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Research Article

Investigating Some Novel Closed Neighborhood Topological Indices of Nanostructures

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Abstract. Chemical graph theory plays an essential role in mathematical chemistry by representing chemical compounds as molecular graphs and utilizing graph-theoretical methods to analyze them. Topological indices (TIs) are numerical parameters that describe the structure of a molecular graph. In this work, we introduced newly defined seven closed neighborhood topological indices and compute the same for some standard classes of graphs. Later we examine these indices with some physical properties of octane isomers. Our indices exhibits highly correlation with acentric factor of octane isomers. Additionally we derive the expression for seven TI's of $TUC_4C_8(R)[p,q]$ nanostructures as well as subdivision graph and the line graph of the subdivision graph of $TUC_4C_8(R)[p,q]$ nanostructures.

Keywords. Closed neighborhood topological indices, Octane isomers

Mathematics Subject Classification (2020). Primary 05C07, Secondary 05C76, 05C35, 05C90

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1. Introduction

In the field of molecular science, one of the key challenges lies in effectively visualizing chemical compounds and accurately predicting their properties. In recent years, graph theory has proven to be a valuable approach in addressing these issues. A molecular graph is a type of simple graph in which atoms are represented by vertices and chemical bonds by edges. A powerful concept

derived from molecular graphs is that of topological indices. These are numerical descriptors that quantify specific aspects of a molecule's structure, such as atom connectivity and path lengths. It provides a bridge between molecular structure and physicochemical properties, and have become indispensable in computational chemistry, particularly in the development of predictive models. These indices are particularly important in QSPR and QSAR modeling, which link molecular structure to properties or biological activities (Karelson [11]).

In this article, we studied simple, connected and undirected graphs. Let $X = (V, E)$ represent a simple, connected graph, where V is the set of vertices and E is the set of edges. The number of vertices in the graph is called the order and is denoted by n, while the number of edges is referred to as the size, denoted by m. When two vertices u and v are directly connected by an edge, we say they are adjacent, and the edge connecting them is written as uv. The degree of a vertex $u \in V(X)$ written as $d_X(u)$, is the number of edges incident to u. The neighborhood of a vertex u is defined as the set of vertices adjacent to u. The degree sum of neighbor of a vertex u is $S_X(u) = \sum_{u \in N_X(u)} d_X(u)$. Let $N_X[u]$ be the closed neighborhood of a vertex u, that includes u and its neighbors. The degree sum of closed neighbor of a vertex u is $S_X[u] = \sum_{u \in N_X[u]} S_X(u) + d_X(u)$ (Basavanagoud *et al*. [3]). For additional graph terms and notations, refer to the works of Bondy and Murty [4], and Harary [10].

First Zagreb index $M_1(X)$ and second Zagreb index $M_2(X)$ were introduced by Gutman and Trinajstić [9]. These indices are defined as follows:

$$M_1(X) = \sum_{uv \in E(X)} (d_X(u) + d_X(v)), \tag{1.1}$$

$$M_2(X) = \sum_{uv \in E(X)} d_X(u) d_X(v). \tag{1.2}$$

In 2015, Furtula and Gutman [5] introduced a graph invariant known as the Forgotten index, or the F-index. This index is defined as follows:

$$F(X) = \sum_{uv \in E(X)} (d_X(u)^2 + d_X(v)^2). \tag{1.3}$$

The Sombor index was recently introduced by Gutman [8] within the field of chemical graph theory. This index is a vertex-degree-based topological measure, denoted as SO and is defined as follows:

$$SO(X) = \sum_{uv \in E(X)} \sqrt{d_X(u)^2 + d_X(v)^2}. \tag{1.4}$$

In 1975, Randic [14] introduced the Randic index, which is defined as:

$$R(X) = \sum_{uv \in E(X)} \frac{1}{\sqrt{d_X(u) d_X(v)}}. \tag{1.5}$$

In 2013, Shirdel *et al*. [15] unveiled the first Hyper-Zagreb index, which is defined as follows:

$$HM_1(X) = \sum_{uv \in E(X)} (d_X(u) + d_X(v))^2. \tag{1.6}$$

In 2016, Gao *et al*. [7] defined a new distance-based Zagreb index, which they referred to as the second Hyper-Zagreb index, and it is given by:

$$HM_2(X) = \sum_{uv \in E(X)} [d_X(u) d_X(v)]^2. \tag{1.7}$$

The first neighborhood Zagreb index (Basavanagoud *et al*. [2]) is defined as

$$NM_1(X) = \sum_{u \in V(X)} S_X(u)^2. \tag{1.8}$$

Another version of first neighborhood Zagreb index is

$$NM_1(X) = \sum_{uv \in E(X)} S_X(u) + S_X(v). \tag{1.9}$$

The first closed neighborhood Zagreb index (Basavanagoud *et al*. [3]) is defined as

$$CM_1(X) = \sum_{u \in V(X)} S_X[u]^2. \tag{1.10}$$

In recent days, several mathematicians and chemists are endeavoring to develop novel indices for forecasting physicochemical behavior of chemical compounds. In this paper we introduce newly defined seven closed neighborhood topological indices. It is expressed as:
The first closed neighborhood modified Zagreb index ($CM_1(X)$) is defined as

$$CM_1(X) = \sum_{uv \in E(X)} S_X[u] + S_X[v]. \tag{1.11}$$

The second closed neighborhood Zagreb index ($CM_2(X)$) is expressed as

$$CM_2(X) = \sum_{uv \in E(X)} S_X[u] S_X[v]. \tag{1.12}$$

The closed neighborhood Forgotten index ($CF(X)$) is given as

$$CF(X) = \sum_{uv \in E(X)} S_X[u]^2 + S_X[v]^2. \tag{1.13}$$

The closed neighborhood sombor index ($CSO(X)$) is defined as

$$CSO(X) = \sum_{uv \in E(X)} \sqrt{S_X[u]^2 + S_X[v]^2}. \tag{1.14}$$

The closed neighborhood randic index ($CR(X)$) is defined as

$$CR(X) = \sum_{uv \in E(X)} \frac{1}{\sqrt{S_X[u] S_X[v]}}. \tag{1.15}$$

The first and second closed neighborhood hyper Zagreb index is expressed as

$$CHM_1(X) = \sum_{uv \in E(X)} (S_X[u] + S_X[v])^2, \tag{1.16}$$

$$CHM_2(X) = \sum_{uv \in E(X)} (S_X[u] S_X[v])^2. \tag{1.17}$$

The following discussion is organized into five sections. In Section 2, we study mathematical properties of closed neighborhood topological indices. In Sections 3 and 4 we explore its chemical applications through regression models of octane isomers. The closed neighborhood topological indices for some standard classes of graphs and some nanostructures is examined in Sections 5 and Section 6.

2. Mathematical Properties of Closed Neighborhood Topological Indices

Theorem 2.1. *Let X be a simple connected graph. Then*

$$CM_1(X) = NM_1(X) + M_1(X).$$

Proof. By using equation (1.11), we have

$$\begin{aligned} CM_1(X) &= \sum_{uv\in E(X)} S_X[u] + S_X[v] \\ &= \sum_{uv\in E(X)} [S_X(u) + d_X(u)] + [S_X(v) + d_X(v)] \\ &= NM_1(X) + M_1(X). \end{aligned}$$

□

Theorem 2.2. *Let X be a simple connected graph. Then*

$$CM_2(X) = NM_1(X) + ND(X) + M_2(X).$$

Proof. By using equation (1.12), we have

$$\begin{aligned} CM_2(X) &= \sum_{uv\in E(X)} S_X[u]S_X[v] \\ &= \sum_{uv\in E(X)} [S_X(u) + d_X(u)][S_X(v) + d_X(v)] \\ &= NM_1(X) + ND(X) + M_2(X), \end{aligned}$$

where $ND(X) = \sum_{uv\in E(X)} [S_X(u)d_X(v) + d_X(u)S_X(v)]$. □

Theorem 2.3. *Let X be a simple connected graph. Then*

$$CF(X) = NF(X) + F(X) + 2ND_1(X).$$

Proof. By using equation (1.13), we have

$$\begin{aligned} CF(X) &= \sum_{uv\in E(X)} S_X[u]^2 + S_X[v]^2 \\ &= \sum_{uv\in E(X)} [S_X(u) + d_X(u)]^2 + [S_X(v) + d_X(v)]^2 \\ &= NF(X) + F(X) + 2ND_1(X), \end{aligned}$$

where $ND_1(X) = \sum_{uv\in E(X)} [S_X(u)d_X(u) + S_X(v)d_X(v)]$. □

Theorem 2.4. *Let X be a simple connected graph. Then*

$$CSO(G) = \sqrt{NF(X) + F(X) + 2ND_1(X)}.$$

Proof. By using equation (1.14), we have

$$\begin{aligned} CSO(X) &= \sum_{uv\in E(X)} \sqrt{S_X[u]^2 + S_X[v]^2} \\ &= \sum_{uv\in E(X)} \sqrt{[S_X(u) + d_X(u)]^2 + [S_X(v) + d_X(v)]^2} \\ &= \sqrt{NF(X) + F(X) + 2ND_1(X)}. \end{aligned}$$

□

Theorem 2.5. *Let X be a simple connected graph. Then*

$$CR(X) = \frac{1}{\sqrt{NM_1(X) + ND(X) + M_2(X)}}.$$

Proof. By using equation (1.15), we have

$$\begin{aligned} CR(X) &= \sum_{uv\in E(X)} \frac{1}{\sqrt{S_X[u]S_X[v]}} \\ &= \sum_{uv\in E(X)} \frac{1}{\sqrt{[S_X(u)+d_X(u)][S_X(v)+d_X(v)]}} \\ &= \frac{1}{\sqrt{NM_1(X)+ND(X)+M_2(X)}}. \end{aligned}$$

□

Theorem 2.6. *Let X be a simple connected graph. Then*

$$CHM_1(X) = NF(X)+F(X)+2ND_1(X)+2(NM_2(X)+ND(X)+M_2(X).$$

Proof. By using equation (1.16), we have

$$\begin{aligned} CHM_1(X) &= \sum_{uv\in E(X)} (S_X[u]+S_X[v])^2 \\ &= \sum_{uv\in E(X)} ([S_X(u)+d_X(u)]+[S_X(v)+d_X(v)])^2 \\ &= \sum_{uv\in E(X)} [S_X(u)+d_X(u)]^2+[S_X(v)+d_X(v)]^2+2([S_X(u)+d_X(u)][S_X(v)+d_X(v)]) \\ &= NF(X)+F(X)+2ND_1(X)+2(NM_2(X)+ND(X)+M_2(X). \end{aligned}$$

□

Theorem 2.7. *Let X be a simple connected graph. Then*

$$CHM_2(X) = (NM_1(X)+ND(X)+M_2(X))^2$$

Proof. By using equation (1.17), we have

$$\begin{aligned} CHM_2(G) &= \sum_{uv\in E(X)} (S_X[u]S_X[v])^2 \\ &= \sum_{uv\in E(X)} ([S_X(u)+d_X(u)][S_X(v)+d_X(v)])^2 \\ &= (NM_1(X)+ND(X)+M_2(X))^2. \end{aligned}$$

□

3. Chemical Applicability of Closed Neighborhood Topological Indices

The correlation coefficient ($|R|$) is an important statistical value for measuring the strength and direction of the linear relationship between predicted and observed values in QSAR and QSPR analysis. In QSPR/QSAR modeling, a correlation coefficient greater than 0.8 is considered statistically significant and very desirable, indicating that the topological index utilized is an excellent predictor that can be confidently included in the model. Thus, determining $|R|$ is an important step in assessing the relevance and quality of descriptors used to create predictive models in computational chemistry and drug design.

This section explores the linear regression analysis between some closed neighborhood topological indices and various properties, such as acentric factor (*AcentFac*) and entropy (S) to octane isomers. We have observed that these topological indices are highly correlated with acentric factor. The physico-chemical properties of octane isomers (column 1-3) were sourced from the International Academy of Mathematical Chemistry website (URL: http://www.iamc-online.org/) (Kuanar *et al*. [12]), and rest of the columns are obtained by the formulae from (1.11)-(1.17) as detailed in Table 1.

Table 1. Physico-chemical properties of Octane isomers

Octane Isomer	*AcentFac*	*S*	$CM_1(X)$	$CM_2(X)$	$CF(X)$	$CR(X)$	$CSO(X)$	$CHM_1(X)$	$CHM_2(X)$
n-octane	0.397898	111.67	74	198	406	1.3815	52.7382	802	6138
2-methyl-heptane	0.377916	109.84	80	228	480	1.2825	57.3700	936	8154
3-methyl-heptane	0.371002	111.26	88	275	626	1.2375	64.2077	1176	13313
4-methyl-heptane	0.371504	109.32	82	244	522	1.2984	59.0711	1010	10196
3-ethyl-hexane	0.362472	109.43	84	257	562	1.2968	60.8847	1076	11899
2,2-dimethyl-hexane	0.339426	103.42	92	300	658	1.1501	66.5696	1258	14688
2,3-dimethyl-hexane	0.348247	108.02	90	285	640	1.1912	65.6140	1210	13067
2,4-dimethyl-hexane	0.344223	106.98	89	278	635	1.2049	64.9887	1191	11340
2,5-dimethyl-hexane	0.356883	105.72	86	259	554	1.1845	61.9475	1072	10339
3,3-dimethyl-hexane	0.322596	104.74	96	326	744	1.1486	70.2541	1396	18566
3,4-dimethyl-hexane	0.340345	106.59	98	335	800	1.1485	72.5292	1470	20953
2-methyl-3-ethyl pentane	0.332433	106.06	92	300	686	1.1949	67.4350	1286	16296
3-methyl-3-ethyl pentane	0.306899	101.48	100	349	830	1.1313	74.0455	1528	22135
2,2,3-trimethyl-pentane	0.300816	101.61	104	368	872	1.0471	76.8235	1608	23024
2,2,4-trimethyl-pentane	0.30537	104.03	98	335	740	1.0622	71.1410	1410	18173
2,3,3-trimethyl-pentane	0.293177	102.02	106	379	916	1.0356	78.730	1674	24813
2,3,4-trimethyl-pentane	0.317422	102.3	98	360	764	1.0888	72.1599	1420	18496
2,2,3,3-tetramethylbutane	0.25294	93.06	118	451	1118	0.8999	88.0546	2022	32791

The linear equation for each physical property acentric factor (*AcentFac*) and entropy (S) with closed neighborhood topological indices are obtained using R software (R Core Team [13]) based on the data provided in Table 1.

4. Regression Models

1. For Acentric factor (AcentFac)

$$AcentFac = 0.6409905(\pm 35.37) - 0.0032800(\pm 0.0001936)CM_1(X),$$

$$AcentFac = 5.060e-01(\pm 1.080e-02) - 5.542e-04(\pm 3.452e-05)CM_2(X),$$

$$AcentFac = 4.729e-01(\pm 1.051e-02) - 1.966e-04(\pm 1.465e-05)CF(X),$$
$$AcentFac = 0.6103346(\pm 0.0179413) - 0.0040358(\pm 0.0002618)CSO(X),$$
$$AcentFac = -0.01197(\pm 0.02355) + 0.29828(\pm 0.02011)CR(X),$$
$$AcentFac = 4.877e-01(\pm 1.054e-02) - 1.161e-04(\pm 7.871e-06)CHM_1(X),$$
$$AcentFac = 4.174e-01(\pm 7.554e-03) - 4.990e-06(\pm 4.290e-07)CHM_2(X).$$

2. For entropy (S)

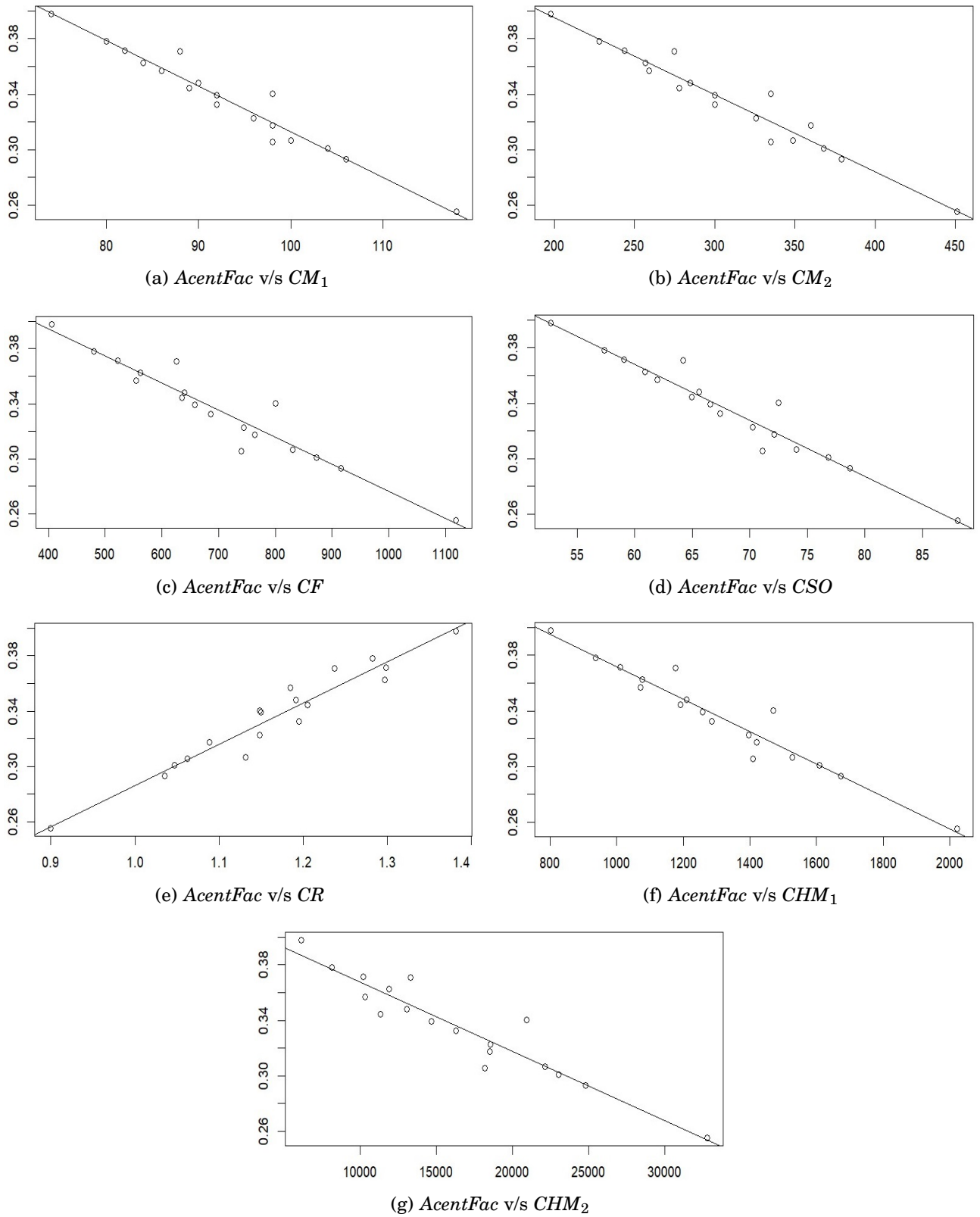
$$S = 142.1534708(\pm 3.95581) - 0.39482(\pm 0.04226)CM_1(X),$$
$$S = 125.982642(\pm 2.227242) - 0.066989(\pm 0.007118)CM_2(X),$$
$$S = 121.885695(\pm 2.010617) - 0.023620(\pm 0.002803)CF(X),$$
$$S = 138.35906(\pm 3.74594) - 0.48427(\pm 0.05466)CSO(X),$$
$$S = 62.612(\pm 4.161) + 36.714(\pm 3.553)CR(X),$$
$$S = 123.668305(\pm 2.126848) - 0.013956(\pm 0.001588)CHM_1(X),$$
$$S = 1.153e+02(\pm 1.324e+00) - 6.015e-04(\pm 7.519e-05)CHM_2(X).$$

Table 2. Correlation coefficient and residual standard error of regression models for Acentric factor

Topological index	Absolute value of the correlation coefficient ($\|R\|$)	Residual standard error
$CM_1(X)$	0.9732	0.0083
$CM_2(X)$	0.9703	0.0088
$CF(X)$	0.9583	0.0104
$CSO(X)$	0.9679	0.0091
$CR(X)$	0.9655	0.0095
$CHM_1(X)$	0.9651	0.0095
$CHM_2(X)$	0.9456	0.0118

Table 3. Correlation coefficient and residual standard error of regression models for Entropy

Topological index	Absolute value of the correlation coefficient ($\|R\|$)	Residual standard error
$CM_1(X)$	0.9193	1.8326
$CM_2(X)$	0.9203	1.8213
$CF(X)$	0.9033	1.9968
$CSO(X)$	0.9114	1.9161
$CR(X)$	0.9325	1.6811
$HM_1(X)$	0.9101	1.9294
$HM_2(X)$	0.8944	2.0826



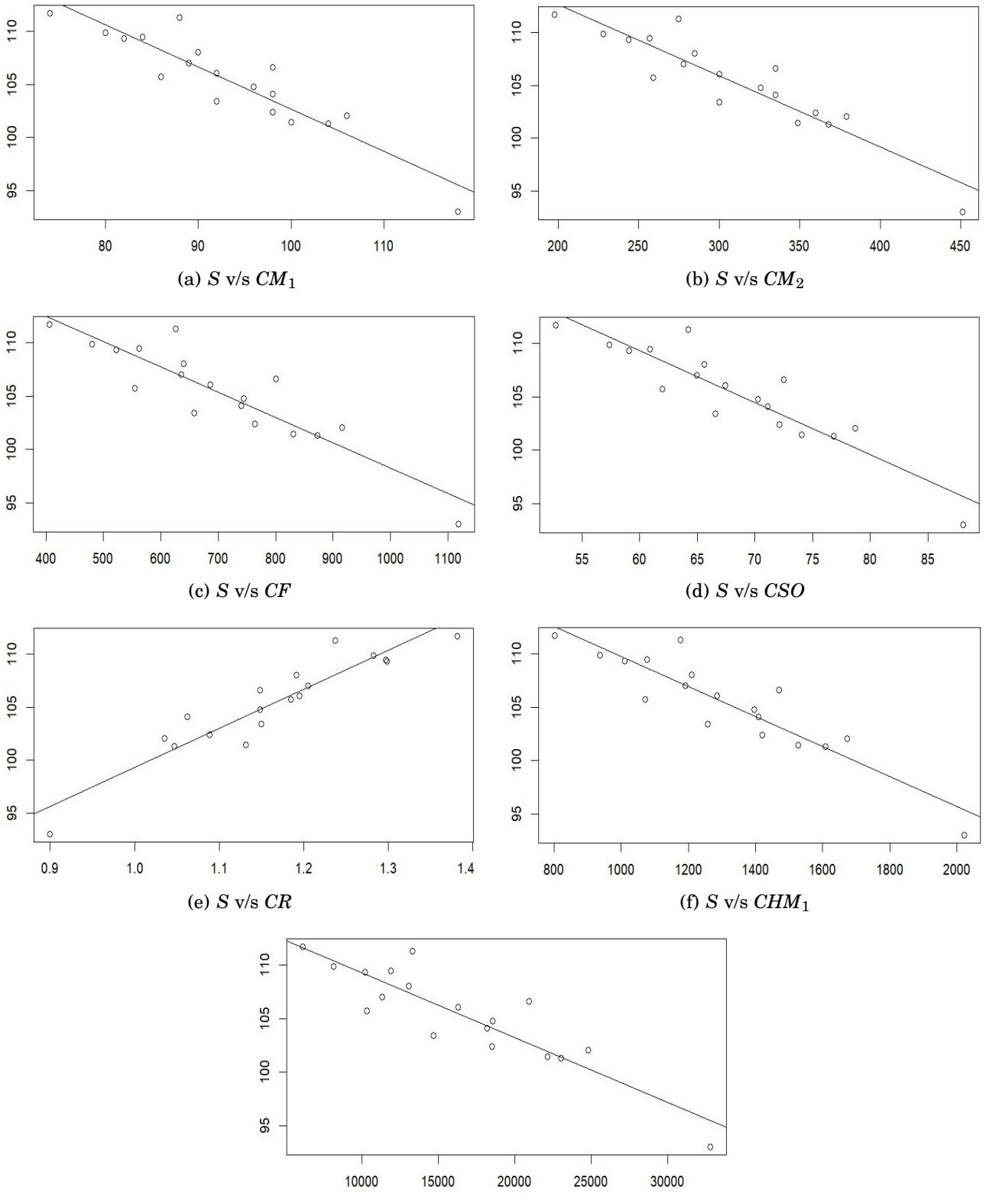
(a) *AcentFac* v/s CM_1 (b) *AcentFac* v/s CM_2

(c) *AcentFac* v/s *CF* (d) *AcentFac* v/s *CSO*

(e) *AcentFac* v/s *CR* (f) *AcentFac* v/s CHM_1

(g) *AcentFac* v/s CHM_2

Figure 1. Linear regression of *AcentFac* v/s topological indices



(a) S v/s CM_1 (b) S v/s CM_2

(c) S v/s CF (d) S v/s CSO

(e) S v/s CR (f) S v/s CHM_1

(g) S v/s CHM_2

Figure 2. Linear regression of S v/s topological indices

5. The Closed Neighborhood Topological Indices of Some Classes of Graphs

In this section, we obtain the expressions of closed neighborhood topological indices for some standard classes of graphs.

Theorem 5.1. *For a path P_n with $n \geq 5$,*

(i) $CM_1(P_n) = 12n - 22$,

(ii) $CM_2(P_n) = 36n - 90$,

(iii) $CF(P_n) = 72n - 170$,

(iv) $CSO(P_n) = 8.4852n - 15.1441$,

(v) $CR(P_n) = 0.1666n - 0.0481$,

(vi) $CHM_1(P_n) = 144n - 350$,

(vii) $CHM_2(P_n) = 1296n - 4230$.

Table 4. Edge partition of the path based on closed neighborhood degree

$(d_{P_n}[u], d_{P_n}[v])$, where $uv \in E(P_n)$	(3,5)	(5,6)	(6,6)
Number of edges	2	2	$n-5$

Proof. The path graph has n vertices and $n-1$ edges. For $n \geq 5$, the closed neighborhood degree of two pendant vertex is 3, the closed neighborhood degree of two vertices which is adjacent to pendant vertex is 5 and the closed neighborhood degree of remaining vertices is 6. Therefore, we get the edge partition based on the closed neighborhood degree of vertices as shown in Table 4. Using information in Table 4 to the formulae (1.11)-(1.17), we get the desired result. □

Theorem 5.2. *For a cycle C_n with $n \geq 3$,*

(i) $CM_1(C_n) = 12n$,

(ii) $CM_2(C_n) = 36n$,

(iii) $CF(C_n) = 72n$,

(iv) $CSO(C_n) = n\sqrt{72}$,

(v) $CR(C_n) = \frac{n}{6}$,

(vi) $CHM_1(C_n) = 144n$,

(vii) $CHM_2(C_n) = 1296n$.

Proof. The cycle graph has n vertices and m edges. For $n \geq 3$, the closed neighborhood degree of each vertex is 6. Therefore, using formulae (1.11)-(1.17) we get the desired result. □

Theorem 5.3. *For a complete graph K_n with $n \geq 3$,*

(i) $CM_1(K_n) = n(n-1)[n^2 - n]$,

(ii) $CM_2(K_n) = \frac{n(n-1)}{2}[n^2 - n]^2$,

(iii) $CF(K_n) = n(n-1)[(n-1)^2 + (n-1)]^2$,

(iv) $CSO(K_n) = \frac{n^2(n-1)^2}{\sqrt{2}}$,

(v) $CR(K_n) = \frac{1}{2}$,

(vi) $CHM_1(K_n) = 2n^3(n-1)^3$,

(vii) $CHM_2(K_n) = \frac{n^5(n-1)^5}{2}$.

Proof. The complete graph has n vertices and $n(n-1)/2$ edges. For $n \geq 3$, the closed neighborhood degree of each vertex is $[(n-1)^2 + (n-1)]$. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 5.4. *For a star graph $K_{1,n}$ with $n \geq 3$,*

(i) $CM_1(K_{1,n}) = n(3n+1)$,

(ii) $CM_2(K_{1,n}) = 2n^2[n+1]$,

(iii) $CF(K_{1,n}) = n[5n^2 + 2n + 1]$,

(iv) $CSO(K_{1,n}) = n\sqrt{5n^2 + 2n + 1}$,

(v) $CR(K_{1,n}) = \frac{1}{\sqrt{2}}\left[\frac{n}{\sqrt{n(n+1)}}\right]$,

(vi) $CHM_1(K_{1,n}) = n(3n+1)^2$,

(vii) $CHM_2(K_{1,n}) = n(2n^2 + 2n)^2$.

Proof. The star graph [10] has $n+1$ vertices and n edges. For $n \geq 3$, the closed neighborhood degree of n pendant vertices are $n+1$ and the closed neighborhood degree of center vertex is $2n$. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 5.5. *For a crown graph S_n^0 with $n \geq 3$,*

(i) $CM_1(S_n^0) = 2n^2(n-1)^2$,

(ii) $CM_2(S_n^0) = n(n-1)^3$,

(iii) $CF(S_n^0) = n(n-1)[2n^4 - 4n^3 + 2n^2]$,

(iv) $CSO(S_n^0) = \sqrt{2}n^2(n-1)^2$,

(v) $CR(S_n^0) = 1$,

(vi) $CHM_1(S_n^0) = 4n^3(n-1)^3$,

(vii) $CHM_2(S_n^0) = n^5(n-1)^5$.

Proof. The crown graph [6] has $2n$ vertices and $n(n-1)$ edges. For $n \geq 3$, the closed neighborhood degree of each vertex is $[(n-1)^2 + (n-1)]$. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 5.6. *For a ladder graph L_n with $n \geq 5$,*

(i) $CM_1(L_n) = 72n - 100$,

(ii) $CM_2(L_n) = 432n - 840$,

(iii) $CF(L_n) = 864n - 1612$,

(iv) $CSO(L_n) = 50.9116n - 69.4075$,

(v) $CR(L_n) = 0.25n + 0.1048$,

(vi) $CHM_1(L_n) = 1728n - 3292$,

(vii) $CHM_2(L_n) = 62208n - 162808$.

Table 5. Edge partition of the ladder graph based on closed neighborhood degree

$(d_{L_n}[u], d_{L_n}[v])$, where $uv \in E(L_n)$	$(7,7)$	$(7,11)$	$(11,11)$	$(11,12)$	$(12,12)$
Number of edges	2	4	2	4	$(3n-14)$

Proof. The ladder graph [6] has $2n$ vertices and $n + 2(n-1)$ edges. For $n \geq 5$, the closed neighborhood degree of both end vertices is 7, the closed neighborhood degree of vertices which is adjacent to end vertex is 11 and the closed neighborhood degree of remaining vertices is 12. Therefore, we get the edge partition based on the closed neighborhood degree of vertices as shown in Table 5. Using information in Table 5 to the formulae (1.11)-(1.17), we get the desired result. □

Theorem 5.7. *For a wheel graph W_n with $n \geq 4$,*

(i) $CM_1(W_n) = n(7n+27)$,

(ii) $CM_2(W_n) = n(5n^2+54n+81)$,

(iii) $CF(W_n) = n(19n^2+54n+243)$,

(iv) $CSO(W_n) = n[\sqrt{2}(n+9) + \sqrt{17n^2+18n+81}]$,

(v) $CR(W_n) = \frac{1}{2}\left[\frac{n}{\sqrt{n(n+9)}}\right]$,

(vi) $CHM_1(W_n) = n(27n^2+126n+243)$,

(vii) $CHM_2(W_n) = n[(n+9)^4 + (4n^2+36n)^2]$.

Proof. The wheel graph [6] has $n+1$ vertices and $2n$ edges. For $n \geq 4$, the closed neighborhood degree of each corner vertex is $9+n$ and the closed neighborhood degree of the center vertex is $4n$. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 5.8. *For a gear graph G_n with $n \geq 3$,*

(i) $CM_1(G_n) = n(7n+37)$,

(ii) $CM_2(G_n) = n(4n^2+44n+112)$,

(iii) $CF(G_n) = n(19n^2+42n+275)$,

(iv) $CSO(G_n) = n[\sqrt{(17n^2+14n+49)} + 2\sqrt{(n^2+14n+113)}]$,

(v) $CR(G_n) = \frac{n}{2\sqrt{n(n+7)}} + \frac{n}{\sqrt{2(n+7)}}$,

(vi) $CHM_1(G_n) = n(27n^2+130n+499)$,

(vii) $CHM_2(G_n) = n(16n^4+224n^3+912n^2+1792n+6272)$.

Proof. The gear graph [1] has $2n+1$ vertices and $3n$ edges. By definition of G_n, the center vertex is of degree n and outer layer vertex is of degree alternative 3 and 2. The closed neighborhood degree of the center vertex is $4n$, the closed neighborhood degree of each corner vertex adjacent to the center vertex is $n+7$ and the closed neighborhood degree of remaining vertices is 8. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 5.9. *For a friendship graph F_n with $n \geq 2$,*

(i) $CM_1(F_n) = n(20n + 16)$,

(ii) $CM_2(F_n) = 4n(7n^2 + 16n + 4)$,

(iii) $CF(F_n) = n(88n^2 + 64n + 64)$,

(iv) $CSO(F_n) = \sqrt{2n}(2n + 4) + 4n\sqrt{(10n^2 + 4n + 4)}$,

(v) $CR(F_n) = \frac{n}{2(n+2)} + \frac{n}{\sqrt{n(3n+6)}}$,

(vi) $CHM_1(F_n) = n(144n^2 + 192n + 96)$,

(vii) $CHM_2(F_n) = n(2n + 4)^4 + 2n(12n^2 + 24n)^2$.

Proof. The friendship graph [6] has $2n+1$ vertices and $3n$ edges. By definition of F_n, $2n$ vertices are of degree 2 and the center vertex is of degree $2n$. The closed neighborhood degree of the center vertex is $6n$ and the closed neighborhood degree of the remaining vertices is $2n + 4$. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 5.10. *For a cocktail party graph $CP_{n,n}$ with $n \geq 2$,*

(i) $CM_1(CP_{n,n}) = 8n(n-1)^2(2n-1)$,

(ii) $CM_2(CP_{n,n}) = 2n(n-1)(4n^2 - 6n + 2)^2$,

(iii) $CF(CP_{n,n}) = 16n(n-1)^3[4(n-1)^2 + 4(n-1) + 1]$,

(iv) $CSO(CP_{n,n}) = 4\sqrt{2}n(n-1)^2(2n-1)$,

(v) $CR(CP_{n,n}) = \frac{n}{2n-1}$,

(vi) $CHM_1(CP_{n,n}) = 16n(n-1)^3[4(n-1)^2 + 4(n-1) + 1]$,

(vii) $CHM_2(CP_{n,n}) = 2n(n-1)[4(n-1)^2 + 2(n-1)]^4$.

Proof. The cocktail party graph [6] has $2n$ vertices and $2n(n-1)$ edges. For $n \geq 2$, the closed neighborhood degree of the each vertex is $4(n-1)^2 + 2(n-1)$. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 5.11. *For a helm graph H_n with $n \geq 3$,*

(i) $CM_1(H_n) = 3n(3n + 19)$,

(ii) $CM_2(H_n) = 6n(13 + n)(n + 3)$,

(iii) $CF(H_n) = n(29n^2 + 104n + 701)$,

(iv) $CSO(H_n) = n[\sqrt{26n^2 + 26n + 169} + \sqrt{2}(13 + n) + \sqrt{(n^2 + 26n + 194)}]$,

(v) $CR(H_n) = n\left[\frac{1}{5n(13+n)} + \frac{1}{13+n} + \frac{1}{5(13+n)}\right]$,

(vi) $CHM_1(H_n) = n(41n^2 + 296n + 1169)$,

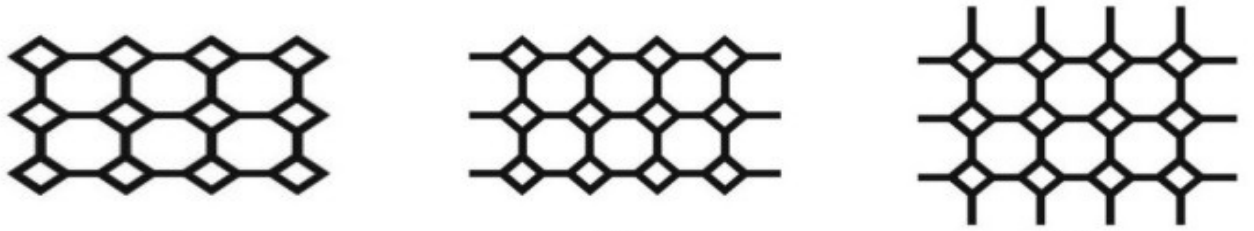
(vii) $CHM_2(H_n) = n(13 + n)^2(26n^2 + 26n + 194)$.

Proof. The helm graph [6] has $2n + 1$ vertices and $3n$ edges. By definition of H_n, the center vertex is of degree n and outer pendent vertex is of degree 1 and the rest is of degree 4. The closed neighborhood degree of center vertex is $5n$, the closed neighborhood degree of outer pendent vertex is 5 and the closed neighborhood degree of remaining vertices is $13 + n$. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

6. Closed Neighborhood Topological Indices of Some Nanostructures

Nanostructures are materials with at least one dimension in the nanometer range, often exhibiting unique physical, chemical, and biological properties due to their small size. These structures can take various forms, including 2D lattices, nanotubes and nanotorus.

A *2D lattice* is a flat, two-dimensional arrangement of atoms or molecules, such as graphene, that exhibits exceptional properties like high conductivity and strength. *Nanotubes* often made of carbon, are cylindrical structures with remarkable mechanical and electrical properties, used in a wide range of applications from electronics to materials science. Meanwhile, a *nanotorus* is a unique toroidal (doughnut-shaped) nanostructure that can possess distinct magnetic, electronic, and catalytic properties due to its circular geometry. Together, these nanostructures represent a versatile toolkit for advancing technologies across fields such as electronics, energy, medicine, and materials science. The nanostructures of $TUC_4C_8(R)[p,q]$, where p and q represents the number of squares in each row and the number of rows of squares.



(a) 2D-lattice $TUC_4C_8(R)[4,3]$ (b) Nanotube $TUC_4C_8(R)[4,3]$ (c) Nanotorus $TUC_4C_8(R)[4,3]$

Figure 3

Theorem 6.1. *Let X be 2D-lattice of $TUC_4C_8(R)[p,q]$. Then*

(i) $CM_1(X) = 92(p+q)+8$,

(ii) $CM_2(X) = 864pq - 462(p+q)+172$,

(iii) $CF(X) = 1728pq - 884(p+q)+8792$,

(iv) $CSO(X) = 101.823pq - 36.044(p+q)+5.231$,

(v) $CR(X) = 0.5pq + 0.0397(p+q) - 0.3772$,

(vi) $CHM_1(X) = 3456pq - 1808(p+q)+656$,

(vii) $CHM_2(X) = 124416pq - 98142(p+q)+69068$.

Table 6. Edge partition of graph X, when $p>1$, $q>1$

$(S_X[u], S_X[v])$, where $uv \in E(X)$	(7,7)	(7,11)	(8,11)	(11,11)	(11,12)	(12,12)
Number of edges	4	8	$4(p+q)-16$	$2(p+q)$	$4(p+q)-16$	$6pq-11(p+q)+20$

Proof. The 2D-lattice of $TUC_4C_8(R)[p,q]$ has $4pq$ vertices and $6pq-p-q$ edges. Therefore, edge partition of X, based on closed neighborhood degree of vertices as shown in Table 6. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 6.2. *Let $S(X)$ be subdivision graph of 2D-lattice of $TUC_4C_8(R)[p,q]$. Then*

(i) $CM_1(S(X)) = 286(p+q) + 204pq$,

(ii) $CM_2(S(X)) = 864pq - 300(p+q) + 24$,

(iii) $CF(S(X)) = 1756 - 590(p+q)$,

(iv) $CSO(S(X)) = 144.498pq - 37.9302(p+q) - 0.756$,

(v) $CR(S(X)) = 1.4142pq - 0.0574(p+q) + 0.0338$,

(vi) $CHM_1(S(X)) = 3468pq - 1190(p+q) + 64$,

(vii) $CHM_2(S(X)) = 62208pq - 28908(p+q) + 5976$.

Table 7. Edge partition of graph $S(X)$, when $p > 1$, $q > 1$

$(S_{S(X)}[u], S_{S(X)}[v])$, where $uv \in E(S(X))$	$(6,6)$	$(6,7)$	$(7,9)$	$(8,9)$
Number of edges	8	$4(p+q)-8$	$4(p+q)-8$	$12pq - 10(p+q) + 8$

Proof. The subdivision graph $S(X)$ has $10pq - p - q$ vertices and $2(6pq - p - q)$ edges. Therefore, edge partition of $S(X)$, based on closed neighborhood degree of vertices as shown in Table 7. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 6.3. *Let $L(S(X))$ be line graph of subdivision graph of 2D-lattice $TUC_4C_8(R)[p,q]$. Then*

(i) $CM_1(L(S(X))) = 432pq - 172(p+q) + 8$,

(ii) $CM_2(L(S(X))) = 2592pq - 1274(p+q) + 240$,

(iii) $CF(L(S(X))) = 5184pq - 2476(p+q) + 344$,

(iv) $CSO(L(S(X))) = 305.470pq - 140.057(p+q) + 3.144$,

(v) $CR(L(S(X))) = 1.5pq - 0.1455(p+q) + 0.120$,

(vi) $CHM_1(L(S(X))) = 10368pq - 5024(p+q) + 824$,

(vii) $CHM_2(L(S(X))) = 373248pq - 226074(p+q) + 88592$.

Table 8. Edge partition of graph $L(S(X))$, when $p > 1, q > 1$

$(S_{L(S(X))}[u], S_{L(S(X))}[v])$, where $uv \in E(L(S(X)))$	$(6,6)$	$(6,7)$	$(7,7)$	$(7,11)$	$(11,12)$	$(12,12)$
Number of edges	4	8	$2(p+q)-8$	$4(p+q)-8$	$8(p+q)-16$	$18pq - 19(p+q) + 20$

Proof. The line graph of subdivision graph $L(S(X))$ has $2(6pq - p - q)$ vertices and $(18pq - 5p - 5q)$ edges. Therefore, edge partition of $L(S(X))$, based on closed neighborhood degree of vertices as shown in Table 8. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 6.4. *Let Y be $TUC_4C_8(R)[p,q]$ nanotubes. Then*

(i) $CM_1(Y) = 4(36pq - 10p - 3q - 11)$,

(ii) $CM_2(Y) = 864pq - 326p - 144q - 450$,

(iii) $CF(Y) = 1728pq - 632p - 252q - 868$,

(iv) $CSO(Y) = 101.823pq - 27.920p - 7.882q - 30.472$,

(v) $CR(Y) = 0.083pq + 0.4857p + 0.0519q + 0.2311$,

(vi) $CHM_1(Y) = 3456pq - 1284p - 2268q - 1768$,

(vii) $CHM_2(Y) = 124416pq - 65534p - 36288q - 93090$.

Table 9. Edge partition of graph Y, when $p > 1$, $q > 1$

$(S_Y[u], S_Y[v])$, where $uv \in E(Y)$	$(8,8)$	$(8,11)$	$(11,11)$	$(8,12)$	$(11,12)$	$(9,12)$	$(12,12)$
Number of edges	4	$2(p+2)$	$2(p-1)$	4	$2(p+2)$	$4(q-2)$	$6pq-7p-4q-6$

Proof. The $TUC_4C_8(R)[p,q]$ nanotube has $4pq$ vertices and $6pq - p$ edges. Therefore, edge partition of $S(Y)$, based on closed neighborhood degree of vertices as shown in Table 9. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 6.5. *Let $S(Y)$ be subdivision graph of $TUC_4C_8(R)[p,q]$ nanotubes. Then*

(i) $CM_1(S(Y)) = 204pq - 54p - 7q$,

(ii) $CM_2(S(Y)) = 864pq - 300p - 59q + 4$,

(iii) $CF(S(Y)) = 1740pq - 590p - 103q$,

(iv) $CSO(S(Y)) = 144.499pq - 37.930p - 4.567q - 0.181$,

(v) $CR(S(Y)) = 1.414pq - 0.0574p + 0.0627q + 0.0023$,

(vi) $CHM_1(S(Y)) = 3468pq - 1190p - 221q + 8$,

(vii) $CHM_2(S(Y)) = 62208pq - 28908p - 7255q + 960$.

Table 10. Edge partition of graph $S(Y)$, when $p > 1$, $q > 1$

$(S_{S(Y)}[u], S_{S(Y)}[v])$, where $uv \in E(S(Y))$	$(5,9)$	$(6,7)$	$(7,7)$	$(7,8)$	$(7,9)$	$(8,9)$
Number of edges	q	$4p$	2	$2q-2$	$4p-2$	$12pq-10p-3q+2$

Proof. The subdivision graph $S(Y)$ has $10pq - p$ vertices and $2(6pq - p)$ edges. Therefore, edge partition of $S(Y)$, based on closed neighborhood degree of vertices as shown in Table 10. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 6.6. *Let $L(S(Y))$ be line graph of subdivision graph of nanotube. Then*

(i) $CM_1(L(S(Y))) = 432pq - 168p - 24q + 8$,

(ii) $CM_2(L(S(Y))) = 2592pq - 1226p - 274q + 96$,

(iii) $CF(L(S(Y))) = 5184pq - 2384p - 528q + 184$,

(iv) $CSO(L(S(Y))) = 305.470pq - 117.490p - 16.627q + 5.534$,

(v) $CR(L(S(Y))) = 0.4330pq - 0.015p + 0.036q - 0.0086$,

(vi) $CHM_1(L(S(Y))) = 10368pq - 4836p - 1076q + 376$,

(vii) $CHM_2(L(S(Y))) = 373248pq - 21282p - 69178q + 26496$.

Table 11. Edge partition of graph $L(S(Y))$, when $p > 1$, $q > 1$

$(S_{L(S(Y))}[u], S_{L(S(Y))}[v])$, where $uv \in E(L(S(Y)))$	(7,7)	(7,11)	(9,11)	(11,11)	(11,12)	(12,12)
Number of edges	$2p$	$4p$	$4q$	$2q$	$4p+4q-8$	$18pq-5(3p+2q)+8$

Proof. The line graph of subdivision graph $L(S(Y))$ has $2(6pq - p)$ vertices and $(18pq - 5p)$ edges. Therefore, edge partition of $L(S(Y))$, based on closed neighborhood degree of vertices as shown in Table 11. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 6.7. *Let Z be $TUC_4C_8(R)[p,q]$ nanotorus. Then*

(i) $CM_1(Z) = 144pq - 12(p+q)$,

(ii) $CM_2(Z) = 864pq - 144(p+q) + 36$,

(iii) $CF(Z) = 1728pq - 252(p+q)$,

(iv) $CSO(Z) = 101.823pq - 7.882(p+q) - 1.206$,

(v) $CR(Z) = 0.5pq + 0.0516(p+q) + 0.7777$,

(vi) $CHM_1(Z) = 3456pq - 540(p+q) + 72$,

(vii) $CHM_2(Z) = 124416pq - 36288(p+q) + 15876$.

Table 12. Edge partition of graph Z, when $p > 1$, $q > 1$

$(S_Z[u], S_Z[v])$, where $uv \in E(Z)$	(9,9)	(9,12)	(12,12)
Number of edges	4	$4(p+q)-8$	$6pq-4(p+q)+4$

Proof. The $TUC_4C_8(R)[p,q]$ nanotorus has $4pq$ vertices and $6pq$ edges. Therefore, edge partition of Z, based on closed neighborhood degree of vertices as shown in Table 12. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 6.8. *Let $S(Z)$ be subdivision graph of $TUC_4C_8(R)[p,q]$ nanotorus. Then*

(i) $CM_1(S(Z)) = 204pq - 7(p+q)$,

(ii) $CM_2(S(Z)) = 864pq - 59(p+q)$,

(iii) $CF(S(Z)) = 1740pq - 103(p+q)$,

(iv) $CSO(S(Z)) = 144.499pq - 4.5689(p+q)$,

(v) $CR(S(Z)) = 1.4142pq + 0.0627(p+q)$,

(vi) $CHM_1(S(Z)) = 3468pq - 221(p+q)$,

(vii) $CHM_2(S(Z)) = 62208pq - 7255(p+q)$.

Table 13. Edge partition of graph $S(Z)$, when $p > 1$, $q > 1$

$(S_{S(Z)}[u], S_{S(Z)}[v])$, where $uv \in E(S(Z))$	(5,9)	(7,8)	(8,9)
Number of edges	$p+q$	$2(p+q)$	$12pq-3(p+q)$

Proof. The subdivision graph $S(Z)$ has $10pq$ vertices and $12pq$ edges. Therefore, edge partition of $S(Z)$, based on closed neighborhood degree of vertices as shown in Table 13. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

Theorem 6.9. *Let $L(S(Z))$ be line graph of subdivision graph of nanotorus. Then*

(i) $CM_1(L(S(Z))) = 432pq - 12(p+q)$,

(ii) $CM_2(L(S(Z))) = 2592pq - 144(p+q)$,

(iii) $CF(L(S(Z))) = 5184pq + 45504(p+q)$,

(iv) $CSO(L(S(Z))) = 305.4701pq - 7.8822(p+q)$,

(v) $CR(L(S(Z))) = 1.5pq + 0.0516(p+q)$,

(vi) $CHM_1(L(S(Z))) = 10368pq - 540(p+q)$,

(vii) $CHM_2(L(S(Z))) = 373248pq - 36288(p+q)$.

Table 14. Edge partition of graph L(S(Z)), when $p > 1$, $q > 1$

$(S_{L(S(Z))}[u], S_{L(S(Z))}[v])$, where $uv \in E(L(S(Z)))$	(9,12)	(12,12)
Number of edges	$4(p+q)$	$18pq-4(p+q)$

Proof. The line graph of subdivision graph $L(S(Z))$ has $12pq$ vertices and $18pq$ edges. Therefore, edge partition of $S(X)$, based on closed neighborhood degree of vertices as shown in Table 14. Therefore, using formulae (1.11)-(1.17) we obtain the desired result. □

7. Conclusion

In this research, we introduced seven closed neighborhood topological indices and we examined its QSPR properties such as entropy and acentric factor to octane isomer. These indices highly correlates with the acentric factor of octane isomers. Later we obtain explicit formulae of these indices to nanostructures. The obtained results shed light on new aspects in the discipline of structural chemistry and also showcase practical relevance in forecasting the characteristics of topological indices at the preliminary analysis.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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