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Analysis of the M-polynomial and NM-Polynomial for Linear chain of indene

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Abstract In this research article, M-polynomial and NM-polynomial of linear chain of indene molecule are computed. These polynomials facilitate the calculation of various topological descriptors, such as degree-based and neighbor degree sum-based indices, like second modified zagreb index, inverse sum index, third version of zagreb index, harmonic index and neighbor version of indices and the results are visually shown.

1 Introduction

A graph is a collection of points, called vertices, connected by lines called edges, denoted by $\alpha(G)$ and $\beta(G)$ respectively. The degree of a vertex is the number of edges connected to it. For more definitions readers can refer following books [1, 10]. A molecular graph represents a molecule's structure by mapping atoms to vertices and chemical bonds to edges. This visual representation helps chemists and researchers understand the structure and properties of molecules, making it easier to analyse and predict their behaviour. A blende of differential and integral operators [13] were used on M polynomial to obtain molecular discriptors based on degree.

The NM-polynomials are refinement of M-polynomials that take into account the neighbor degree sum of each vertex in the graph and they have been used to derive various neighbor degree sum-based indices [14]. These topological indices have a wide range of applications in various fields, particularly in chemistry and materials science, including QSAR, QSPR and drug design. This makes them essential tools in modern scientific research and industry [14, 7, 16].

In this paper, the first Zagreb (M_1^1), second Zagreb (M_2), second modified Zagreb ($^mM_2$), forgotten (F), redefined third Zagreb (ReZG_3), symmetric division (SDD), inverse sum indeg (I) and augmented Zagreb (A) indices are degree-based molecular descriptors. Additionally, the third version of Zagreb (NM_1^1), neighborhood second modified Zagreb (M_2^*), neighborhood second modified Zagreb ($^mNM_2$), neighborhood forgotten (NF), third NDe (ND_3), fifth NDe (ND_5), neighborhood inverse sum indeg (NI) and Sanskruti (S) indices are neighborhood degree-based descriptors.

1.1 Indene molecule

Indene is a bicyclic chemical compound made up of a cyclopentene ring fused to a benzene ring. It is employed as a precursor in the production of many different compounds, including resins and polymers. It is a colourless liquid with a distinct smell. Because of its distinct aromatic qualities, indene is also of interest in organic synthesis and materials science.

Figure 1. Indene molecule.

1.2 Linear chain of indene molecule

Structural derivatives of indene that are expanded in a linear configuration, frequently adding more conjugated systems or functional groups, are referred to as linear chain of indene molecule. These changes have the ability to change the molecule's chemical makeup, which can make it helpful in specific applications like advanced material synthesis or organic semiconductors.

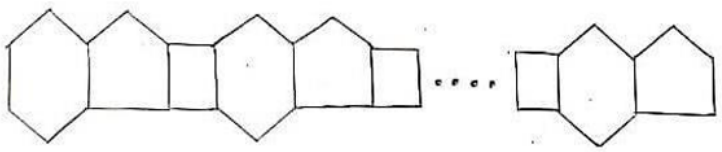

Figure 2. Linear chain of indene molecule.

Closed-forms for M-polynomial and NM-polynomial of linear chain of indene molecular graphs are derived. Additionally, various topological indices are computed by using these polynomials.
The remainder of the manuscript is organized as follows. Section 2 presents the necessary preliminaries for deriving the main findings. Section 3 outlines the methodology used in the study. Section 4 focuses on the computational aspects of linear chain of indene molecule. A comparative analysis of the results is provided in Section 5. Finally, the conclusions of the study are presented in Section 6.

2 Preliminary analysis of linear chain of indene through M-polynomial and NM-polynomial

Definition 2.1. A degree-based topological index defined on graph G as follows:

$$M(G) = \sum_{u,v\in\beta(G)} f(d_u, d_v) \tag{2.1}$$

Where $f(d_u, d_v)$ is the function of degree d_u and d_v of vertices u and v.

Definition 2.2. Neighbor degree sum based topological indices are defined on graph G as follows:

$$NM(G) = \sum_{u,v\in\beta(G)} f(\delta_u, \delta_v) \tag{2.2}$$

Where $f(\delta_u, \delta_v)$ is the function of neighbor degree sum $\delta_u$and δ_v of vertices u and v.

Definition 2.3. M-polynomial [4] of a graph G is formulated as

$$M(G; x, y) = \sum_{i\leq j} m_{(i,j)}(G) x^i y^j \tag{2.3}$$

Where $m_{(i,j)}(G)$, $(i, j \geq 1)$ be the number of edges $u, v \in \beta(G)$ such that $(d_u, d_v) = (i, j)$.

Definition 2.4. NM-polynomial [2] of a graph G is formulated as

$$NM(G;x,y)=\sum_{i\leq j} m^{*}_{(i,j)}(G)x^{i}y^{j} \tag{2.4}$$

Where $m^{*}_{(i,j)}(G)$, $(i,j\geq 1)$ be the number of edges $u,v\in\beta(G)$ such that $(\delta_u,\delta_v)=(i,j)$.

For degree-based topological indices $\eta_u=d_u$, $\eta_v=d_v$, $\lambda(x,y)=M(G;x,y)$ and similarly for neighbor degree sum-based topological indices $\eta_u=\delta_u$, $\eta_v=\delta_v$, $\lambda(x,y)=NM(G;x,y)$.

Table 1. Derivation of degree based and neighbor degree sum based indices.

Topological Indices	**f(η_u,η_v)**	**Derivation from $\lambda(x,y)=M(G;x,y)$ or $NM(G;x,y)$**
M_1^1/NM_1^1	$\sum_{uv\in\beta(G)}(\eta_u+\eta_v)$	$(D_x+D_y)(\lambda(x,y))\Big\vert_{x=1,y=1}$
M_2/M_2^*	$\sum_{uv\in\beta(G)}(\eta_u\eta_v)$	$(D_xD_y)(\lambda(x,y))\Big\vert_{x=1,y=1}$
${}^mM_2/{}^mNM_2$	$\sum_{uv\in\beta(G)}\frac{1}{\eta_u\eta_v}$	$(S_xS_y)(\lambda(x,y))\Big\vert_{x=1,y=1}$
$ReZG_3/ND_3$	$\sum_{uv\in\beta(G)}\eta_u\eta_v(\eta_u+\eta_v)$	$D_xD_y(D_x+D_y)(\lambda(x,y))\Big\vert_{x=1,y=1}$
SDD/ND_5	$\sum_{uv\in\beta(G)}\frac{\eta_u^2+\eta_v^2}{\eta_u\eta_v}$	$(D_xS_y+S_xD_y)(\lambda(x,y))\Big\vert_{x=1,y=1}$
A/S	$\sum_{uv\in\beta(G)}(\frac{\eta_u\eta_v}{\eta_u+\eta_v-2})^3$	$S_x^3Q-2JD_x^3D_y^3(\lambda(x,y))\Big\vert_{x=1}$
I/NI	$\sum_{uv\in\beta(G)}\frac{\eta_u\eta_v}{\eta_u+\eta_v}$	$S_xJD_xD_y(\lambda(x,y))\Big\vert_{x=1}$
F/NF	$\sum_{uv\in\beta(G)}(\eta_u^2+\eta_v^2)$	$(D_x^2+D_y^2)(\lambda(x,y))\Big\vert_{x=1,y=1}$

Where, $D_x(\lambda(x,y))=x\left(\frac{\partial\lambda(x,y)}{\partial x}\right)$, $D_y(\lambda(x,y))=y\left(\frac{\partial\lambda(x,y)}{\partial y}\right)$, $J(\lambda(x,y))=f(x,x)$, $S_x(\lambda(x,y))=\int_0^x\frac{f(t,y)}{t}\,dt$, $S_y(\lambda(x,y))=\int_0^y\frac{f(x,t)}{t}\,dt$, $Q_{-2}\lambda(x,y)=x^{-2}\lambda(x,y)$.

3 A mathematical framework for indices based on M-Polynomial and NM polynomial

We apply the edge partition method to obtain the M-polynomial and NM-polynomial of molecular graph of linear chain of indene molecule and then several degree-based indices and neighbor degree sum-based indices are recovered using a few calculus operators. Further, the correlation between molecular weight and topological indices for linear chain of indene molecule is established.

4 Computational aspects of Linear chain of indene

The structure of indene and linear chain of indene are shown in Figure 1.1 and Figure 1.2 respectively. in the following theorem, the M-polynomial and similarly NM-polynomial of linear chain of indene are computed.

Table 2. Edge partition based on degrees of their end vertices.

(d_u,d_v)	(2,2)	(2,3)	(3,3)
Edge count	5	$6n-2$	$6n-5$

Table 3. Edge partition based on neighbor degree sum of their end vertices.

(δ_u, δ_v)	(4,4)	(4,5)	(5,7)	(5,8)	(6,7)	(6, 8)	(7,7)	(7,8)	(8,8)	(8,9)
Edge count	1	4	3	1	$2n-1$	$4n-5$	1	$n-1$	$2n-2$	$3n-3$

Theorem 4.1. *The M-polynomial of linear chain of indene is* $5x^2y^2+(6n-2)x^2y^3+(6n-5)x^3y^3$.

Proof. The molecular graph of the linear chain of indene is of order $9n$ and size $12n-2$.
From Table 2, $|\beta_1(G)| = 5, \quad |\beta_2(G)| = 6n-2, \quad |\beta_3(G)| = 6n-5$.
From the definition of M polynomial,
$M(G;x,y) = 5x^2y^2 + (6n-2)x^2y^3 + (6n-5)x^3y^3$. □

Theorem 4.2. *For the molecular graph of linear chain of indene molecule,*

(i) $M_1^1 = 66n - 20$.

(ii) $M_2 = 90n - 37$.

(iii) ${}^mM_2 = \frac{5n}{3} + \frac{13}{36}$.

(iv) $ReZG_3 = 250 + 504n$.

(v) $SDD = \frac{3723n}{32} - \frac{2109}{64}$.

(vi) $A = 25n - \frac{13}{3}$.

(vii) $I = \frac{81n}{5} - \frac{49}{10}$.

(viii) $F = 186n - 76$.

Proof. The required results are obtained by substituting Table 1 results into M-polynomial. □

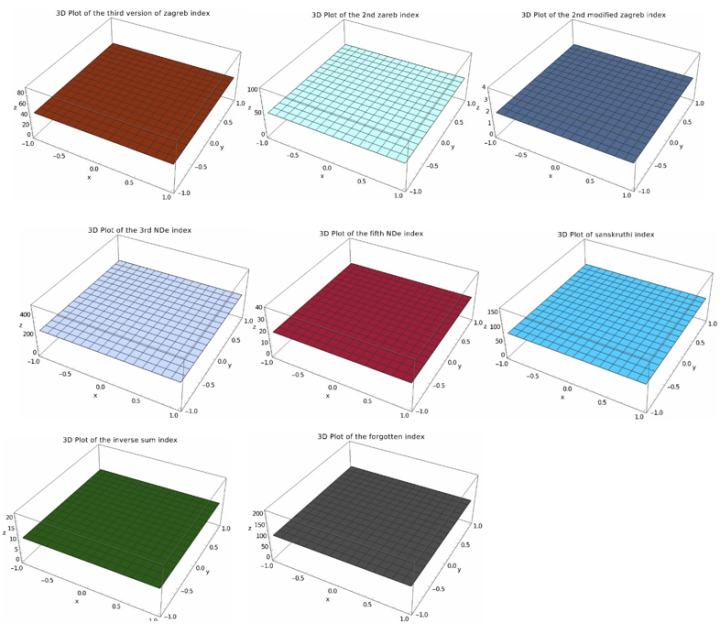

Figure 3. 3D plot of degree based indices of linear chain of indene molecule.

Theorem 4.3. *The NM-polynomial of linear chain of indene molecule is* $x^4y^4+4x^4y^5+3x^5y^7+x^5y^8+(2n-1)x^6y^7+(4n-5)x^6y^8+(n-1)x^7y^8+(2n-2)x^8y^8+(3n-3)x^8y^9$.

Proof. The molecular graph of a linear chain of indene consists of $9n$ vertices and $12n-2$ edges. From Table 3,

$$|\beta_1(G)|=1,\quad |\beta_2(G)|=4,\quad |\beta_3(G)|=3,\quad |\beta_4(G)|=1,$$
$$|\beta_5(G)|=2n-1,\quad |\beta_6(G)|=4n-5,\quad |\beta_7(G)|=1,\quad |\beta_8(G)|=n-1,$$
$$|\beta_9(G)|=2n-2,\quad |\beta_{10}(G)|=3n-3$$

By using the definition of the NM-polynomial:

$$NM(G;x,y)=x^4y^4+4x^4y^5+3x^5y^7+x^5y^8+(2n-1)x^6y^7+(4n-5)x^6y^8 + x^7y^7+(n-1)x^7y^8+(2n-2)x^8y^8+(3n-3)x^8y^9$$

□

Theorem 4.4. *For the molecular graph of linear chain of indene molecule,*

(i) $NM_1^1=180n-74$.

(ii) $M_2^*=676n-392$.

(iii) ${}^mNM_2=\frac{149n}{672}+\frac{1371}{7840}$.

(iv) $ND_3=10340n-7152$.

(v) $ND_5=\frac{2053n}{84}-\frac{209}{56}$.

(vi) $S=\frac{121627194711472n}{125375375125}-\frac{4986051805211833}{804024008000}$.

(vii) $NI=\frac{1035292n}{23205}-\frac{51785299}{278460}$.

(viii) $NF=1374n-784$.

Proof. The required results are obtained by substituting Table 2 results into NM-polynomial. □

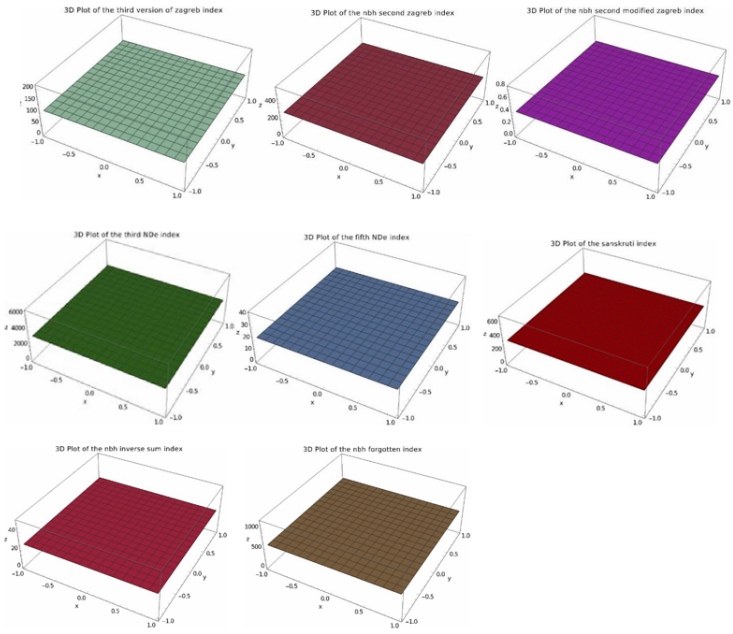

Figure 4. 3D plot of neighbor degree sum based indices of linear chain of indene molecule.

5 Exploring the correlation between molecular weight and topological indices in linear chain of indene

In this section, The relationship between molecular weight of linear chain of indene molecule and a few topological indices, specifically degree based and neighbor degree sum-based indices, is established.

Table 4. Measured values of molecular weight and degree-based indices of the linear chain of indene.

n	$M_w(g/mol)$	M_1^1	M_2	${}^mM_2$	$ReZG_3$	SDD	A	I	F
1	116.16	46	53	2.0277	254	20.6666	83.3906	11.3	110
2	232.32	112	143	3.6944	758	45.6666	199.734	327.5	296
3	348.48	178	233	5.3611	1262	70.6666	316.078	143.7	482
4	464.64	244	323	7.0277	1766	95.6666	432.421	859.9	668
5	580.80	310	413	8.6944	2270	120.6666	548.765	676.1	854
6	696.96	376	503	10.3611	2774	145.6666	665.109	392.3	1040
7	813.12	442	593	12.0277	3278	170.6666	781.453	1108.5	1226
8	929.28	508	683	13.6944	3782	195.6666	897.796	8124.7	1412
9	1045.44	574	773	15.3611	4286	220.6666	1014.14	140.9	1598
10	1161.60	640	863	17.0277	4790	245.6666	1130.48	4157.1	1784

The linear regression model for the molecular weight M_w was developed using the line-of-best-fit approach, which minimizes the sum of squared error terms to provide the most accurate predictions based on the data Table 4.

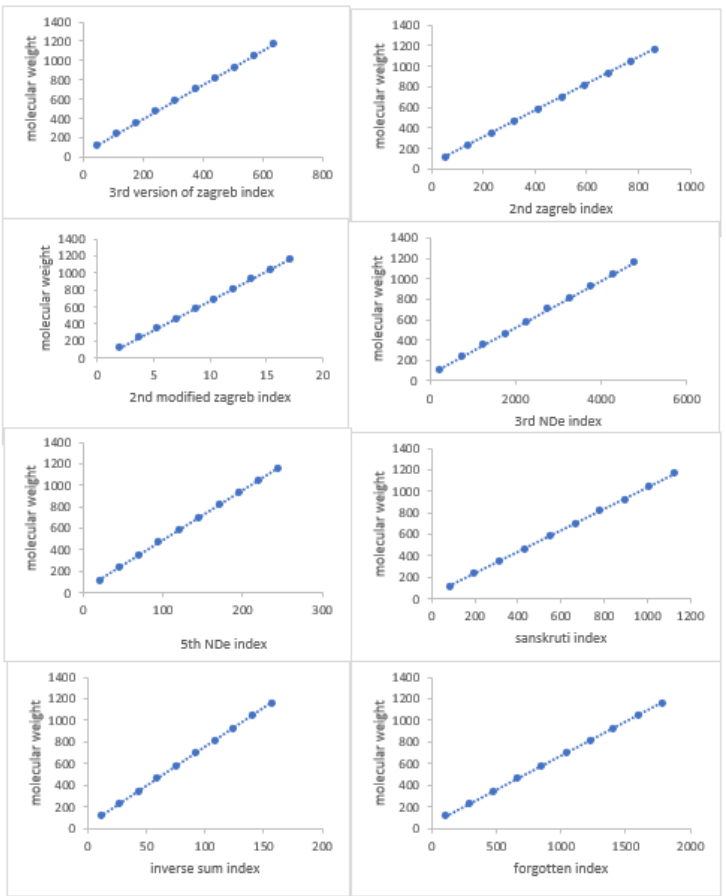

Figure 5. Scatter plot between molecular weight and degree based indices.

$$M_w = 1.759(\pm 0.001606)M_1^1 + 35.37(\pm 0.6295)$$
$$M_w = 1.290(\pm 0.001178)M_2 + 47.92(\pm 0.6195)$$
$$M_w = 69.64(\pm 0.06366)^m M_2 + -24.91(\pm 0.6788)$$
$$M_w = 0.2303(\pm 0.0002104)ReZG_3 + 57.777(\pm 0.6117)$$
$$M_w = 4.643(\pm 0.004241)SDD + 20.35(\pm 0.6416)$$
$$M_w = 0.9976(\pm 0.0009111)A + 33.08(\pm 0.6313)$$
$$M_w = 7.165(\pm 0.006544)I + 35.31(\pm 0.6296)$$
$$M_w = 0.6240(\pm 0.0005700)F + 47.63(\pm 0.6197)$$

Table 5. Correlation coefficient (R) of degree based indices.

Indices	$M_1^1(G)$	$M_2(G)$	${}^mM_2(G)$	$ReZG_3(G)$	$SDD(G)$	$A(G)$	$I(G)$	$F(G)$
Correlation coeffecient(R)	1	1	1	1	1	1	1	1

Table 6. Measured values of molecular weight and neighbor degree sum based indices of the linear chain of indene.

n	M_w	NM_1^1	M_2^*	${}^mNM_2$	ND_3	ND_5	S	NI	NF
1	116.16	106	284	0.3965	3188	20.7083	348.7138	26.0180	590
2	232.32	286	960	0.6183	13528	45.1488	1318.818	270.6330	1964
3	348.48	466	1636	0.8400	23868	69.5892	2288.922	5115.248	3338
4	464.64	646	2312	1.0617	34208	94.0297	3259.026	8159.863	14712
5	580.80	826	2988	1.2835	44548	118.470	24229.131	2204.478	16086
6	696.96	1006	3664	1.5052	54888	142.910	75199.235	5249.093	27460
7	813.12	1186	4340	1.7269	65228	167.351	16169.339	8293.708	28834
8	929.28	1366	5016	1.9486	75568	191.791	7139.444	2338.323	210208
9	1045.44	1546	5692	2.1704	85908	216.232	8109.548	5382.938	311582
10	1161.60	1726	6368	2.3921	96248	240.672	69079.652	8427.553	12956

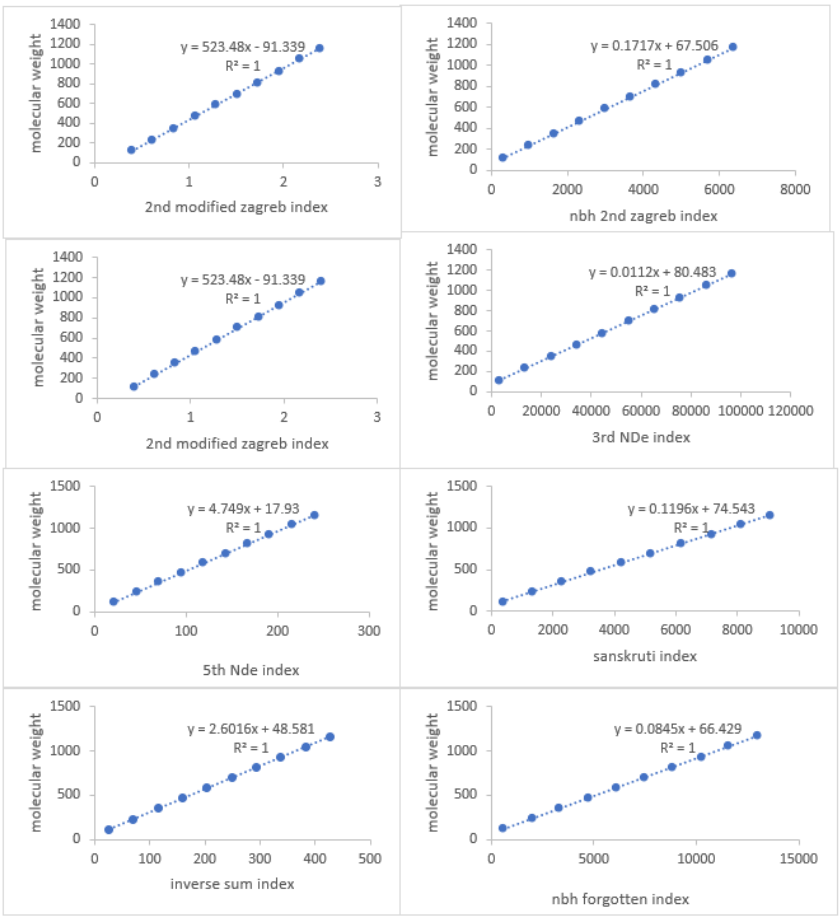

Figure 6. Scatter plot between molecular weight and neibhor degree sum based indices.

The linear regression model for the molecular weight (Mw) was developed using the lineof best-fit approach, which minimizes the sum of squared error terms to provide the most accurate predictions based on the data Table 6.

$$M_w = 0.6453NM_1^1 + 47.75$$
$$M_w = 0.1718M_2^* + 67.36$$
$$M_w = 523.9(\pm 0.0008819)^m NM_2 - 91.61(\pm 0.0001352)$$
$$M_w = 0.01123ND_3 + 80.35$$
$$M_w = 4.753(\pm 3.884 \times 10^{-5})ND_5 + 17.74(\pm 0.005761)$$
$$M_w = 0.1197(\pm 4.821 \times 10^{-9})S + 74.41(\pm 2.640 \times 10^{-5})$$
$$M_w = 2.604(\pm 5.755 \times 10^{-7})NI + 48.42(\pm 0.0001499)$$
$$M_w = 0.08452(\pm 1.453 \times 10^{-5})NF + +66.35(\pm 0.1139)$$

Table 7. Correlation coefficient (R) of the indices

Indices	$NM_1^1(G)$	$M_2^*(G)$	${}^mNM_2(G)$	$ND_3(G)$	$ND_5(G)$	$S(G)$	$NI(G)$	$NF(G)$
Correlation coeffecient(R)	1	1	1	1	1	1	1	1

From the above Table 5 and Table 7, We've found that our research has produced notable outcomes, with linear regression models exhibiting a perfect correlation (R=1) between the molecular weight of indene molecules and degree and neighbour degree sumbased topological indices, indicating the models are highly effective in predicting molecular weight based on these indices. To further authenticate our findings, we investigate the relationship between topological indices and molecular weight (Mw), outlined below.
Molecular weight and index interconnections via M-polynomials.

$$M_w(M_1^1) = 1.76(66n - 20) + 35.2.$$
$$M_w(M_2) = 1.29(-37 + 90n) + 47.76.$$
$$M_w(mM_2) = 69.7\left(\frac{5n}{3} + \frac{13}{36}\right) + 24.86.$$
$$M_w(ND_3) = 0.23 \times (-250 + 504n) + 57.74.$$
$$M_w(ND_5) = 4.64\left(25n - \frac{13}{3}\right) + 20.16.$$
$$M_w(S) = \left(\frac{3723n}{32} - \frac{2109}{64}\right) + 32.77.$$
$$M_w(I) = 7.17\left(\frac{81n}{5} - \frac{49}{10}\right) + 35.16.$$
$$M_w(F) = 0.625(186n - 76) + 47.41.$$

Molecular weight and neighbor degree sum based index via NM-polynomials,

$$\begin{aligned}
Mw(NM_1^1) &= 116.15994n.\\
Mw(M_2^*) &= 116.1368n.\\
Mw({}^mNM_2) &= 293\left(\frac{149n}{672}+\frac{1371}{7840}\right).\\
Mw(ND_3) &= 116.1182n.\\
Mw(ND_5) &= 5.61\left(\frac{2053n}{84}-\frac{209}{56}\right).\\
Mw(S) &= 0.11973\,(970.1043n-621.3904)+74.405.\\
Mw(NI) &= 116.1597n.\\
Mw(NF) &= 116.13048n.
\end{aligned}$$

6 Conclusion

This paper investigates a linear chain of indene using graph theoretical approach. Edge partitions based on vertex degree and vertex neighbor degrees are derived. Further, various molecular descriptors are computed using M and NM-polynomial approach.Additionally, Correlation between molecular weight and a few topological indices for a linear chain of indene molecule is established. Notably, these indices demonstrate remarkable isomer discrimination ability compared to others. As valuable molecular descriptors in chemical graph theory, they facilitate establishing structure-property and structure-activity relationships. Through mathematical formulations, our findings provide insights into the properties and activities of the considered structures.

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