1$, $i = 1, 2, \ldots, p$, then:*

1. $Ecc_1(\mathcal{H}) = \frac{1}{2}(3p^2-2p-1) + (p+2)a_{\frac{p+1}{2}} + \sum_{i=1}^{\frac{p-1}{2}}(2p-2i+3)(a_i + a_{p+1-i})$.
2. $Ecc_2(\mathcal{H}) = \frac{1}{12}(7p^3-3p^2-7p+3) + \frac{1}{4}(p+1)(p+3)a_{\frac{p+1}{2}}$
$$+\sum_{i=1}^{\frac{p-1}{2}}(p+1-i)(p+2-i)(a_i + a_{p+1-i}).$$

Proof: From Definition 4, then:

1. $Ecc_1(\mathcal{H}) = \sum_{vu \in E}(e(v)+e(u))$

$$= \sum_{i=1}^{p-1}(e(v_i)+e(v_{i+1})) + \sum_{i=1}^{p}\sum_{j=1}^{a_i}(e(v_i)+e(u_{i,j}))$$

$$= 2\sum_{i=1}^{\frac{p-1}{2}}(e(v_i)+e(v_{i+1})) + \sum_{i=1}^{\frac{p+1}{2}}\sum_{j=1}^{a_i}(e(v_i)+e(u_{i,j})) + \sum_{i=\frac{p+3}{2}}^{p}\sum_{j=1}^{a_i}(e(v_i)+e(u_{i,j}))$$

$$= 2\sum_{i=1}^{\frac{p-1}{2}}(e(v_i)+e(v_{i+1})) + \sum_{i=1}^{\frac{p+1}{2}}\sum_{j=1}^{a_i}(e(v_i)+e(u_{i,j})) + \sum_{i=1}^{\frac{p-1}{2}}\sum_{j=1}^{a_{p+1-i}}(e(v_{p+1-i})+e(u_{p+1-i,j}))$$

$$= 2\sum_{i=1}^{\frac{p-1}{2}}(p+1-i+p+1-i-1) + \sum_{i=1}^{\frac{p+1}{2}}\sum_{j=1}^{a_i}(p+1-i+p+1-i+1)$$

$$+ \sum_{i=1}^{\frac{p-1}{2}}\sum_{j=1}^{a_{p+1-i}}(p+1-i+p+1-i+1)$$

$$= 2\sum_{i=1}^{\frac{p-1}{2}}(2p-2i+1) + \sum_{i=1}^{\frac{p+1}{2}}\sum_{j=1}^{a_i}(2p-2i+3) + \sum_{i=1}^{\frac{p-1}{2}}\sum_{j=1}^{a_{p+1-i}}(2p-2i+3)$$

$$= 2\sum_{i=1}^{\frac{p-1}{2}}(2p-2i+1) + \sum_{i=1}^{\frac{p+1}{2}}(2p-2i+3)\,a_i + \sum_{i=1}^{\frac{p-1}{2}}(2p-2i+3)\,a_{p+1-i}$$

$$= 2\sum_{i=1}^{\frac{p-1}{2}}(2p-2i+1) + (p+2)\,a_{\frac{p+1}{2}} + \sum_{i=1}^{\frac{p-1}{2}}(2p-2i+3)\left(a_i+a_{p+1-i}\right)$$

$$= \frac{1}{2}\left(3p^2-2p-1\right) + (p+2)\,a_{\frac{p+1}{2}} + \sum_{i=1}^{\frac{p-1}{2}}(2p-2i+3)\left(a_i+a_{p+1-i}\right).$$

2. $Ecc_2(\mathcal{H}) = \sum_{vu \in E}(e(v)\times e(u))$

$$= \sum_{i=1}^{p-1}(e(v_i)\times e(v_{i+1})) + \sum_{i=1}^{p}\sum_{j=1}^{a_i}(e(v_i)\times e(u_{i,j}))$$

$$= 2\sum_{i=1}^{\frac{p-1}{2}}(e(v_i)\times e(v_{i+1})) + \sum_{i=1}^{\frac{p+1}{2}}\sum_{j=1}^{a_i}(e(v_i)\times e(u_{i,j})) + \sum_{i=\frac{p+3}{2}}^{p}\sum_{j=1}^{a_i}(e(v_i)\times e(u_{i,j}))$$

$$= 2\sum_{i=1}^{\frac{p-1}{2}}(e(v_i)\times e(v_{i+1})) + \sum_{i=1}^{\frac{p+1}{2}}\sum_{j=1}^{a_i}(e(v_i)\times e(u_{i,j})) + \sum_{i=1}^{\frac{p-1}{2}}\sum_{j=1}^{a_{p+1-i}}(e(v_{p+1-i})\times e(u_{p+1-i,j}))$$

$$= 2\sum_{i=1}^{\frac{p-1}{2}}(p+1-i)(p+1-i-1) + \sum_{i=1}^{\frac{p+1}{2}}\sum_{j=1}^{a_i}(p+1-i)(p+1-i+1)$$

$$+ \sum_{i=1}^{\frac{p-1}{2}}\sum_{j=1}^{a_{p+1-i}}(p+1-i)(p+1-i+1)$$

$$= 2\sum_{i=1}^{\frac{p-1}{2}}(p+1-i)(p-i) + \sum_{i=1}^{\frac{p+1}{2}}\sum_{j=1}^{a_i}(p+1-i)(p+2-i)$$

$$+ \sum_{i=1}^{\frac{p-1}{2}}\sum_{j=1}^{a_{p+1-i}}(p+1-i)(p+2-i)$$

$$= 2\sum_{i=1}^{\frac{p-1}{2}}(p+1-i)(p-i) + \sum_{i=1}^{\frac{p+1}{2}}(p+1-i)(p+2-i)\,a_i + \sum_{i=1}^{\frac{p-1}{2}}(p+1-i)(p+2-i)\,a_{p+1-i}$$
$$= 2\sum_{i=1}^{\frac{p-1}{2}}(p+1-i)(p-i) + \frac{1}{4}(p+1)(p+3)\,a_{\frac{p+1}{2}} + \sum_{i=1}^{\frac{p-1}{2}}(p+1-i)(p+2-i)\left(a_i + a_{p+1-i}\right)$$
$$= \frac{1}{12}\left(7p^3 - 3p^2 - 7p + 3\right) + \frac{1}{4}(p+1)(p+3)\,a_{\frac{p+1}{2}} + \sum_{i=1}^{\frac{p-1}{2}}(p+1-i)(p+2-i)\left(a_i + a_{p+1-i}\right). \quad \blacksquare$$

Corollary 4: *For all $p \geq 3$ and $a_i = a$, $i = 1, 2, \ldots, p$, then:*

1. $Ecc_1(\mathcal{H}) = \frac{1}{2}(a+1)(3p^2-1) + p(2a-1)$.
2. $Ecc_2(\mathcal{H}) = \frac{1}{12}(p^2-1)(7p(a+1)+3(5a-1)) + \frac{1}{4}(p+1)(p+3)a$. $\blacksquare$

Theorem 5: *For all ≥ 4, p is an even and $a_i \geq 1$, $i = 1, 2, \ldots, p$, then:*

1. $Ecc_1(\mathcal{H}) = \frac{3}{2}p^2 - p + \sum_{i=1}^{\frac{p}{2}}(2p-2i+3)(a_i + a_{p+1-i})$.
2. $Ecc_2(\mathcal{H}) = \frac{1}{12}(7p^3 - 3p^2 - 4p + 12) + \sum_{i=1}^{\frac{p}{2}}(p+1-i)(p+2-i)(a_i + a_{p+1-i})$.

Proof: From Definition 4, then:

1. $Ecc_1(\mathcal{H}) = \sum_{vu\in E}(e(v) + e(u))$

$$= \sum_{i=1}^{p-1}(e(v_i) + e(v_{i+1})) + \sum_{i=1}^{p}\sum_{j=1}^{a_i}(e(v_i) + e(u_{i,j}))$$
$$= 2\sum_{i=1}^{\frac{p}{2}-1}(e(v_i) + e(v_{i+1})) + e(v_{\frac{p}{2}}) + e\left(v_{\frac{p}{2}+1}\right) + \sum_{i=1}^{\frac{p}{2}}\sum_{j=1}^{a_i}(e(v_i) + e(u_{i,j}))$$
$$+ \sum_{i=\frac{p}{2}+1}^{p}\sum_{j=1}^{a_i}(e(v_i) + e(u_{i,j}))$$
$$= 2\sum_{i=1}^{\frac{p}{2}-1}(e(v_i) + e(v_{i+1})) + e(v_{\frac{p}{2}}) + e\left(v_{\frac{p}{2}+1}\right) + \sum_{i=1}^{\frac{p}{2}}\sum_{j=1}^{a_i}(e(v_i) + e(u_{i,j}))$$
$$+ \sum_{i=1}^{\frac{p}{2}}\sum_{j=1}^{a_{p+1-i}}\left(e\left(v_{p+1-i}\right) + e\left(u_{p+1-i,j}\right)\right)$$
$$= 2\sum_{i=1}^{\frac{p}{2}-1}(p+1-i+p+1-i-1) + \left(\frac{p}{2}+1+\frac{p}{2}+1\right) + \sum_{i=1}^{\frac{p}{2}}\sum_{j=1}^{a_i}(p+1-i+p+1-i+1)$$
$$+ \sum_{i=1}^{\frac{p}{2}}\sum_{j=1}^{a_{p+1-i}}(p+1-i+p+1-i+1)$$
$$= 2\sum_{i=1}^{\frac{p}{2}-1}(2p-2i+1) + (p+2) + \sum_{i=1}^{\frac{p}{2}}\sum_{j=1}^{a_i}(2p-2i+3) + \sum_{i=1}^{\frac{p}{2}}\sum_{j=1}^{a_{p+1-i}}(2p-2i+3)$$
$$= p+2+2\sum_{i=1}^{\frac{p}{2}-1}(2p-2i+1) + \sum_{i=1}^{\frac{p}{2}}(2p-2i+3)\,a_i + \sum_{i=1}^{\frac{p}{2}}(2p-2i+3)\,a_{p+1-i}$$
$$= p+2+2\sum_{i=1}^{\frac{p}{2}-1}(2p-2i+1) + \sum_{i=1}^{\frac{p}{2}}(2p-2i+3)\left(a_i + a_{p+1-i}\right)$$

$$= \frac{3}{2}p^2 - p + \sum_{i=1}^{\frac{p}{2}} (2p - 2i + 3)\left(a_i + a_{p+1-i}\right).$$

2. $Ecc_2(\mathcal{H}) = \sum_{vu\in E}(e(v) \times e(u))$

$$= \sum_{i=1}^{p-1}(e(v_i) \times e(v_{i+1})) + \sum_{i=1}^{p}\sum_{j=1}^{a_i}(e(v_i) \times e(u_{i,j}))$$
$$= 2\sum_{i=1}^{\frac{p}{2}-1}(e(v_i) \times e(v_{i+1})) + e(v_{\frac{p}{2}}) \times e\left(v_{\frac{p}{2}+1}\right) + \sum_{i=1}^{\frac{p}{2}}\sum_{j=1}^{a_i}(e(v_i) \times e(u_{i,j}))$$
$$+ \sum_{i=\frac{p}{2}+1}^{p}\sum_{j=1}^{a_i}(e(v_i) \times e(u_{i,j}))$$
$$= 2\sum_{i=1}^{\frac{p}{2}-1}(e(v_i) \times e(v_{i+1})) + e(v_{\frac{p}{2}}) \times e\left(v_{\frac{p}{2}+1}\right) + \sum_{i=1}^{\frac{p}{2}}\sum_{j=1}^{a_i}(e(v_i) \times e(u_{i,j}))$$
$$+ \sum_{i=1}^{\frac{p}{2}}\sum_{j=1}^{a_{p+1-i}}\left(e\left(v_{p+1-i}\right) \times e\left(u_{p+1-i,j}\right)\right)$$
$$= 2\sum_{i=1}^{\frac{p}{2}-1}(p+1-i)(p+1-i-1) + \left(\frac{p}{2}+1\right)\left(\frac{p}{2}+1\right) + \sum_{i=1}^{\frac{p}{2}}\sum_{j=1}^{a_i}(p+1-i)(p+1-i+1)$$
$$+ \sum_{i=1}^{\frac{p}{2}}\sum_{j=1}^{a_{p+1-i}}(p+1-i)(p+1-i+1)$$
$$= 2\sum_{i=1}^{\frac{p}{2}-1}(p+1-i)(p-i) + \left(\frac{p}{2}+1\right)^2 + \sum_{i=1}^{\frac{p}{2}}(p+1-i)(p+2-i)\,a_i$$
$$+ \sum_{i=1}^{\frac{p}{2}}(p+1-i)(p+2-i)\,a_{p+1-i}$$
$$= \frac{1}{12}\left(7p^3 - 3p^2 - 4p + 12\right) + \sum_{i=1}^{\frac{p}{2}}(p+1-i)(p+2-i)(a_i + a_{p+1-i}). \quad \blacksquare$$

Corollary 5: *For all $p \geq 3$ and $a_i = a$, $i = 1, 2, \ldots, p$, then:*

1. $Ecc_1(\mathcal{H}) = \frac{3}{2}p^2(a+1) + p(2a-1)$.
2. $Ecc_2(\mathcal{H}) = \frac{1}{12}(7p^3(a+1) + 3p^2(6a-1) + 4p(2a-1) + 12)$. ■

Applications

From Theorems 1 to 5, when $a_i = 0,\ i = 1, p$ and $a_i = 2,\ i = 2, 3, \ldots, p-1$.The following corollaries will be obtained respectively.

Corollary 6: *For all $p \geq 3$, then:*

1. $M_1(\mathcal{H}) = 18p - 34$.
2. $M_2(\mathcal{H}) = 24p - 56$. ■

Corollary 7: *For all $p \geq 3$, then:*

1. $M_1^c(\mathcal{H}) = 18p^2 - 78p + 84$.
2. $M_2^c(\mathcal{H}) = 18p^2 - 93p + 123$. ■

Corollary 8: *For all $p \geq 3$, then:*

1. $M_1^m(\mathcal{H}) = 625(200)^{p-3}$.
2. $M_2^m(\mathcal{H}) = (256)^{p-2}$. ■

Corollary 9: *For all $p \geq 5$, p is an odd, then:*

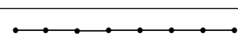
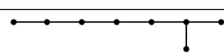
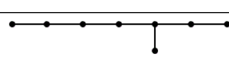
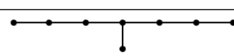
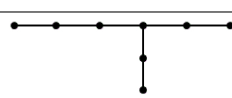
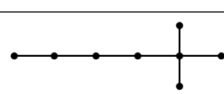
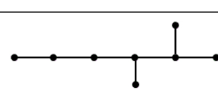
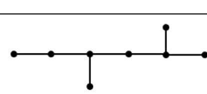
1. $Ecc_1(\mathcal{H}) = \frac{1}{2}(9p^2 - 22p + 9)$.
2. $Ecc_2(\mathcal{H}) = \frac{1}{4}(7p^3 - 23p^2 + 17p - 1)$. ■

Corollary 10: *For all $p \geq 4$, p is an even, then:*

1. $Ecc_1(\mathcal{H}) = \frac{9}{2}p^2 - 11p + 6$.
2. $Ecc_2(\mathcal{H}) = \frac{1}{4}p(7p^2 - 23p + 20)$. ■

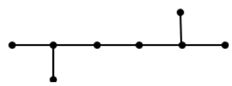
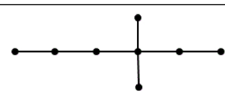
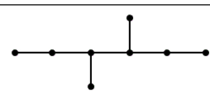
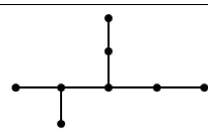
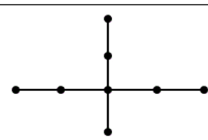
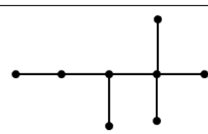
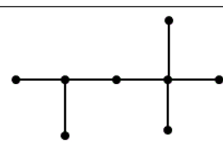
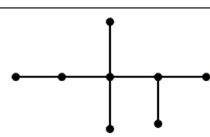
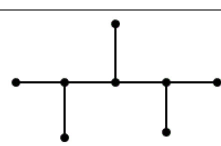
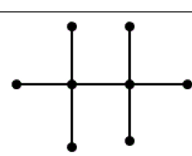
Alkanes are a basic class of hydrocarbons made up only of single-bonded carbon and hydrogen atoms.[16,17] The usual molecular formula for them is C_pH_{2p+2}, where p is the number of carbon atoms. In graph theory, this linear configuration of carbon atoms can be represented as a particular class of caterpillar graphs. A caterpillar graph has all of its vertices situated within a single distance from a central "spine," which is similar to the structure of alkanes, which are made up of hydrogen atoms as branches and carbon atoms as the backbone. Table 1 gives the information about 18 alkanes, their ascent fact, and entropy. Further columns in Table 1 represent their Zagreb-type topological indices. With the help of this information, mathematical models were investigated to predict entropy and ascent factor by using Zagreb-type indices. These mathematical models and their behaviors are shown in Figs. 3 and 4. From Table 1, it was also observed that the second Zagreb coindex gives the best result when predicting the entropy with a standard error of 1.39, while the other Zagreb-type indices have a greater standard error, meaning they have less power to predict entropy. From Figs. 3 and 4, it is clear that all the Zagreb-type indices are good to predict the ascent factor of the alkanes, but the first and the second Zagreb coindices give the lowest standard error. Hence, these two indices can be used to predict the ascent factor of alkanes.

Table 1. Alkanes with molecular structure, ascent fact, entropy and Zagreb type indices.

	Name	Isomers structure	Ascent. Fact	Entropy	M_1	M_2	M_1^m	M_2^m	M_1^c	M_2^c	Ecc_1	Ecc_2
1	Octane		0.397898	111.67	26	24	9216	4096	72	61	74	200
2	Methylheptane		0.377916	109.84	28	26	15360	6912	70	58	65	154
3	3-Methylheptane		0.371002	111.26	28	27	14400	6912	70	57	63	144
4	Methylheptane		0.371504	109.32	28	27	14400	6912	70	57	61	136
5	3-Ethylhexane		0.362472	109.43	28	28	13500	6912	70	56	54	105
6	2,2-dimethylhexane		0.339426	103.42	32	30	36000	4096	66	52	56	113
7	2,3-Dimethylhexane		0.348247	108.02	30	30	23040	11664	68	53	54	105
8	2,4-dimethylhexane		0.344223	106.98	30	29	24000	11664	68	54	54	105

(Continued.)

Table 1. Continued.

	Name	Isomers structure	Ascent. Fact	Entropy	M_1	M_2	M_1^m	M_2^m	M_1^c	M_2^c	Ecc_1	Ecc_2
9	2,5-Dimethylhexane		0.356830	105.72	30	28	25600	11664	68	55	56	113
10	3,3-Dimethylhexane		0.322596	104.74	32	32	32400	16384	66	50	52	97
11	3,4-Dimethylhexane		0.340345	106.59	30	31	21600	11664	68	52	52	97
12	3-Ethyl-2-methylpentane		0.332433	106.06	30	31	21600	11664	68	52	43	66
13	3-Ethyl-3-methylpentane		0.306899	101.48	32	34	29160	16384	66	48	41	60
14	2,2,3-Trimethylpentane		0.300816	101.31	34	35	52500	27648	64	46	43	66
15	2,2,4-Trimethylpentane		0.305370	104.09	34	32	60000	54000	64	49	45	72
16	2,3,3-Trimethylpentane		0.293177	102.06	34	36	27648	50400	64	45	41	60
17	2,3,4-Trimethylpentane		0.317422	102.39	32	33	36864	19683	69	49	43	66
18	Tetramethylbutane		0.255294	93.06	38	40	125000	65536	60	39	34	40

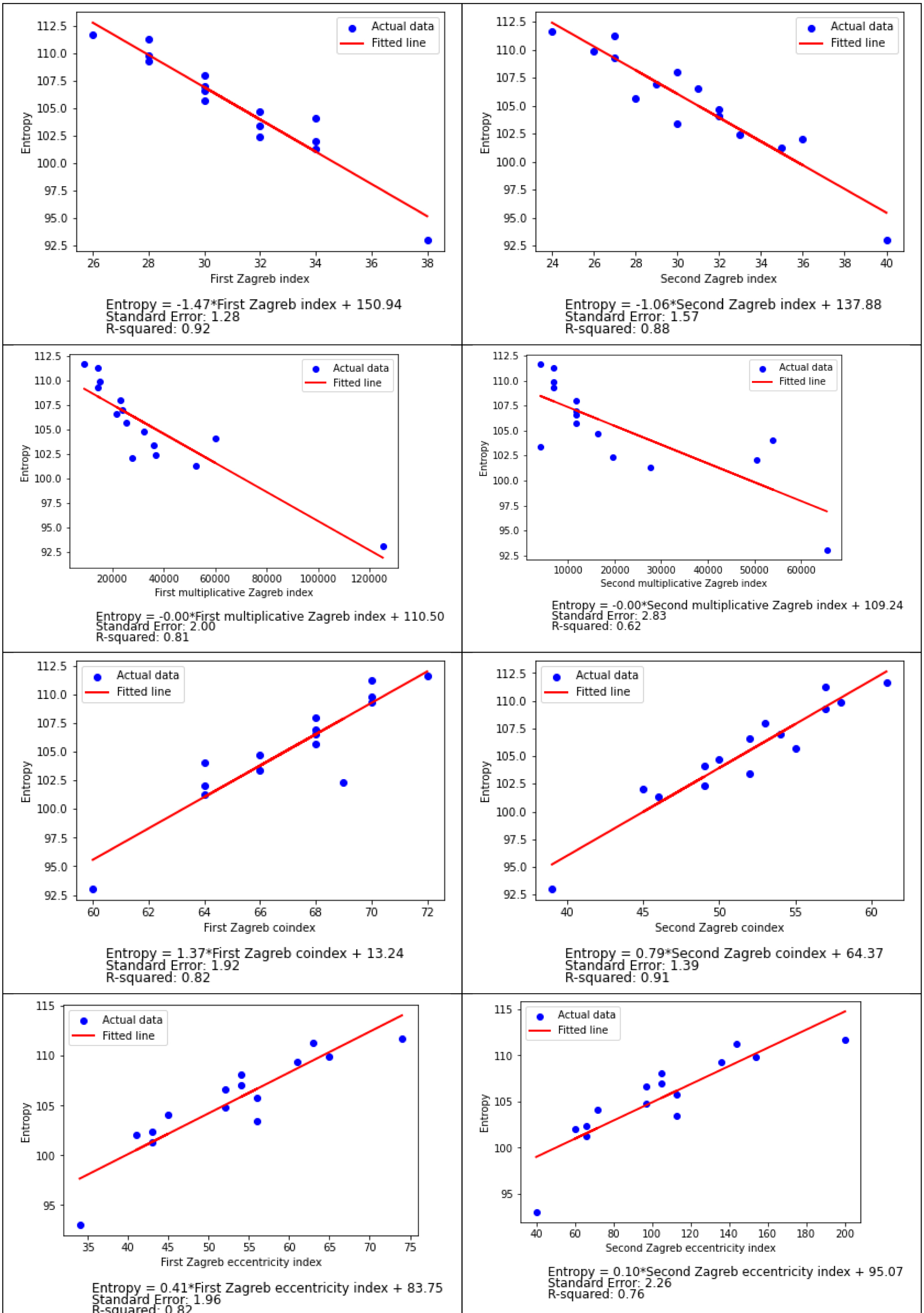


Fig. 3. Mathematical Models for entropy via Zagreb type indices.

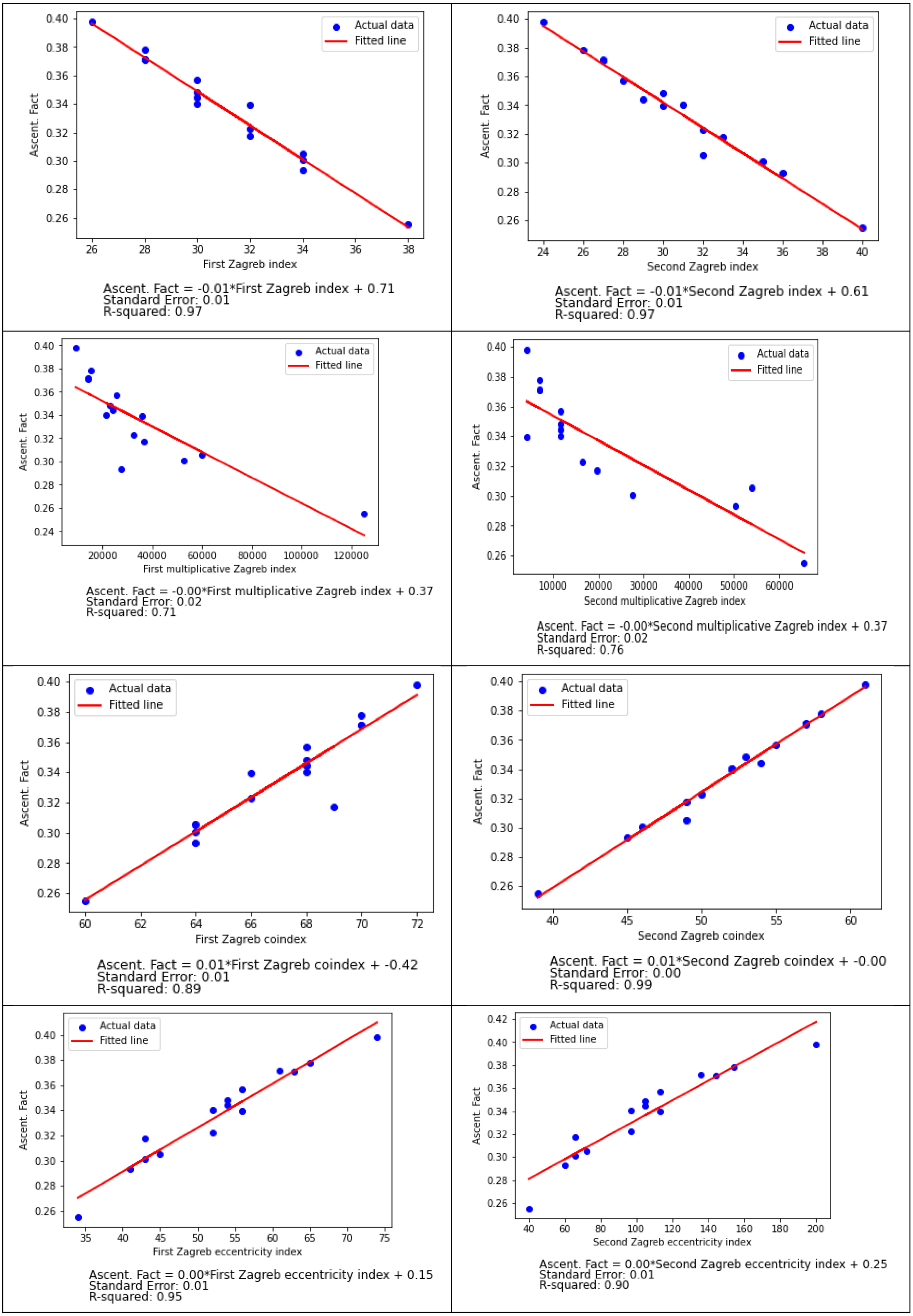


Fig. 4. Mathematical Models for ascent fact via Zagreb type indices.

The proposed method offers several advantages over existing approaches, including analytical tractability, predictive accuracy, strong chemical correlation, and broad applicability.

The proposed method offers several advantages over current methods: ease of analysis, predictive accuracy, strong chemical correlation, and general applicability.

Conclusions

The analysis shows that the Zagreb index M_2 achieves the highest accuracy in predicting entropy among the studied indices, registering the lowest error $\cong 1.39$, as shown in Table 1 and Fig. 3 also shows that the two indices M_1 and M_2 exhibit the lowest standard errors in estimating the uplift factor, supporting their adoption as reliable predictive indices. Furthermore, general formulas for these two indices and their caterpillar graph analogs have been derived, providing a practical framework for efficiently calculating the topological indices of alkanes and predicting the properties of unstudied compounds. The approach can be extended in the future to include broader classes of graphs and evaluate additional indices within more diverse molecular structures, thus enhancing the applications of structure – property relationship modeling.

Authors' declaration

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are ours. Furthermore, any Figures and images that are not ours have been included with the necessary permission for republication, which is attached to the manuscript.
- No animal studies are present in the manuscript.
- No human studies are present in the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee at the University of Mosul.

Authors' contributions statement

The problem was presented in detail by researcher A.M.A. The theoretical results (Theorems and corollary formulas) were found by researchers M.M.F and M.S.A., while the researcher M.K.J. applied the results to chemical compounds and compared the theoretical results with the real results. All authors read and approved the final manuscript.

References

1. Chartrand G, Jordon H, Vatter V, Zhang P. Graphs and Digraphs. 7th edition. New York: Chapman and Hall/CRC; 2024;364 p. https://doi.org/10.1201/9781003461289
2. Gutman I, Trinajstic N. Graph Theory and Molecular Orbitals, Total φ-Electron Energy of Alternant Hydrocarbons. Chem Phys Lett. 1972;17(4):535–538. https://doi.org/10.1016/0009-2614(72)85099-1
3. Randic M. Characterization of molecular branching. J Am Chem. Soc. 1975;97(23):6609–6615. https://doi.org/10.1021/ja00856a001
4. Akhmejanova M, Olmezov K, Volostnov A, Vorobyev I, Vorob'ev K, Yarovikov Y. Wiener index and graphs, almost half of whose vertices satisfy Šoltés property. Discrete Appl. Math. 2023;325:37–42. https://doi.org/10.1016/j.dam.2022.09.021
5. Movahedi F, Akhbari MH, Kamarulhaili H. On the Hosoya Index of Some Families of Graph. Math. Interdiscip. Res. 2021;6(3):225–234. https://doi.org/10.22052/MIR.2021.240266.1238
6. Rashad I, Fawad A, Rakhshanda Q, Muhammad N, Wali K M, Shahid K. Several Zagreb indices of power graphs of finite non-abelian groups. Heliyon. 2023;9(9):e19560. https://doi.org/10.1016/j.heliyon.2023.e19560
7. Umadi VS, Sangogi AM. Computing Topological Indices of Certain Networks. Commun Appl Nonlinear Anal. 2023;31(2):416–429. https://doi.org/10.52783/cana.v31.611
8. Rai S, Deb B. On the first and second Zagreb indices of some products of signed graphs. AKCE Int. J Graphs Comb. 2023;20(2):185–192. https://doi.org/10.1080/09728600.2023.2237092
9. Tratnik N, Pleteršek PZ. Zagreb Root-Indices of Graphs with Chemical Applications. Mathematics. 2024;12(23):3871. https://doi.org/10.3390/math12233871
10. Alex L, Gopal I. Zagreb Indices of some Chemical Structures using New Products of Graphs. J Hyperstructures. 2023;12(2):257–275. https://doi.org/10.22098/jhs.2023.2803
11. Došlic T. Vertex–weighted Wiener polynomials for composite graphs, Ars Math. Contemp. 2008;1(1):66–80. https://doi.org/10.26493/1855-3974.15.895

12. Todeschini R, Consonni V. New local vertex invariants and molecular descriptors based on functions of the vertex degrees. MATCH Commun Math Comput Chem. 2010;64:359–372.
13. Abdullah MM, Ali AM. Schultz and modified Schultz polynomials for edge – Identification chain and ring – for square graphs. Baghdad Sci. J. 2022;19(3):560–568. https://doi.org/10.21123/bsj.2022.19.3.0560
14. Azari M. On the Zagreb and Eccentricity Coindices of Graph Products. Iran J Math Sci Inform. 2023;18(1):165–178. https://doi.org/10.52547/ijmsi.18.1.165
15. Andrade E., Helena G., Marıa R. Spectra and Randic spectra of caterpillar graphs and applications to the energy. MATCH Commun Math Comput Chem 77(2017):61–75.
16. Yan-yan JIA. Thermodynamic Properties of Saturated Alkanes. Natural Science of Hainan University 28.1 (2025):28–31. https://doi.org/10.15886/j.cnki.hdxbzkb.2010.01.005
17. Mehling H, Mary AW. Analysis of trends in phase change enthalpy, entropy and temperature for alkanes, alcohols and fatty acids. Chem. Phys. Impacts, 6(2023):100222. https://doi.org/10.1016/j.chphi.2023.100222

بعض أنواع أدلة زغرب لبيان الدرب الشوكي العام وتطبيقاتها في التنبؤ بخصائص الجزيئات

مؤيد مهيدي فتحي [1] ، محمد شاكر احمد[1] ، محمد كامران جميل [2] ، احمد محمد علي[3]

[1]مدرسة موهوبين نينوى، المديرية العامة لتربية نينوى، الموصل، العراق
[2]قسم الرياضيات، الكلية الحديثة، جامعة ريفا الدولية، لاهور، باكستان.
[3]قسم الرياضيات، كلية علوم الحاسوب والرياضيات، جامعة الموصل، الموصل، العراق.

الخلاصة

تُعدّ الادلة التبولوجيا في نظرية البيان موضوعًا بالغ الأهمية، نظرًا لأهميتها العملية في بعض فروع العلوم، وخاصةً في الكيمياء والفيزياء والشبكات، وذلك لارتباطها الوثيق بالخواص الكيميائية والفيزيائية، بما في ذلك درجة الغليان ودرجة الانصهار وضغط البخار والحجم المولي وغيرها. هناك عدة أنواع من الادلة التبولوجيا، أهمها الادلة التي تعتمد على درجات الرؤوس، وخاصةً الرؤوس المتجاورة وغير المتجاورة. تُعتبر أدلة زغرب للرؤوس المتجاورة وغير المتجاورة، والضربية واللامركزية للرؤوس المتجاورة في البيان البسيط المتصل من الادلة التبولوجيا التي لها دور في معرفة العديد من الخصائص الكيميائية والفيزيائية. في هذا البحث، ناقشنا الادلة التبولوجيا من نوع زغرب لبيان الدرب الشوكي المعمم، بالإضافة إلى جزيئات الألكانات ذات الصيغة C_p H_(2p+2)، وهي حالة خاصة من بيان الدرب الشوكي المعمم ، إضافة الى ذلك، درسنا بعض خصائصه. أما في فقرة التطبيق، أوضحنا أن مؤشري زغرب الأول والثاني (المؤشران المتقابلان) يُعطيان ارتباطًا عاليًا بين مؤشرات زغرب الأخرى عند التنبؤ بالإنتروبيا وعامل الصعود للألكانات.

الكلمات المفتاحية: بيان كاتربيلر، المركبات الكيميائية، أدلة زغرب للاختلاف المركزي، أدلة زغرب المضاعفة، أدلة زغرب و الادلة المقابلة.