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Reduced Reversed Degree-Based Topological Indices Of Line Graph Of Alkanes

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Abstract:
Topological indices are numerical values associated with the structure of a molecule that can be used to predict various chemical and physical properties. The line graph of an alkane is a graph derived from the molecular graph of the alkane, where each vertex represents a bond and edges represent adjacency between bonds. Reduced reversed degree-based topological indices are a new class of indices that take into account the degrees of the vertices in a reverse and reduced manner, providing potentially more accurate descriptors for molecular properties.In this article, we introduce and explore the reduced reversed degree-based topological indices for the line graph of alkanes. A formula for calculating reduced reverse (RR) degree-based topological indices for alkane line graphs is presented, and mathematical expressions unique to alkane structures are derived. The results demonstrate that reduced reversed degree-based topological indices offer significant insights and improved accuracy in predicting alkane properties, highlighting their potential utility in cheminformatics and molecular modelling.
Keywords: *Line Graph, Alkane graph, Reduced Reverse Topological Indices.*

INTRODUCTION

Topological Indices (TI) are an effective tool in mathematical chemistry for examining the physico-chemical characteristics of medications and other chemical substances. One of the main topics of study in chemical graph theory is the analysis of molecular graphs' topological indices. These investigations aid in examining the connection between a drug's physico-chemical characteristics and its molecular structure. The atoms in a molecular graph are called vertices, and the covalent connections that bind them together are called edges. A vertex's degree [1], which is represented by the symbol d(v), indicates how many edges are incident on it. Any vertex in a chemical network has a maximum degree of 4. Among degree-based topological indices, the oldest and most significant are the Zagreb indices [2], [3].

Let v be a vertex in graph G, then Reverse vertex degree, or R(v), was first proposed by G. Kulli [4] and is defined as

$$\mathcal{R}(\mathrm{v}) = \Delta(\mathrm{G}) - \mathrm{d}(\mathrm{v}) + 1$$

Where $\Delta(\mathrm{G})$ is the maximum degree of the graph G and $\mathrm{d}(\mathrm{v})$ is the degree of the vertex v.

Inspired by this definition, Ravi et.al.[5] define the reduced reverse degree as

$$\mathcal{RR}(\mathrm{G}) = \Delta(\mathrm{G}) - \mathrm{d}(\mathrm{v}) + 2$$

In the development of pharmaceutical drugs, a compound's physico-chemical characteristics and biological activities are crucial. Topological indices, derived from chemical graph theory, offer a cost-effective way to predict these properties without laboratory testing. As part of the Quantitative Structure–Property Relationship (QSPR) and Quantitative Structure–Activity Relationship (QSAR) analyses, researchers use these indices to model and understand compound behavior [6]. Recently, studies have focused on COVID-19 medications' topological indices, applying methods such as M-polynomials, NM-polynomials, and RNM-polynomials. Various topological indices—such as degree-based and distance-based indices—have been developed and computed for different graph structures, including those formed through diverse graph operations [7-16]

Definition 1.1.

Alkanes are made entirely of single-bonded hydrogen and carbon atoms, which are organized in patterns resembling like trees as shown in Figure 1. The alkanes' standard formula is $C_K H_{2K+2}$. where, $K \geq 1$. The first four alkanes are mostly utilized for power production, cooking, and heating, but they are also the main component of lubricants and gasoline, making them extremely useful commercially (see Sardar et al. [17]). Chemical graph theory, along with certain other sciences, relies heavily on graph operations. By using graph operations on alkanes, a unique chemical structure is analysed in this study.

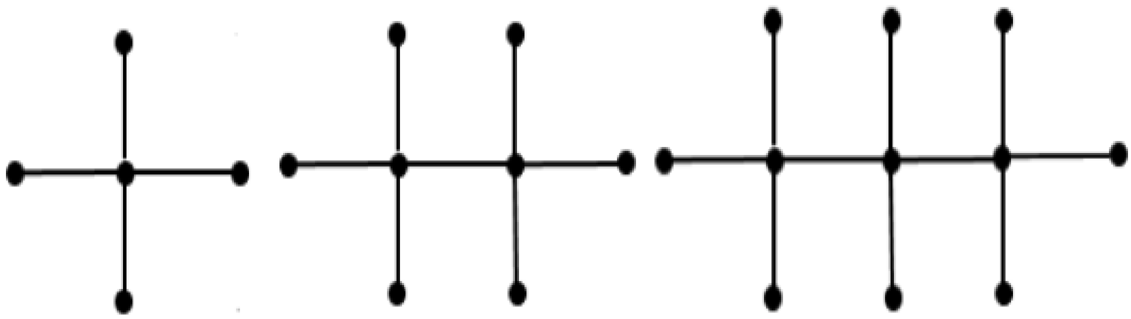

Figure 1: Alkanes (CH_4, C_2H_6, C_3H_8)

Definition 1.2.

In graph theory, a line graph L(G) of a given graph G is a graph that represents the adjacency between edges of G. In the line graph L(G): -

- Every vertex in L(G) is corresponding to an edge in G.
- Two vertices in L(G) are adjacent and coincide with the same vertex in G if and only if their related edges share a common end vertex see Nithya et al. [18].

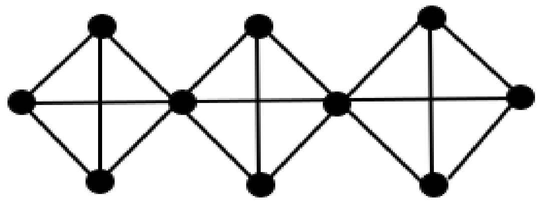

Figure 2: Line graph of Alkane $L(C_3H_8)$

Definition 1.3

In this paper, we define the reduced reverse degree-based versions of Randic index [19], Atom bond connectivity index [20-21], Geometric-arithmetic index [21], Zagreb indices [2],[3],[22-24], Balaban index[16].

$$\mathcal{RRR}_{\alpha}(G) = \sum_{u,v \in E(G)} [\mathcal{RR}d(u) \times \mathcal{RR}d(v)]^{\alpha}\,;\, \alpha = 1, -1, \frac{1}{2}, -\frac{1}{2} \qquad (1.3.1)$$

Reduced Reverse second Zagreb index $\mathcal{RR}M_2(G)$ is the term used if α = 1.

$$\mathcal{RR}ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{\mathcal{RR}d(u) + \mathcal{RR}d(v) - 2}{\mathcal{RR}d(u) \times \mathcal{RR}d(v)}} \qquad (1.3.2)$$

$$\mathcal{RR}GA(G) = \sum_{u,v \in E(G)} 2\sqrt{\frac{\mathcal{RR}d(u) \times \mathcal{RR}d(v)}{\mathcal{RR}d(u) + \mathcal{RR}d(v)}} \qquad (1.3.3)$$

$$\mathcal{RRM}_1(G) = \sum_{u,v\in E(G)} \mathcal{R}\mathcal{R}d(u) + \mathcal{RR}d(v) \quad (1.3.4)$$

$$\mathcal{RRM}_2(G) = \sum_{u,v\in E(G)} \mathcal{R}\mathcal{R}d(u) \times \mathcal{RR}d(v) \quad (1.3.5)$$

$$\mathcal{RR}\overline{M_1}(G) = 2|E(G)|(|V(G)| - 1) - \mathcal{RRM}_1(G) \quad (1.3.6)$$

$$\mathcal{RR}\overline{M_2}(G) = 2|E(G)|^2 - \frac{1}{2}\mathcal{RRM}_1(G) - \mathcal{RRM}_2(G) \quad (1.3.7)$$

$$\mathcal{RRHM}(G) = \sum_{u,v\in E(G)} [\mathcal{RR}d(u) \times \mathcal{RR}d(v)]^2 \quad (1.3.8)$$

$$\mathcal{RRF}(G) = \sum_{u,v\in E(G)} (\mathcal{RR}d(u))^2 + (\mathcal{RR}d(v))^2 \quad (1.3.9)$$

$$\mathcal{RRJ}(G) = \frac{u}{u - v + 2} \sum_{u,v\in E(G)} \frac{1}{\sqrt{\mathcal{RR}d(u) \times \mathcal{RR}d(v)}} \quad (1.3.10)$$

$$\mathcal{RR}\mathrm{P}M_1(G) = \prod\nolimits_{u,v\in E(G)} \mathcal{RR}d(u) + \mathcal{RR}d(v) \quad (1.3.11)$$

$$\mathcal{RR}\mathrm{P}M_2(G) = \prod\nolimits_{u,v\in E(G)} \mathcal{RR}d(u) \times \mathcal{RR}d(v) \quad (1.3.12)$$

$$\mathcal{RR}\mathrm{ReZ}G_1(G) = \sum_{u,v\in E(G)} \frac{\mathcal{RR}d(u) + \mathcal{RR}d(v)}{\mathcal{RR}d(u) \times \mathcal{RR}d(v)}, \quad (1.3.13)$$

$$\mathcal{RR}\mathrm{ReZ}G_2(G) = \sum_{u,v\in E(G)} \frac{\mathcal{RR}d(u) \times \mathcal{RR}d(v)}{\mathcal{RR}d(u) + \mathcal{RR}d(v)}, \quad (1.3.14)$$

$$\mathcal{RR}\mathrm{ReZ}G_3(G) = \sum_{u,v\in E(G)} (\mathcal{RR}d(u) + \mathcal{RR}d(v))(\mathcal{RR}d(u) \times \mathcal{RR}d(v)) \quad (1.3.15)$$

Main Results

The edge set of the line graph of alkanes is partitioned into four sets based on the reduced reverse degree of end vertices.

The first edge set of the partition contains $K-2$ edges uv, where $\mathcal{RR}\mathrm{d(u)} = 2$ and $\mathcal{RR}\mathrm{d(v)} = 2$.

The second edge set of the partition contains $4k-2$ edges uv, where $\mathcal{RR}\mathrm{d(u)} = 2$ and $\mathcal{RR}\mathrm{d(v)} = 5$.

The third edge set of the partition contains $K+4$ edges uv, where $\mathcal{RR}\mathrm{d(u)} = 5$ and $\mathcal{RR}\mathrm{d}(v) = 5$.

The Line graph of Alkanes has a maximum degree of 5. Using the reduced reverse vertex degree definition $\mathcal{RR}(\mathrm{G}) = \Delta(\mathrm{G}) - \mathrm{d(v)} + 2$, Table 1 shows the reduced reverse degree-based edge partition of the Alkanes line graph.

Table 1. Reduced Reverse edge set of the partition of Line Graph of Alkanes.

$\mathcal{RR}\mathrm{d(u)}, \mathcal{RR}\mathrm{d}(v)$	(2,2)	(2,5)	(5,5)
Frequency	$K-2$	$4K-2$	$K+4$

Theorem 2.1. The reduced reverse Randić index, for different values of α, of the Line graph of Alkanes is given by:

i. $\mathcal{RRR}_1\big(L(C_K H_{2K+2})\big) = 69K + 72$
ii. $\mathcal{RRR}_{-1}\big(L(C_K H_{2K+2})\big) = 0.69K - 0.54$
iii. $\mathcal{RRR}_{\frac{1}{2}}\big(L(C_K H_{2K+2})\big) = 19.6491K + 9.6754$
iv. $\mathcal{RRR}_{-\frac{1}{2}}\big(L(C_K H_{2K+2})\big) = 1.9649K - 0.8324$

Proof:
From Table 2, we compute the reduced reverse Randić index as below,

$$\mathcal{RRR}_{\alpha}\big(L(C_K H_{2K+2})\big) = \sum_{u,v \in E(L(C_K H_{2K+2}))} [\mathrm{R}\mathcal{R}d(u) \times R\mathcal{R}d(v)]^{\alpha}, \qquad K \geq 3$$

i. For $\alpha = 1$,

$$\mathcal{RRR}_{1}\big(L(C_K H_{2K+2})\big)$$
$$= [(K-2)\times(2\times 2)] + [(4K-2)\times(2\times 5)] + [(K+4)\times(5\times 5\,)]$$
$$= 69K + 72$$

ii. For $\alpha = -1$,

$$\mathcal{RRR}_{-1}\big(L(C_K H_{2K+2})\big)$$
$$= \left[(K-2)\times\frac{1}{2\times 2}\right] + \left[(4K-2)\times\frac{1}{2\times 5}\right] + \left[(K+4)\times\frac{1}{5\times 5}\right]$$
$$= 0.69K - 0.54$$

iii. For $\alpha = \frac{1}{2}$,

$$\mathcal{RRR}_{\frac{1}{2}}\big(L(C_K H_{2K+2})\big)$$
$$= \left[(K-2)\times\sqrt{2\times 2}\,\right] + \left[(4K-2)\times\sqrt{2\times 5}\,\right] + \left[(K+4)\times\sqrt{5\times 5}\,\right]$$
$$= 19.6491K + 9.6754$$

iv. For $\alpha = -\frac{1}{2}$,

$$\mathcal{RRR}_{-\frac{1}{2}}\big(L(C_K H_{2K+2})\big)$$
$$= \left[(K-2)\times\frac{1}{\sqrt{2\times 2}}\right] + \left[(4K-2)\times\frac{1}{\sqrt{2\times 5}}\right] + \left[(K+4)\times\frac{1}{\sqrt{5\times 5}}\right]$$
$$= 1.9649K - 0.8324$$

Theorem 2.2. The reduced reverse atomic bond connectivity index, reduced reverse geometric arithmetic index of the line graph of Alkanes are given by:

i. $\mathcal{RRABC}\big(L(C_K H_{2K+2})\big) = 4.1012\mathrm{K} - 0.56568$
ii. $\mathcal{RRGA}\big(L(C_K H_{2K+2})\big) = 5.6140K + 0.19298$

Proof:

i. From table 2, we compute the reduced reverse atomic bond connectivity index as below,

$$\mathcal{RRABC}\big(L(C_K H_{2K+2})\big) = \sum_{u,v \in E(L(C_K H_{2K+2}))} \sqrt{\frac{\mathcal{RR}d(u) + \mathcal{RR}d(v) - 2}{\mathcal{RR}d(u) \times \mathcal{RR}d(v)}}, \qquad K \geq 3$$
$$= \left[(K-2)\times\sqrt{\frac{2+2-2}{2\times 2}}\,\right] + \left[(4K-2)\times\sqrt{\frac{2+5-2}{2\times 5}}\,\right] + \left[(K+4)\times\sqrt{\frac{5+5-2}{5\times 5}}\,\right]$$
$$= 4.1012\mathrm{K} - 0.56568$$

ii. From Table 2, we compute the reduced reverse geometric arithmetic index as below,

$$\mathcal{RRGA}\big(L(C_K H_{2K+2})\big) = \sum_{u,v \in E(L(C_K H_{2K+2}))} \frac{2\sqrt{\mathcal{RR}d(u) \times \mathcal{RR}d(v)}}{\mathcal{RR}d(u) + \mathcal{RR}d(v)}, \qquad K \geq 3$$
$$= \left[(K-2)\times\frac{2\sqrt{2\times 2}}{2+2}\,\right] + \left[(4K-2)\times\frac{2\sqrt{2\times 5}}{2+5}\,\right] + \left[(K+4)\times\frac{2\sqrt{5\times 5}}{5+5}\,\right]$$
$$= 5.6140K + 0.19298$$

Theorem 2.3. The reduced reverse first Zagreb index, reduced reverse second Zagreb index, reduced reverse first Zagreb co-index and reduced reverse second Zagreb co-index of the line graph of Alkanes are given by:

i. $\mathcal{RR}\mathrm{M}_1\big(L(C_K H_{2K+2})\big) = 42\mathrm{K} + 18$
ii. $\mathcal{RR}\mathrm{M}_2\big(L(C_K H_{2K+2})\big) = 69\mathrm{K} + 72$
iii. $\mathcal{RR}\overline{M}_1\big(L(C_K H_{2K+2})\big) = 6(6K^2 - 7K - 3)$
iv. $\mathcal{RR}\overline{M}_2\big(L(C_K H_{2K+2})\big) = 9(8\mathrm{K}^2 - 10\mathrm{K} - 9)$

Proof:

i. From Table 2, we compute the reduced reverse first Zagreb index as below,

$$\mathcal{RR}\mathrm{M}_1\big(L(C_K H_{2K+2})\big) = \sum_{u,v\in E(L(C_K H_{2K+2}))} \mathcal{RR}d(u) + \mathcal{RR}d(v), \qquad K \geq 3$$
$$= [(K-2)\times(2+2)] + [(4K-2)\times(2+5)] + [(K+4)\times(5+5)]$$
$$= 42K + 18$$

ii. From Table 2, we compute the reduced reverse second Zagreb index as below,

$$\mathcal{RR}\mathrm{M}_2\big(L(C_K H_{2K+2})\big) = \sum_{u,v\in E(L(C_K H_{2K+2}))} \mathcal{RR}d(u) \times \mathcal{RR}d(v), \qquad K \geq 3$$
$$= [(K-2)\times(2\times 2)] + [(4K-2)\times(2\times 5)] + [(K+4)\times(5\times 5)]$$
$$= 69K + 72$$

iii. From Table 2, we compute the reduced reverse first Zagreb co-index as below,

$$\mathcal{RR}\overline{M}_1\big(L(C_K H_{2K+2})\big) = 2\mid E\big(L(C_K H_{2K+2})\big)\mid \big(\mid V\big(L(C_K H_{2K+2})\big)\mid -1\big) - \mathcal{RR}\mathrm{M}_1\big(L(C_K H_{2K+2})\big)$$
$$= 2|6K| \quad (|3K+1| - 1) - (42K+18) = 6(6K^2 - 7K - 3)$$

iv. From Table 2, we compute the reduced reverse second Zagreb co-index as below,

$$\mathcal{RR}\overline{M}_2\big(L(C_K H_{2K+2})\big) = 2\mid E(L(C_K H_{2K+2}))\mid^2 - \frac{1}{2}\,\mathcal{RR}\mathrm{M}_1\big(L(C_K H_{2K+2})\big) - \mathcal{RR}\mathrm{M}_2\big(L(C_K H_{2K+2})\big)$$
$$= 2|6K|^2 - \frac{1}{2}(42K+18) - (69K+72) = 9(8K^2 - 10K - 9)$$

Theorem 2.4. The reduced reverse hyper Zagreb index, reduced reverse forgotten index and reduced reverse Balaban index of the line graph of Alkanes are given by:

i. $\mathcal{RR}\mathrm{HM}\big(L(C_K H_{2K+2})\big) = 1041K + 2268$
ii. $\mathcal{RR}\mathrm{F}\big(L(C_K H_{2K+2})\big) = 174K + 126$
iii. $\mathcal{RR}\mathrm{J}\big(L(C_K H_{2K+2})\big) = \frac{6K}{3K+1}(1.9649K - 0.8324)$

Proof:

i. From Table 2, we compute the reduced reverse hyper Zagreb index as below,

$$\mathcal{RR}\mathrm{HM}\big(L(C_K H_{2K+2})\big) = \sum_{u,v\in E(L(C_K H_{2K+2}))} [\mathcal{RR}d(u)\times\mathcal{RR}d(v)]^2, \quad K \geq 3$$
$$=[(K-2)\times(2\times 2)^2]+[(4K-2)\times(2\times 5)^2] + [(K+4)\times(5\times 5)^2]$$
$$= 1041K + 2268$$

ii. From Table 2, we compute the reduced reverse forgotten index as below,

$$\mathcal{RR}\mathrm{F}\big(L(C_K H_{2K+2})\big) = \sum_{u,v\in E(L(C_K H_{2K+2}))} \big(\mathcal{RR}d(u)\big)^2 + \big(\mathcal{RR}d(v)\big)^2, \quad K \geq 3$$
$$= [(K-2)\times(2^2+2^2)] + [(4K-2)\times(2^2+5^2)] + [(K+4)\times(5^2+5^2)]$$
$$= 174K + 126$$

iii. From Table 2, we compute the reduced reverse Balaban index as below,

$$\mathfrak{RR}J(L(C_K H_{2K+2})) = \frac{u}{u-v+2}\sum_{u,v\in E(L(C_K H_{2K+2}))}\frac{1}{\sqrt{\mathfrak{RR}d(u)\times\mathfrak{RR}d(v)}}, K \geq 3$$
$$= \frac{6K}{6K-(3K+1)+2}\left\{\left[(K-2)\times\frac{1}{\sqrt{2\times 2}}\right] + \left[(4K-2)\times\frac{1}{\sqrt{2\times 5}}\right] + \left[(K+4)\times\frac{1}{\sqrt{5\times 5}}\right]\right\}$$

$$= \frac{6K}{3K+1}(1.9649K - 0.8324)$$

Theorem 2.5. The reduced reverse first multiple Zagreb index, reduced reverse second multiple Zagreb index of the Line graph of Alkanes is given by:

i. $\mathcal{RR}\mathrm{PM}_1\big(L(C_K H_{2K+2})\big) = 160(7K^3 + 10.5K^2 - 63K + 28)$
ii. $\mathcal{RR}\mathrm{PM}_2\big(L(C_K H_{2K+2})\big) = 400(10K^3 + 15K^2 - 90K + 40)$

Proof.

i. From Table 2, we compute the reduced reverse first multiple Zagreb index as below,

$$\mathcal{RR}\mathrm{PM}_1\big(L(C_K H_{2K+2})\big) = \prod_{u,v \in E(L(C_K H_{2K+2}))} \mathcal{RR}d(u) + \mathcal{RR}d(v), \quad K \geq 3$$

$$= [(K-2) \times (2+2)] \times [(4K-2) \times (2+5)] \times [(K+4) \times (5+5)]$$

$$= 160(7K^3 + 10.5K^2 - 63K + 28)$$

ii. From Table 2, we compute the reduced reverse second multiple Zagreb index as below,

$$\mathcal{RR}\mathrm{PM}_2\big(L(C_K H_{2K+2})\big) = \prod_{u,v \in E(L(C_K H_{2K+2}))} \mathcal{RR}d(u) \times \mathcal{RR}d(v), \quad K \geq 3$$

$$= [(K-2) \times (2 \times 2)] \times [(4K-2) \times (2 \times 5)] \times [(K+4) \times (5 \times 5)]$$

$$= 400(10K^3 + 15K^2 - 90K + 40)$$

Theorem 2.6. The reduced reverse first redefined Zagreb index, reduced reverse second redefined Zagreb index, and reduced reverse third redefined Zagreb index of the line graph of Alkanes are given by:

i. $\mathcal{RR}\mathrm{ReZG}_1\big(L(C_K H_{2K+2})\big) = 4.2K - 1.8$
ii. $\mathcal{RR}\mathrm{ReZG}_2\big(L(C_K H_{2K+2})\big) = 9.21428K + 5.1428$
iii. $\mathcal{RR}\mathrm{ReZG}_3\big(L(C_K H_{2K+2})\big) = 546K + 828$

Proof.

i. From Table 2, we compute the reduced reverse first redefined Zagreb index as below,

$$\Re\Re\,\mathrm{Re}\,ZG_1(L(C_K H_{2K+2})) = \sum_{u,v \in E(L(C_K H_{2K+2}))} \frac{\Re\Re d(u) + \Re\Re d(v)}{\Re\Re d(u) \times \Re\Re d(v)}, K \geq 3$$

$$= \left[(K-2) \times \left(\frac{2+2}{2 \times 2}\right)\right] + \left[(4K-2) \times \left(\frac{2+5}{2 \times 5}\right)\right] + \left[(K+4) \times \left(\frac{5+5}{5 \times 5}\right)\right]$$

$$= 4.2K - 1.8$$

ii. From Table 2, we compute the reduced reverse second redefined Zagreb index as below,

$$\Re\Re\,\mathrm{Re}\,ZG_2(L(C_K H_{2K+2})) = \sum_{u,v \in E(L(C_K H_{2K+2}))} \frac{\Re\Re d(u) \times \Re\Re d(v)}{\Re\Re d(u) + \Re\Re d(v)}, K \geq 3$$

$$= \left[(K-2) \times \left(\frac{2 \times 2}{2+2}\right)\right] + \left[(4K-2) \times \left(\frac{2 \times 5}{2+5}\right)\right] + \left[(K+4) \times \left(\frac{5 \times 5}{5+5}\right)\right]$$

$$= 9.21428K + 5.1428$$

iii. From Table 2, we compute the reduced reverse third redefined Zagreb index as below,

$$\Re\Re\,\mathrm{Re}\,ZG_3(L(C_K H_{2K+2})) = \sum_{u,v \in E(L(C_K H_{2K+2}))} \big(\Re\Re d(u) + \Re\Re d(v)\big)\big(\Re\Re d(u) \times \Re\Re d(v)\big), K \geq 3$$

$$= [(K-2) \times (2+2) \times (2+2)] + [(4K-2) \times (2+5) \times (2+5)] + [(K+4) \times (5+5) \times (5+5)]$$

$$= 546K + 828$$

Hence, we get the required results by using table 1.

Graphical Comparison

The topological indices, which are based on the Reduced reverse degree of the vertices in the Line graph of Alkanes $L(C_K H_{2K+2})$, are compared here both numerically and graphically.

Table 2. The numerical behaviour of topological indices for the Line graph of Alkanes $L(C_K H_{2K+2})$ $Where\ K \geq 3$.

K	Reduced reverse first Zagreb co-index $\mathcal{RR}\overline{M}_1$	Reduced reverse second Zagreb co-index $\mathcal{RR}\overline{M}_2$	Reduced reverse Forgotten index $\mathcal{RRF}$	Reduced reverse hyper Zagreb index $\mathcal{RR}$HM	Reduced reverse first multiple Zagreb index $\mathcal{RR}PM_1$	Reduced reverse second multiple Zagreb index $\mathcal{RR}PM_2$	Reduced reverse third redefined Zagreb index $\mathcal{RR}ReZG_3$
3	180	297	5391	648	19600	70000	2466
4	390	711	6432	822	62720	224000	3012
5	672	1269	7473	996	136080	486000	3558
6	1026	1971	8514	1170	246400	880000	4104
7	1452	2817	9555	1344	400400	1430000	4650
8	1950	3807	10596	1518	604800	2160000	5196
9	2520	4941	11637	1692	866320	3094000	5742
10	3162	6219	12678	1866	1191680	4256000	6288
11	3876	7641	13719	2040	1587600	5670000	6834
12	4662	9207	14760	2214	2060800	7360000	7380
13	5520	10917	15801	2388	2618000	9350000	7926
14	6450	12771	16842	2562	3265920	11664000	8472
15	7452	14769	17883	2736	4011280	14326000	9018
16	8526	16911	18924	2910	4860800	17360000	9564
17	9672	19197	19965	3084	5821200	20790000	10110
18	10890	21627	21006	3258	6899200	24640000	10656
19	12180	24201	22047	3432	8101520	28934000	11202
20	13542	26919	23088	3606	9434880	33696000	11748

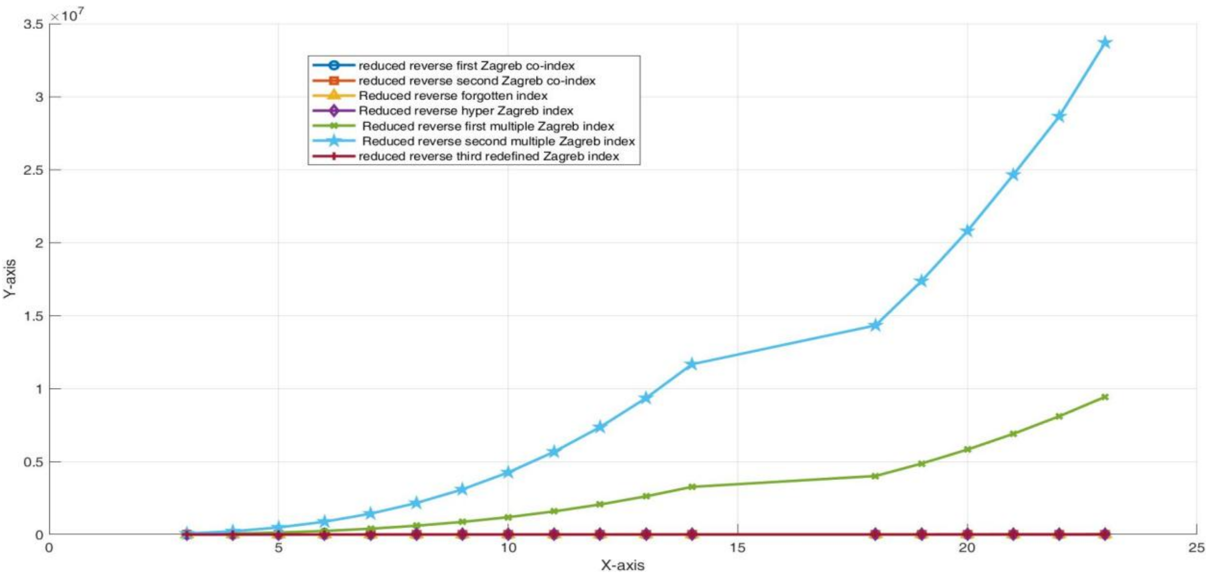

Figure 3: Graphical representation of Topological indices of Line graph of Alkanes $L(C_K H_{2K+2})$.

CONCLUSION

In this study, we examined the topological indices of the line graphs of alkanes, with particular emphasis on the reduced reverse degree as a fundamental parameter. The analysis revealed a range of structural properties inherent to the transformed graphs. However, it was observed that the line graph of an alkane does not correspond to a chemically realizable compound, thereby limiting the direct applicability of the computed indices for predicting chemical properties. This disconnect arises from the fact that line graphs, while mathematically derived from molecular structures, do not retain the chemical validity or interpretability of the original molecules. As a result, although the indices may possess theoretical importance within graph theory, they lack chemical significance as molecular descriptors.

A comparative graphical analysis of the topological indices was conducted, showing that the reduced reverse second multiple Zagreb index not only attained the highest values but also exhibited the most promising predictive performance among all descriptors considered.

Future investigations may focus on alternative graph transformation techniques that better preserve chemical meaning, or on hybrid methodologies that integrate these theoretical indices with data-driven models to enhance their practical utility in cheminformatics.

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