Hindawi
Journal of Mathematics
Volume 2022, Article ID 2006084, 14 pages
https://doi.org/10.1155/2022/2006084

Research Article

Two Dimensional Descriptors Based on Degree, Neighborhood Degree, and Reverse Degree for HEX (Hexagonal) Lattice

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Received 6 March 2022; Revised 29 March 2022; Accepted 31 March 2022; Published 14 May 2022

Academic Editor: Gohar Ali

Crystal structures are of great scrutiny due to the elegant and well-ordered symmetry that influences a significant role in determining numerous physical properties. Our aim is to perceive the role of topological descriptors in the field of crystallography using chemical graph theory to examine symmetrical crystal structure HEX. Simple hexagonal (HEX) is a crystal structure formed by arranging the same layer of atoms in a hexagon with one additional atom at the center. Chemical graph theory allows us to study a variety of molecular structures via graphical representation where each atom is denoted as a vertex and the bond form between them is defined as edge. In this research work, we compute the general Randi$\widehat{c}$ index, atom bond connectivity index, geometric arithmetic index, first and second Zagreb indices. Furthermore, we will compute their neighborhood and reverse degree-based versions and visualize which descriptor stands high in accordance with its numerical value.

1. Introduction

HEX (hexagonal) crystal structure, due to its prominent symmetry following by the atoms arranged in it, portrays a critical role in determining wide range of physiochemical properties such as sublimation point, heat of fusion, and molar heat capacity etc to establish strong metallic bodies. There are very few elements which attains this crystal structure namely, H, C, N, Se, and Te. Chemical graph theory allows us to study vast and complex structures by considering the vertex set as atom set, and the edges in the corresponding graphs formed by the structure are defined as bond between two atoms. The unit cell of the HEX structure [1] is formed by considering two hexagonal layers formed by atoms arranged in hexagon with an atom that lies in their center, as shown in Figure 1, and each of the layers forms bond between each atoms that lies exactly around its symmetry.

The lattice is formed by arranging its unit cells in one dimension, as shown in Figure 2. In this paper, we present closed formulas for two dimensional topological descriptors based on degree, reverse degree, and neighborhood degree, and for this purpose, we calculate these degrees for each atom (vertex) of a lattice formed by HEX. This kind of crystal lattice has a vertex set $V_n = 7n + 7$ and edge set $E_n = 19n + 12$, where n is the no. of unit cells that forms lattice.

2. Preliminaries

In this section, we give a brief view for the two-dimensional topological descriptors for which we compute closed formulas for HEX(n).

The first Zagreb index [2] is defined as

$$M_1(G) = \sum_{fg\in E(G)} \left(d_f + d_g\right). \tag{1}$$

Zagreb index is one of the oldest and important indices introduced by Gutman and Das [3] defined as

$$M_2(G) = \sum_{fg\in E(G)} d_f d_g. \tag{2}$$

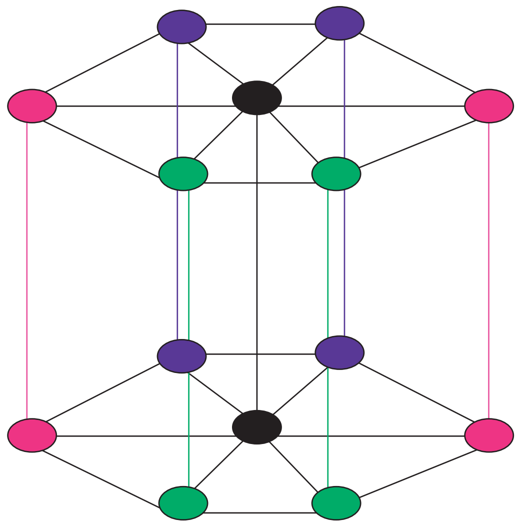

Figure 1: HEX unit cell.

The general Randić index [4] is defined as

$$R_\alpha(G) = \sum_{fg\in E(G)} \left(d_f d_g\right)^\alpha. \tag{3}$$

The atom bond connectivity index [5] is defined as

$$ABC(G) = \sum_{fg\in E(G)} \sqrt{\frac{d_f + d_g - 2}{d_f d_g}}. \tag{4}$$

The geometric arithmetic index [6] is defined as

$$\mathrm{GA}(G) = \sum_{fg\in E(G)} \frac{2\sqrt{d_f d_g}}{d_f + d_g}. \tag{5}$$

Mondal et al. introduced some prominent neighborhood degree-based versions of topological descriptors, namely, neighborhood forgotten and harmonic index [7], given as

$$\begin{aligned} F_N^*(G) &= \sum_{fg\in E(G)} \left(\delta_f^2 + \delta_g^2\right), \\ \mathrm{NH}(G) &= \sum_{fg\in E(G)} \frac{2}{\delta_f + \delta_g}. \end{aligned} \tag{6}$$

Neighbor versions of first [8] and second Zagreb index [7] are defined as

$$\begin{aligned} M_1^*(G) &= \sum_{fg\in E(G)} \left(\delta_f + \delta_g\right), \\ M_2^*(G) &= \sum_{fg\in E(G)} \left(\delta_f \delta_g\right). \end{aligned} \tag{7}$$

Sanskruti index [9] is given as

$$S(G) = \sum_{fg\in E(G)} \left(\frac{\delta_f \delta_g}{\delta_f + \delta_g - 2}\right)^3. \tag{8}$$

Neighborhood inverse sum index [10] is defined as

$$\mathrm{NI}(G) = \sum_{fg\in E(G)} \frac{\delta_f \delta_g}{\delta_f + \delta_g}. \tag{9}$$

The neighborhood modified second Zagreb index [11] is defined as

$$M_2^{nm}(G) = \sum_{fg\in E(G)} \frac{1}{\delta_f \delta_g}. \tag{10}$$

3rd and 5th NDe index [12] is defined as

$$\begin{aligned} \mathrm{ND}_3(G) &= \sum_{fg\in E(G)} \delta_f \delta_g \left(\delta_f + \delta_g\right), \\ \mathrm{ND}_5(G) &= \sum_{fg\in E(G)} \left[\frac{\delta_f}{\delta_g} + \frac{\delta_g}{\delta_f}\right]. \end{aligned} \tag{11}$$

Reverse degree-based Randić index [13] is defined as

$$\Re R_\alpha(G) = \sum_{fg\in E(G)} \left[\Re_f \Re_g\right]^\alpha, \tag{12}$$

where α is real.

The atom bond connectivity index is presented by Estrada et al. [14]. The reverse atom bond connectivity index is defined as

$$\Re ABC(G) = \sum_{fg\in E(G)} \sqrt{\frac{\Re_f + \Re_g - 2}{\Re_f \Re_g}}. \tag{13}$$

The geometric arithmetic index of a graph G is presented by Vukičević and Furtula [15]. The reverse geometric arithmetic index is defined as

$$\Re \mathrm{GA}(G) = \sum_{fg\in E(G)} \frac{2\sqrt{\Re_f \Re_g}}{\Re_f + \Re_g}. \tag{14}$$

Shirdel et al. [16] presented a reverse hyper Zagreb index defined as

$$\Re \mathrm{HM}(G) = \sum_{fg\in E(G)} \left(\Re_f + \Re_g\right)^2. \tag{15}$$

Metallic structures are of great importance and are using widely in the scientific environment. To study them and investigate their properties is one of the greatest aspects because of their toxicity and strong physio chemical and electrical properties, in order to utilize the best chemical formed by metallic crystal structures that required the right amount of data. For this purpose, we examine HEX crystal structure which found rarely in a few elements, and many of its existence are unknown. Newly, the metallic structures due to their end-to-end symmetry attaining by its atoms bonding and arrangement become the noteworthy idea. Mujahed and Nagy measured Wiener index on diamond cubic crystal [17]. Siddiqui et al. investigated FCC for various degree based and their polynomial indices in [18]. Admiring their works, we present and investigate HEX crystal lattice by means of two-dimensional descriptors. As our work is depending on the crystal structures that uniquely found in

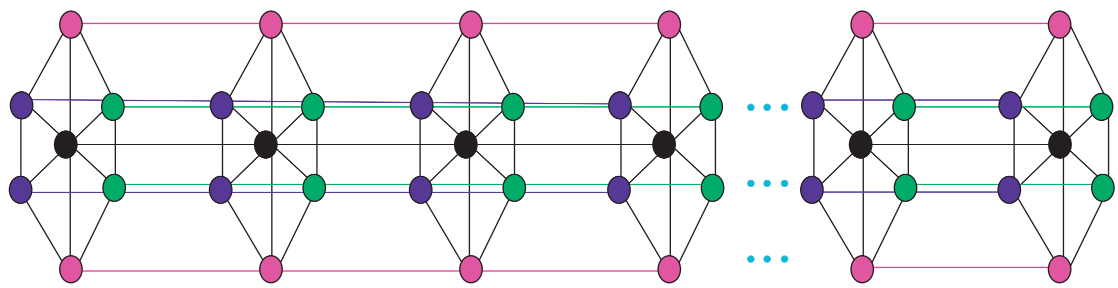

Figure 2: HEX(n) crystal lattice.

Table 1: Degree-based edge partition.

Edge notation	(d_f, d_g)	order of (d_f, d_g)
E_1	(4, 4)	12
E_2	(5, 5)	$12n - 18$
E_3	(4, 5)	12
E_4	(4, 7)	12
E_5	(5, 8)	$6n - 6$
E_6	(8, 8)	$n - 2$
E_7	(7, 8)	2

metals, so to basically study the simple one-dimensional hexagonal system through descriptors, we refer the viewer to the following works: Ahmad and Imran [19] computed the exact values for vertex edge degree-based topological descriptors for HEX derived networks, namely, $HDN_1(p)$ and $HDN_2(p)$, where p is the dimension. In [20], Ahmad et al. computed degree-based topological indices for metal organic networks (MONs). Amić et al. [21] recommended that a improved version of the (valence) vertex-connectivity index should be routinely employed in the structure-property modeling instead of the standard version of the index.

3. Results

In this section, we discuss how to compute the closed formulas for descriptors based on degree reverse degree and neighborhood degree.

3.1. Topological Descriptors based on Degree.

The degree of a vertex f is the no. of edges incident with that vertex defined as d_f [22]. In the first and last layer for each n unit cell lattice, the vertices arranged in hexagon have degree 4, and the degree of centered vertex is 7, and as we add unit cells, the degree of the other hexagonal layer vertices increases. To compute well-defined formulas in the theorems for each descriptor, we compute each vertex degree and categorize them in Table 1.

3.1.1. Evaluation and Discussion

Theorem 1. *We consider the HEX(n) (hexagonal lattice); then, its first and second Zagreb index is equal to*

(a) First Zagreb index of $HEX(n) = 76 + 214n$

(b) Second Zagreb index of $HEX(n) = 62 + 604n$

Proof. We consider hexagonal lattice. We prove the above results for first and second Zagreb index by using Table 1 and formula for these indices.

(a) Computations for the first Zagreb index:

$$\begin{aligned} M_1(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} (d_f + d_g) \\ &= \sum_{fg\in E_1} (d_f + d_g) + \sum_{fg\in E_2} (d_f + d_g) + \sum_{fg\in E_3} (d_f + d_g) + \cdots + \sum_{fg\in E_7} (d_f + d_g) \\ &= 12(4+4) + (12n-18)(5+5) + 12(4+5) + 12(4+7) + (6n-6)(5+8) + (n-2)(8+8) + 2(7+8) \\ &= 76 + 214n. \end{aligned} \tag{16}$$

(b) Computations for the second Zagreb index:

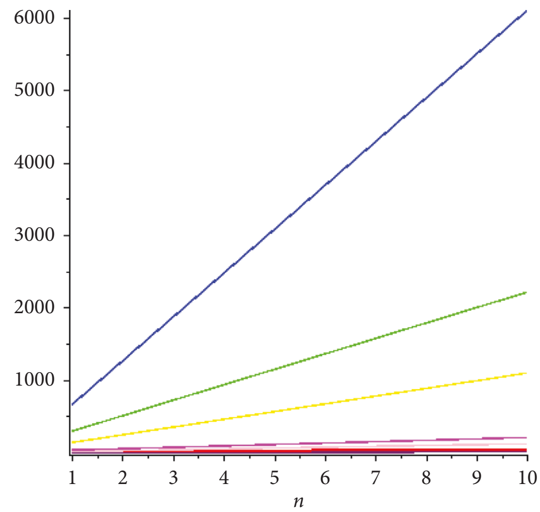

Figure 3: Graphical analysis of degree-based topological descriptors.

$$\begin{aligned} M_2(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} d_f d_g \\ &= \sum_{fg\in E_1} d_f d_g + \sum_{fg\in E_2} d_f d_g + \sum_{fg\in E_3} d_f d_g + \cdots + \sum_{fg\in E_7} d_f d_g \\ &= 12(4\times 4) + (12n-18)(5\times 5) + 12(4\times 5) + 12(4\times 7) + (6n-6)(5\times 8) + (n-2)(8\times 8) + 2(7\times 8) \\ &= 62 + 604n. \end{aligned} \tag{17}$$

□

Theorem 2. *We consider the HEX(n) (hexagonal lattice); then, its general Randić index is equal to*

$$R_\alpha(\mathrm{HEX}(n)) = \begin{cases} M_2(\mathrm{HEX}(n)) = 62 + 604n, & \text{if } \alpha = 1\,(a), \\ \dfrac{5113}{5600} + \dfrac{1033}{1600}n, & \text{if } \alpha = -1\,(b), \\ 36.18296055 + 105.9473319n, & \text{if } \alpha = \dfrac{1}{2}\,(c), \\ 3.419646355 + 3.473683298n, & \text{if } \alpha = -\dfrac{1}{2}\,(d). \end{cases} \tag{18}$$

Proof. We consider the HEX(n) and formula for general Randić index to compute results.

$$\begin{aligned} R_\alpha(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \left(d_f d_g\right)^\alpha \\ &= \sum_{fg\in E_1} \left(d_f d_g\right)^\alpha + \sum_{fg\varepsilon E_2} \left(d_f d_g\right)^\alpha + \sum_{fg\varepsilon E_3} \left(d_f d_g\right)^\alpha + \cdots + \sum_{fg\varepsilon E_7} \left(d_f d_g\right)^\alpha. \end{aligned} \tag{19}$$

Table 2: Neighborhood degree-based edge partition.

Edge notation	(N_f, N_g)	order of (N_f, N_g)
E_1	$(20, 20)$	12
E_2	$(27, 27)$	12
E_3	$(28, 28)$	$12n - 42$
E_4	$(20, 32)$	12
E_5	$(20, 27)$	12
E_6	$(32, 45)$	2
E_7	$(27, 45)$	12
E_8	$(27, 28)$	12
E_9	$(28, 46)$	$6n - 18$
E_{10}	$(45, 46)$	2
E_{11}	$(46, 46)$	$n - 4$

We obtain the following results by using Table 1:

(a) When $\alpha = 1$, general Randić index is equal to second Zagreb index

(b) When $\alpha = -1$,

$$R_{-1}(\text{HEX}(n)) = \sum_{fg\in E(\text{HEX}(n))} \left(d_f d_g\right)^{-1}$$
$$= \sum_{fg\in E_1} \left(d_f d_g\right)^{-1} + \sum_{fg\varepsilon E_2} \left(d_f d_g\right)^{-1} + \sum_{fg\varepsilon E_3} \left(d_f d_g\right)^{-1} + \cdots + \sum_{fg\varepsilon E_7} \left(d_f d_g\right)^{-1} \tag{20}$$
$$= \frac{12}{4\times 4} + \frac{(12n-18)}{5\times 5} + \frac{12}{4\times 5} + \frac{12}{4\times 7} + \frac{6n-6}{5\times 8} + \frac{n-2}{8\times 8} + \frac{2}{7\times 8}$$

(c) When $\alpha = (1/2)$,

$$R_{(1/2)}(\text{HEX}(n)) = \sum_{fg\in E(\text{HEX}(n))} \sqrt{d_f d_g}$$
$$= 12\sqrt{4\times 4} + (12n-18)\sqrt{5\times 5} + 12\sqrt{4\times 5} + 12\sqrt{4\times 7} + (6n-6)\sqrt{5\times 8} + (n-2)\sqrt{8\times 8} + 2\sqrt{7\times 8}$$
$$= 36.18296055 + 105.9473319n \tag{21}$$

(d) When $\alpha = -(1/2)$,

$$R_{-(1/2)}(\text{HEX}(n)) = \sum_{fg\in E(\text{HEX}(n))} \frac{1}{\sqrt{d_f d_g}}$$
$$= \frac{12}{\sqrt{4\times 4}} + \frac{(12n-18)}{\sqrt{5\times 5}} + \frac{12}{\sqrt{4\times 5}} + \frac{12}{\sqrt{4\times 7}} + \frac{(6n-6)}{\sqrt{5\times 8}} + \frac{(n-2)}{\sqrt{8\times 8}} + \frac{2}{\sqrt{7\times 8}} \tag{22}$$
$$= 3.419646355 + 3.473683298n$$

□

Theorem 3. *We consider the HEX(n); then,*

(a) Atom bond connectivity index of $HEX(n) = 10.402355882n + 7.950571054$

(b) Geometric arithmetic index of $HEX(n) = 18.83805106n + 11.62829205$

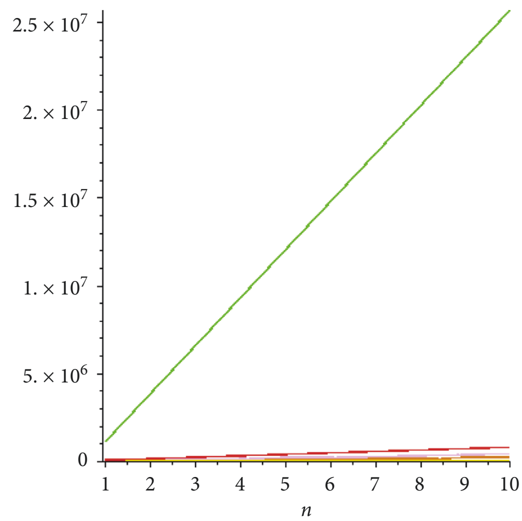

FIGURE 4: Graphical analysis of neighborhood degree-based topological descriptors.

Proof. We consider the hexagonal lattice. We use Table 1 and general formulas for the following indices to compute results.

(a) The atom bond connectivity index is given as

$$\begin{aligned} ABC(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \sqrt{\frac{d_f + d_g - 2}{d_f d_g}} \\ &= 12\sqrt{\frac{4+4-2}{4\times 4}} + (12n-18)\sqrt{\frac{5+5-2}{5\times 5}} + 12\sqrt{\frac{4+5-2}{4\times 5}} + 12\sqrt{\frac{4+7-2}{4\times 7}} + (6n-6)\sqrt{\frac{5+8-2}{5\times 8}} + (n-2)\sqrt{\frac{8+8-2}{8\times 8}} + 2\sqrt{\frac{7+8-2}{7\times 8}} \\ &= 10.402355882n + 7.950571054. \end{aligned} \tag{23}$$

(b) The geometric arithmetic index is given as

$$\begin{aligned} \mathrm{GA}(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \frac{2\sqrt{d_f d_g}}{d_f + d_g} \\ &= 12\frac{2\sqrt{4\times 4}}{4+4} + (12n-18)\frac{2\sqrt{5\times 5}}{5+5} + 12\frac{2\sqrt{4\times 5}}{4+5} + 12\frac{2\sqrt{4\times 7}}{4+7} + (6n-6)\frac{2\sqrt{5\times 8}}{5+8} + (n-2)\frac{2\sqrt{8\times 8}}{8+8} + 2\frac{2\sqrt{7\times 8}}{7+8} \\ &= 18.83805106n + 11.62829205. \end{aligned} \tag{24}$$

Amongst all the computed degree-based indices, we encounter for $n = 1, \ldots, 10$ that the second Zagreb index $M_2(\mathrm{HEX}(n))$ ranks high and Randić index for $\alpha = -1$, $R_{-1}(\mathrm{HEX}(n))$ ranks lowest, where we use the colors green, blue, purple, yellow, red, pink and magenta for the descriptors, namely, $M_1(\mathrm{HEX}(n))$, $M_2(\mathrm{HEX}(n))$, $R_{-1}(\mathrm{HEX}(n))$, $R_{(1/2)}(\mathrm{HEX}(n))$, $R_{-(1/2)}(\mathrm{HEX}(n))$, $ABC(\mathrm{HEX}(n))$, and $\mathrm{GA}(\mathrm{HEX}(n))$ as shown in Figure 3. □

3.2. Topological Descriptors based on Neighborhood Degree. The neighborhood degree is defined as δ_f denoted the degree sum of neighbors of vertex f [22]. All the neighborhood degrees are categorized in Table 2 corresponding to their edge sets to depict exact values for the descriptors based on neighborhood degree in the following theorems.

Table 3: Reverse degree-based edge partition.

Edge notation	$(\mathfrak{R}_f, \mathfrak{R}_g)$	order of $(\mathfrak{R}_f, \mathfrak{R}_g)$
E_1	$(5, 5)$	12
E_2	$(4, 4)$	$12n - 18$
E_3	$(5, 4)$	12
E_4	$(5, 2)$	12
E_5	$(4, 1)$	$6n - 6$
E_6	$(1, 1)$	$n - 2$
E_7	$(2, 1)$	2

3.2.1. Evaluation and Discussion

Theorem 4. *We consider HEX(n). The neighborhood versions of Zagreb indices for HEX(n) are*

(a) First neighborhood Zagreb index for $HEX(n) = 124 + 1208n$

(b) Second neighborhood Zagreb index of $HEX(n) = 19252n - 6196$

(c) The neighborhood second modified Zagreb index of $HEX(n) = 0.0461008161 + 0.02043709733n$

Proof. We consider the general formula for neighborhood versions of Zagreb indices and evaluate results for HEX(n) by using Table 2.

(a) Calculations for $M_1^*(\mathrm{HEX}(n))$:

$$\begin{aligned} M_1^*(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \left(\delta_f + \delta_g\right) \\ &= \sum_{fg\in E_1} \left(\delta_f + \delta_g\right) + \sum_{fg\in E_2} \left(\delta_f + \delta_g\right) + \sum_{fg\in E_3} \left(\delta_f + \delta_g\right) + \cdots + \sum_{fg\in E_{11}} \left(\delta_f + \delta_g\right) \\ &= 12(40) + 12(54) + (12n - 42)(56) + 12(52) + 12(47) + 2(77) + 12(72) + 12(55) \\ &\quad + (6n - 18)(74) + 2(91) + (n - 4)(92) \\ &= 124 + 1208n. \end{aligned} \tag{25}$$

(b) Calculations for $M_2^*(\mathrm{HEX}(n))$:

$$\begin{aligned} M_2^*(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \left(\delta_f \delta_g\right) \\ &= \sum_{fg\in E_1} \left(\delta_f \delta_g\right) + \sum_{fg\in E_2} \left(\delta_f \delta_{gg}\right) + \sum_{fg\in E_3} \left(\delta_f \delta_g\right) + \cdots + \sum_{fg\in E_{11}} \left(\delta_f \delta_g\right) \\ &= 12(400) + 12(729) + (12n - 42)(784) + 12(640) + 12(540) + 2(1440) + 12(1215) \\ &\quad + 12(756) + (6n - 18)(1288) + 2(2070) + (n - 4)(2116) \\ &= 19252n - 6196. \end{aligned} \tag{26}$$

(c) Calculations for $M_2^{nm}(\mathrm{HEX}(n))$:

$$\begin{aligned} M_2^{nm}(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \frac{1}{\delta_f \delta_g} \\ &= \sum_{fg\in E_1} \frac{1}{\delta_f \delta_g} + \sum_{fg\in E_2} \frac{1}{\delta_f \delta_g} + \sum_{fg\in E_3} \frac{1}{\delta_f \delta_g} + \cdots + \sum_{fg\in E_{11}} \frac{1}{\delta_f \delta_g} \\ &= 12\left(\frac{1}{400}\right) + 12\left(\frac{1}{729}\right) + (12n - 42)\left(\frac{1}{784}\right) + 12\left(\frac{1}{640}\right) + 12\left(\frac{1}{540}\right) + 2\left(\frac{1}{1440}\right) + 12\left(\frac{1}{1215}\right) + 12\left(\frac{1}{756}\right) \\ &\quad + (6n - 18)\left(\frac{1}{1288}\right) + 2\left(\frac{1}{2070}\right) + (n - 4)\left(\frac{1}{2116}\right) \\ &= 0.0461008161 + 0.02043709733n. \end{aligned} \tag{27}$$

□

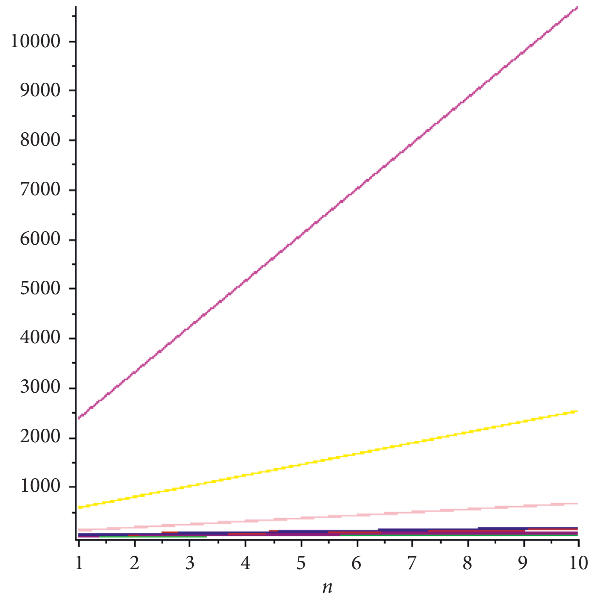

Figure 5: Graphical analysis of reverse degree-based topological descriptors.

Theorem 5. *We consider the neighborhood forgotten topological index of HEX* $(n) = 40448n - 11668$.

Proof. We consider HEX(n), and using Table 2, we have the following evaluations for the neighborhood forgotten topological index:

$$\begin{aligned}
F_N^*(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))}\left(\delta_f^2+\delta_g^2\right)\\
&= \sum_{fg\in E_1}\left(\delta_f^2+\delta_g^2\right)+\sum_{fg\in E_2}\left(\delta_f^2+\delta_g^2\right)+\sum_{fg\in E_3}\left(\delta_f^2+\delta_g^2\right)+\cdots+\sum_{fg\in E_{11}}\left(\delta_f^2+\delta_g^2\right)\\
&= 12(800)+12(1458)+(12n-42)(1568)+12(1424)+12(1129)+2(3049)+12(2754)+12(1513)+(6n\\
&\quad -18)(2900)+2(4141)+(n-4)(4232)\\
&= 40448n-11668.
\end{aligned} \tag{28}$$

□

Theorem 6. *The third and fifth NDe index of HEX* (n):

$$\mathrm{NDe}=\begin{cases}\mathrm{ND}_3 = 2730640n - 1652752 \ (a),\\ \mathrm{ND}_5 = 26.7125 + 39.50931677n \ (b).\end{cases} \tag{29}$$

Proof. We consider HEX(n). we compute the results using Table 2 and general formulas for the indices as mentioned in this theorem.

(a) The computations for ND_3 are given as

$$\begin{aligned}
\mathrm{ND}_3(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))}\delta_f\delta_g\left(\delta_f+\delta_g\right)\\
&= \sum_{fg\in E_1}\delta_f\delta_g\left(\delta_f+\delta_g\right)+\sum_{fg\in E_2}\delta_f\delta_g\left(\delta_f+\delta_g\right)+\sum_{fg\in E_3}\delta_f\delta_g\left(\delta_f+\delta_g\right)+\cdots+\sum_{fg\in E_{11}}\delta_f\delta_g\left(\delta_f+\delta_g\right)\\
&= 12(800)(40)+12(1458)(54)+(12n-42)(1568)(56)+12(1424)(52)+12(1129)(47)+2(3049)(77)\\
&\quad +12(2754)(72)+12(1513)(55)+(6n-18)(2900)(74)+2(4141)(91)+(n-4)(4232)(92)\\
&= 2730640n-1652752.
\end{aligned} \tag{30}$$

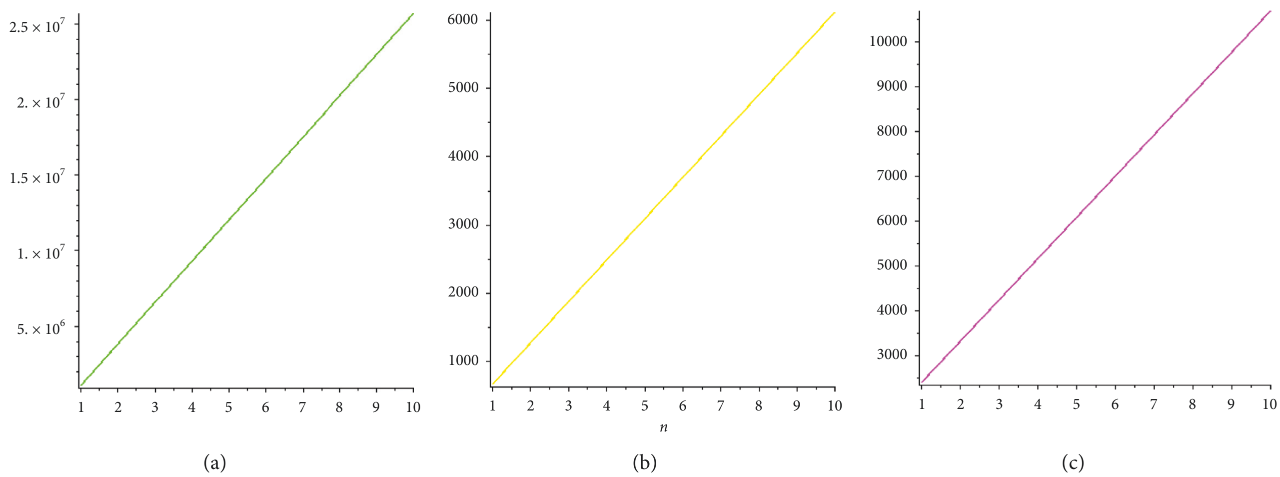

FIGURE 6: (a)$\mathrm{ND}_3(\mathrm{HEX}(n))$, (b)$M_2(\mathrm{HEX}(n))$, and (c)$\mathfrak{R}\mathrm{HM}(\mathrm{HEX}(n))$.

(b) The computations for ND_5 are given as

$$\begin{aligned}\mathrm{ND}_5(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))}\left[\frac{\delta_f}{\delta_g}+\frac{\delta_g}{\delta_f}\right]\\ &= \sum_{fg\in E_1}\left[\frac{\delta_f}{\delta_g}+\frac{\delta_g}{\delta_f}\right]+\sum_{fg\in E_2}\left[\frac{\delta_f}{\delta_g}+\frac{\delta_g}{\delta_f}\right]+\sum_{fg\in E_3}\left[\frac{\delta_f}{\delta_g}+\frac{\delta_g}{\delta_f}\right]+\cdots+\sum_{fg\in E_{11}}\left[\frac{\delta_f}{\delta_g}+\frac{\delta_g}{\delta_f}\right]\\ &= 12(2)+12(2)+(12n-42)(2)+12\left(\frac{89}{40}\right)+12\left(\frac{1129}{540}\right)+2\left(\frac{3049}{1440}\right)+12\left(\frac{34}{15}\right)+12\left(\frac{1513}{756}\right)+(6n-18)\left(\frac{725}{322}\right)\\ &\quad+2\left(\frac{4141}{2070}\right)+(n-4)(2)\\ &= 26.7125+39.50931677n.\end{aligned} \tag{31}$$

□

Theorem 7. *In this theorem, we compute closed formulas for the following indices:*

(a) The neighborhood Harmonic index of HEX$(n) = 0.2087792612 + 0.6124727212n$

(b) The neighborhood inverse sum index of HEX$(n) = 24.60990826 + 295.4324324n$

(c) The Sanskruti index of HEX$(n) = 84068.12956n - 53703.85814$

Proof. To prove the results (a), (b), and (c), we consider the hexagonal crystal lattice. Next, we consider the general formulas for the indices and evaluate them, respectively, by using Table 2.

(a) The neighborhood Harmonic index of $\mathrm{HEX}(n)$:

$$
\begin{aligned}
\mathrm{NH}(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))}\frac{2}{\delta_f+\delta_g}\\
&= \sum_{fg\in E_1}\frac{2}{\delta_f+\delta_g}+\sum_{fg\in E_2}\frac{2}{\delta_f+\delta_g}+\sum_{fg\in E_3}\frac{2}{\delta_f+\delta_g}+\cdots+\sum_{fg\in E_{11}}\frac{2}{\delta_f+\delta_g}\\
&= \frac{12(2)}{40}+\frac{12(2)}{54}+\frac{(12n-42)(2)}{56}+\frac{12(2)}{52}+\frac{12(2)}{47}+\frac{2(2)}{77}+\frac{12(2)}{72}+\frac{12(2)}{55}+\frac{(6n-18)(2)}{74}+\frac{2(2)}{91}+\frac{(n-4)(2)}{92}\\
&= 0.2087792612+0.6124727212n.
\end{aligned}
\tag{32}
$$

(b) The neighborhood inverse sum index of $\mathrm{HEX}(n)$:

$$
\begin{aligned}
\mathrm{NI}(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))}\frac{\delta_f\delta_g}{\delta_f+\delta_g}\\
&= \sum_{fg\in E_1}\frac{\delta_f\delta_g}{\delta_f+\delta_g}+\sum_{fg\in E_2}\frac{\delta_f\delta_g}{\delta_f+\delta_g}+\sum_{fg\in E_3}\frac{\delta_f\delta_g}{\delta_f+\delta_g}+\cdots+\sum_{fg\in E_{11}}\frac{\delta_f\delta_g}{\delta_f+\delta_g}\\
&= \frac{12(400)}{40}+\frac{12(729)}{54}+\frac{(12n-42)(784)}{56}+\frac{12(640)}{52}+\frac{12(540)}{47}+\frac{2(1440)}{77}+\frac{12(1215)}{72}+\frac{12(756)}{55}\\
&\quad+\frac{(6n-18)(1288)}{74}+\frac{2(2070)}{91}+\frac{(n-4)(2116)}{92}\\
&= 24.60990826+295.4324324n.
\end{aligned}
\tag{33}
$$

(c) The Sanskruti index of $\mathrm{HEX}(n)$:

$$
\begin{aligned}
S(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))}\left(\frac{\delta_f\delta_g}{\delta_f+\delta_g-2}\right)^3\\
&= \sum_{fg\in E_1}\left(\frac{\delta_f\delta_g}{\delta_f+\delta_g-2}\right)^3+\sum_{fg\in E_2}\left(\frac{\delta_f\delta_g}{\delta_f+\delta_g-2}\right)^3+\sum_{fg\in E_3}\left(\frac{\delta_f\delta_g}{\delta_s+\delta_t-2}\right)^3+\cdots+\sum_{fg\in E_{11}}\left(\frac{\delta_f\delta_g}{\delta_f+\delta_g-2}\right)^3\\
&= \frac{12(400)^3}{54872}+\frac{12(729)^3}{140608}+\frac{(12n-42)(784)^3}{157464}+\frac{12(640)^3}{125000}+\frac{12(540)^3}{91125}+\frac{2(1440)^3}{421875}+\frac{12(1215)^3}{343000}+\frac{12(756)^3}{148877}\\
&\quad+\frac{(6n-18)(1288)^3}{373248}+\frac{2(2070)^3}{704969}+\frac{(n-4)(2116)^3}{729000}\\
&= 84068.12956n-53703.85814.
\end{aligned}
\tag{34}
$$

Amongst all the computed neighborhood degree-based indices, we can visualize from the graphical representation that the index ND_3 ranks highest and $M_2^{nm}(\mathrm{HEX}(n))$ ranks lowest for hexagonal lattice by substituting it for n ranging from 1 to10. Here, we use colors cyan, gold, plum, violet, green, purple, blue, yellow, and orange for the descriptors named as $M_1^*(\mathrm{HEX}(n)), M_2^*(\mathrm{HEX}(n)), F_N^*(\mathrm{HEX}(n)), M_2^{nm}(\mathrm{HEX}(n)), ND_3(\mathrm{HEX}(n)), ND_5(\mathrm{HEX}(n))$, $NH(\mathrm{HEX}(n)), NI(\mathrm{HEX}(n)), S(\mathrm{HEX}(n))$, respectively, as shown in Figure 4. □

3.3. Topological Descriptors based on Reverse Degree. Reverse degree of the vertex depends on the maximum degree in a graph and d_f. It is defined as $\mathfrak{R}_f = \Delta(\mathrm{HEX}(n)) - d_f + 1$, where $\Delta(\mathrm{HEX}(n)) = 8$. We compute neighborhood degree for the n dimensional lattice. In Table 3, we mention all the neighborhood degrees for the entire lattice or for each value of n, and we categorized these values through the edge distributions according to the edges having same degrees, and we also mention cardinality of each edge having vertices with same reverse degree. For each no. of unit cells n, we use Table 3 to compute results for the following theorems.

3.3.1. Evaluation and Discussion. In this section, we compute results in the form of theorems.

Theorem 8. *We consider the HEX(n) (hexagonal lattice); then, its general Randić index is equal to*

$$\mathfrak{R}R_\alpha(\mathrm{HEX}(n)) = \begin{cases} 350 + 217n, & \text{if } \alpha = 1\ (a), \\ \dfrac{13}{4}n - \dfrac{5}{8}, & \text{if } \alpha = -1\ (b), \\ 68.44139051 + 61n, & \text{if } \alpha = \dfrac{1}{2}\ (c), \\ 0.7922283276 + 7n, & \text{if } \alpha = -\dfrac{1}{2}\ (d). \end{cases} \tag{35}$$

Proof. We consider the HEX(n) and formula for general reverse Randić index to compute results. We perform evaluations by using Table 3.

(a) When $\alpha = 1, \mathfrak{R}R_1(\mathrm{HEX}(n))$ is given as

$$\begin{aligned} \mathfrak{R}R_1(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \left[\mathfrak{R}_f\mathfrak{R}_g\right]^1 \\ &= \sum_{fg\in E_1}\left[\mathfrak{R}_f\mathfrak{R}_g\right] + \sum_{fg\in E_2}\left[\mathfrak{R}_f\mathfrak{R}_g\right] + \cdots + \sum_{fg\in E_7}\left[\mathfrak{R}_f\mathfrak{R}_g\right] \\ &= 12(5\times 5) + (12n-18)(4\times 4) + 12(5\times 4) + 12(5\times 2) + (6n-6)(4\times 1) + (n-2)(1\times 1) + 2(2\times 1) \\ &= 350 + 217n \end{aligned} \tag{36}$$

(b) When $\alpha = -1, \mathfrak{R}R_{-1}(\mathrm{HEX}(n))$ is given as

$$\begin{aligned} \mathfrak{R}R_{-1}(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \left[\mathfrak{R}_f\mathfrak{R}_g\right]^{-1} \\ &= \sum_{fg\in E_1}\left[\mathfrak{R}_f\mathfrak{R}_g\right]^{-1} + \sum_{fg\in E_2}\left[\mathfrak{R}_f\mathfrak{R}_g\right]^{-1} + \cdots + \sum_{fg\in E_7}\left[\mathfrak{R}_f\mathfrak{R}_g\right]^{-1} \\ &= 12(5\times 5)^{-1} + (12n-18)(4\times 4)^{-1} + 12(5\times 4)^{-1} + 12(5\times 2)^{-1} + (6n-6)(4\times 1)^{-1} + (n-2)(1\times 1)^{-1} \\ &+ 2(2\times 1)^{-1} \\ &= \frac{13}{4}n - \frac{5}{8}. \end{aligned} \tag{37}$$

(c) When $\alpha = (1/2)$, $\mathfrak{R}R_{(1/2)}(\mathrm{HEX}(n))$ is given as

$$\begin{aligned}
\Re R_{(1/2)}(\mathrm{HEX}(n)) = \Re R_{(1/2)}(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \left[\Re_f \Re_g\right]^{(1/2)} \\
&= \sum_{fg\in E_1} \left[\Re_f \Re_g\right]^{(1/2)} + \sum_{fg\in E_2} \left[\Re_f \Re_g\right]^{(1/2)} + \cdots + \sum_{fg\in E_7} \left[\Re_f \Re_g\right]^{(1/2)} \\
&= 12\sqrt{5\times 5} + (12n-18)\sqrt{4\times 4} + 12\sqrt{5\times 4} + 12\sqrt{5\times 2} + (6n-6)\sqrt{4\times 1} + (n-2)\sqrt{1\times 1} + 2\sqrt{2\times 1} \\
&= 68.44139051 + 61n
\end{aligned} \tag{38}$$

(d) When $\alpha = -(1/2), \Re R_{-(1/2)}(\mathrm{HEX}(n))$ is given as

$$\begin{aligned}
\Re R_{-(1/2)}(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \left[\Re_f \Re_g\right]^{-(1/2)} \\
&= \sum_{fg\in E_1} \left[\Re_f \Re_g\right]^{-(1/2)} + \sum_{fg\in E_2} \left[\Re_f \Re_g\right]^{-(1/2)} + \cdots + \sum_{fg\in E_7} \left[\Re_f \Re_g\right]^{-(1/2)} \\
&= \frac{12}{\sqrt{5\times 5}} + \frac{12n-18}{\sqrt{4\times 4}} + \frac{12}{\sqrt{5\times 4}} + \frac{12}{\sqrt{5\times 2}} + \frac{6n-6}{\sqrt{4\times 1}} + \frac{n-2}{\sqrt{1\times 1}} + \frac{2}{\sqrt{2\times 1}} \\
&= 0.7922283276 + 7n.
\end{aligned} \tag{39}$$

□

Theorem 9. *In this theorem, we evaluate closed forms for the following indices:*

(a) *Reverse atom bond connectivity index of* $HEX(n) = ((12\sqrt{15} + 15\sqrt{3})/5)n + 7.56815951$

(b) *Reverse geometric arithmetic index of* $HEX(n) = (89/5)n + 9.967790715$

(c) *Reverse hyper Zagreb index of* $HEX(n) = 1468 + 922n$

Proof. We consider HEX(n). We use general formulas for the reverse atom bond connectivity, geometric, and hyper Zagreb indices by using Table 3.

(a) Computations for reverse atom bond connectivity index are given as

$$\begin{aligned}
\Re ABC(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \sqrt{\frac{\Re_f + \Re_g - 2}{\Re_f \Re_g}} \\
&= \sum_{fg\in E_1} \sqrt{\frac{\Re_f + \Re_g - 2}{\Re_f \Re_g}} + \sum_{fg\in E_2} \sqrt{\frac{\Re_f + \Re_g - 2}{\Re_f \Re_g}} + \cdots + \sum_{fg\in E_7} \sqrt{\frac{\Re_f + \Re_g - 2}{\Re_f \Re_g}} \\
&= 12\sqrt{\frac{5+5-2}{5\times 5}} + (12n-18)\sqrt{\frac{4+4-2}{4\times 4}} + 12\sqrt{\frac{5+4-2}{5\times 4}} + 12\sqrt{\frac{5+2-2}{5\times 2}} + (6n-6)\sqrt{\frac{4+1-2}{4\times 1}} \\
&\quad + (n-2)\sqrt{\frac{1+1-2}{1\times 1}} + 2\sqrt{\frac{2+1-2}{2\times 1}} \\
&= \left(\frac{12\sqrt{15} + 15\sqrt{3}}{5}\right)n + 7.56815951.
\end{aligned} \tag{40}$$

(b) Computations for reverse geometric connectivity index are given as

$$\begin{aligned}
\Re\mathrm{GA}(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \frac{2\sqrt{\Re_f\Re_g}}{\Re_f+\Re_g} \\
&= \sum_{fg\in E_1} \frac{2\sqrt{\Re_f\Re_g}}{\Re_f+\Re_g} + \sum_{fg\in E_2} \frac{2\sqrt{\Re_f\Re_g}}{\Re_f+\Re_g} + \sum_{fg\in E_3} \frac{2\sqrt{\Re_f\Re_g}}{\Re_f+\Re_g} + \cdots + \sum_{fg\in E_7} \frac{2\sqrt{\Re_f\Re_g}}{\Re_f+\Re_g} \\
&= 12\left(\frac{2\sqrt{5\times 5}}{5+5}\right) + (12n-18)\left(\frac{2\sqrt{4\times 4}}{4+4}\right) + 12\left(\frac{2\sqrt{5\times 4}}{5+4}\right) + 12\left(\frac{2\sqrt{5\times 2}}{5+2}\right) + (6n-6)\left(\frac{2\sqrt{4\times 1}}{4+1}\right) \\
&\quad + (n-2)\left(\frac{2\sqrt{1\times 1}}{1+1}\right) + 2\left(\frac{2\sqrt{2\times 1}}{2+1}\right) \\
&= \frac{89}{5}n + 9.967790715.
\end{aligned} \tag{41}$$

(c) Computations for reverse hyper Zagreb index are given as

$$\begin{aligned}
\Re\mathrm{HM}(\mathrm{HEX}(n)) &= \sum_{fg\in E(\mathrm{HEX}(n))} \left(\Re_f+\Re_g\right)^2 \\
&= \sum_{fg\in E_1} \left(\Re_f+\Re_g\right)^2 + \sum_{fg\in E_2} \left(\Re_f+\Re_g\right)^2 + \sum_{fg\in E_3} \left(\Re_f+\Re_g\right)^2 + \cdots + \sum_{fg\in E_7} \left(\left(\Re_f+\Re_g\right)^2\right. \\
&= 12(5+5)^2 + (12n-18)(4+4)^2 + 12(5+4)^2 + 12(5+2)^2 + (6n-6)(4+1)^2 + (n-2)(1+1)^2 + 2(2+1)^2 \\
&= 1468 + 922n.
\end{aligned} \tag{42}$$

Amongst all the evaluated reverse degree-based indices, reverse hyper Zagreb index ranks first and reverse Randić index for $\alpha = -1$, $R_{-1}(\mathrm{HEX}(n))$ ranks lowest, where n varies from 1 to 10. We use color palette in the following way for individual descriptor as yellow, green, pink, purple, brown, blue, and magenta for $\Re R_1(\mathrm{HEX}(n))$, $\Re R_{-1}(\mathrm{HEX}(n))$, $\Re R_{(1/2)}(\mathrm{HEX}(n))$, $\Re R_{-(1/2)}(\mathrm{HEX}(n))$, $\Re ABC(\mathrm{HEX}(n))$, and $\Re\mathrm{GA}(\mathrm{HEX}(n))$, $\Re\mathrm{HM}(\mathrm{HEX}(n))$, as shown in Figure 5. □

4. Conclusion

After evaluating the results, we have concluded that the ND_3 two-dimensional descriptor is of virtuous quality for the hexagonal crystal structure lattice as it ranks high among all the computed descriptors based on degree, neighborhood degree, and reverse degree. These calculations and closed form theorems will benefit math chemists by utilizing it in many mathematical techniques, and worthy quantitative studies include QSAR/QSPR/QSTR to study in depth the metallic crystallography formed in both inorganic and organic compounds attaining crystal structures. Below is the individual graphical representation of the descriptors that ranks high from each subsection of results, namely, degree based, neighborhood degree, and reverse degree, where green color graph representing $ND_3(\mathrm{HEX}(n))$, yellow representing $M_2(\mathrm{HEX}(n))$, and magenta representing $\Re\mathrm{HM}(\mathrm{HEX}(n))$ to visualize the best ranking descriptor for hexagonal crystal structure lattice HEX(n), as shown in Figures 6(a)–6(c).

Data Availability

The data used to support the findings of this study are cited at relevant places within the article as references.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

This work was supported by the Deanship of Scientific Research, Vice Presidency for Graduate Studies, and Scientific Research, King Faisal University Saudi Arabia (Project no. GRANT304).

References

[1] M. J. H. C. Belger and N. J. A. Sloane, *Sphere Packings, Lattices and Groups*, Springer-Verlag, Berlin, Germany, 1989.

[2] I. Gutman, B. Ruscic, N. Trinajstic, and C. F. Wilcox, "Graph theory and molecular orbitals. XII. Acyclic polyenes," *The Journal of Chemical Physics*, vol. 62, no. 9, pp. 3399–3409, 1975.
[3] I. Gutman and K. C. Das, "The first Zagreb index 30 years after," *MATCH Communications in Mathematical and in Computer*, vol. 50, no. 1, pp. 83–92, 2004.
[4] X. Li and Y. Shi, "A survey on the Randic index," *MATCH Communications in Mathematical and in Computer*, vol. 59, no. 1, pp. 127–156, 2008.
[5] K. C. Das, I. Gutman, and B. Furtula, "On atom-bond connectivity index," *Chemical Physics Letters*, vol. 511, no. 4–6, pp. 452–454, 2011.
[6] M. Numan, N. Naz, and F. Uddin, "New results on topological indices for Benes and butterfly networks," *University Politehnica of Bucharest Scientific Bulletin-Series A-Applied Mathematics and Physics*, vol. 82, no. 3, pp. 33–42, 2020.
[7] S. Mondal, N. De, and A. Pal, "On some new neighbourhood degree based indices," 2019, https://arxiv.org/abs/1906.11215.
[8] M. Ghorbani and M. A. Hosseinzadeh, "A note of Zagreb indices of nanostar dendrimers," *Optoelectronics and Advanced Materials, Rapid Communications*, vol. 4, pp. 1877–1880, 2010.
[9] M. S. Sardar, X. F. Pan, X.-F. Pan, W. Gao, and M. R. Farahani, "Computing Sanskruti index of titania nanotubes," *Open Journal of Mathematical Sciences*, vol. 1, no. 1, pp. 126–131, 2017.
[10] V. R. Kulli, "Some new status neighborhood indices of graphs," *IJMTT*, vol. 66, no. 9, pp. 139–153, 2020.
[11] S. Mondal, A. Dey, N. De, and A. Pal, "QSPR analysis of some novel neighbourhood degree-based topological descriptors," *Complex & Intelligent Systems*, vol. 7, no. 2, pp. 977–996, 2021.
[12] S. Mondal, M. K. Siddiqui, N. De, and A. Pal, "Neighborhood M-polynomial of crystallographic structures," *Biointerface Research in Applied Chemistry*, vol. 11, pp. 9372–9381, 2021.
[13] D. Zhao, Y.-M. Chu, M. K. Siddiqui et al., "On reverse degree based topological indices of polycyclic metal organic network," *Polycyclic Aromatic Compounds*, pp. 1–18. In press, 2021.
[14] E. Estrada, L. Torres, L. Rodriguez, and I. Gutman, "An atom-bond connectivity index: modelling the enthalpy of formation of alkanes," *Indian Journal of Chemistry*, vol. 37, pp. 849–855, 1998.
[15] D. Vukičević and B. Furtula, "Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges," *Journal of Mathematical Chemistry*, vol. 46, no. 4, pp. 1369–1376, 2009.
[16] G. H. Shirdel, H. Rezapour, and A. M. Sayadi, "The hyper-Zagreb index of graph operations," *Iranian Journal of Mathematical Chemistry*, vol. 4, pp. 213–220, 2013.
[17] H. Mujahed and B. Nagy, "Exact formula computing the wiener index on rows of unit cells of the diamond cubic grid connected in a row," *PJTAS*, vol. 26, no. 2, 2019.
[18] M. K. Siddiqui, M. Imran, and M. Saeed, "Topological properties of face-centred cubic lattice," *Hacettepe Journal of Mathematics and Statistics*, vol. 49, pp. 1–13, 2020.
[19] A. Ahmad and M. Imran, "Vertex-edge-degree-based topological properties for hex-derived networks," *Complexity*, vol. 2022, Article ID 7025480, 13 pages, 2022.
[20] A. Ahmad, M. A. Asim, and M. F. Nadeem, "Polynomials of degree-based indices of metal-organic networks," *Combinatorial Chemistry & High Throughput Screening*, vol. 25, 2020.
[21] D. Amić, D. Bešlo, B. Lucić, S. Nikolić, and N. Trinajstić, "The vertex-connectivity index revisited," *Journal of Chemical Information and Computer Sciences*, vol. 38, no. 5, pp. 819–822, 1998.
[22] B. Bollobás, *Graph Theory: An Introductory Course*, Springer, Berlin, Germany, 2012.