

Research Article

Topological Properties of Nano Sheets Based on Octa Graphene

Fozia Bashir Farooq 

Department of Mathematics and Statistics, Faculty of Science, Imam Mohammad Ibn Saud Islamic University(IMSU),
P.O. Box 90950, Riyadh 11623, Saudi Arabia

Correspondence should be addressed to Fozia Bashir Farooq; fozia.gc@gmail.com

Received 28 February 2022; Accepted 7 April 2022; Published 20 May 2022

Academic Editor: Gohar Ali

Copyright © 2022 Fozia Bashir Farooq. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

Octa Graphene is a carbon nanosheet constructed by octagons and squares to build a unit cell. Topological properties of nano sheets based on Octa graphene are investigated in this article for the first time. Octa Graphene play a role as a Nano carrier for drug delivery and plays vital role in cell base drug delivery applications. Two structures, Namely Octa-Grayphyne and Octa-Graphdine are investigated topically in this article. Mechanically Octa-Grayphyne and Octa-Graphdine are of immense interest in Nano structural batteries and other Nano devices. The ultimate value of these Nano sheets in nano electronics can be interpreted by observing their electronic structure and vibrational properties.

1. Introduction

Nano sheets are two dimensional Nano structures. Carbon Nano sheets from the last decades are of great interest for researchers. These sheets were produced by heating the fibers at a temperature of over 350 F for 24 hours. Graphene is crystal like Nano structure of carbon atoms, with a strong bond and of thickness of one atom. Whereas Graphene Nano sheet is a 2D Nano structure consist of a single lyre of carbon atoms with hexagonal lattices. Wu et al. [1] investigated Graphene oxide sheet can be used as a carrier for Adriamcine, can reverse drug resistance in breast cancer. Moreover, in [2] it was shown that Graphene oxide sheet was also an anti-cancer agent. Without loss of generality we can state that Grephene oxide sheet is a source to decrease death rate due to cancer. The novel 2D Nano sheets have open new horizons to solve the serious environmental water pollution problem of the time by serving as a favorable candidate to reduce heavy metal pollution from water. To read about Nanosheets read [3].

Octa Grephene is a carbon Nano sheet, consisting of octagons and squares. Poupitz at el [4] introduces Octa-Grayphyne and Octa-Graphdine Nano sheets. Before going to further investigation of theses nano sheets, authors would

like to recall some history of Topological indices for chemical graphs;

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$ with $|V(G)| = p$ and $|E(G)| = q$ respectively. Degree of a vertex $u \in V(G)$, means number of edges incident with u and symbolically written as d_u . A chemical Graph is the graphical representation of a chemical structure where vertices represents the atoms and edges represents the bond between atoms. In chemical graphs the maximum degree of vertex that can have is 4.

The Molecular Descriptor is a procedure to transform chemical information of a compound to a numerical value. Topological indices are one of the types of molecular descriptors. These indices are numerical values calculated from graphical representation of chemical compounds. Topological indices play an important role for Quantitative Structure Activity relationship (QSAR) by correlating psychochemical and biological properties of chemical compounds. Harry wiener is the founder of chemical graph theory. His contribution towards study of Topological indices is radical and about QSAR methods can be found in [5] commendable. He introduced structure-base invariants correlating boiling points of paraffin. He introduced the Winer index, which plays a major role in nanotechnology.

One of the classical topological index was introduced by Milan Randić in 1975. Randić index is the Sum of bond contribution of the degrees of vertices (atoms) making that bond, defined in [6] as;

$$\chi(\mathbb{G}) = \sum_{uv \in E(\mathbb{G})} \frac{1}{\sqrt{d_u d_v}} \quad (1)$$

Idea of general Randić index was given by Bollobás and Erdős in [7] as:

$$R_\alpha(\mathbb{G}) = \sum_{uv \in E(\mathbb{G})} (d_u d_v)^\alpha \quad (2)$$

Gutman and Trinajstić [8], introduces first and second Zagreb indices $M_1(\mathbb{G})$ and $M_2(\mathbb{G})$ as;

$$\begin{aligned} M_1(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} [d_u + d_v], \\ M_2(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} [d_u d_v]. \end{aligned} \quad (3)$$

History of topological index will not complete without discussion of Atom Bond connectivity index (ABC index) as it has extraordinary applications in rationalizing alkanes. ABC index was introduced by Estrada et al. [9] as;

$$I(\mathbb{G}) = \sum_{uv \in E(\mathbb{G})} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \quad (4)$$

Harmonic index $H(\mathbb{G})$ of a graph \mathbb{G} is defined [10] as;

$$H(\mathbb{G}) = \sum_{uv \in E(\mathbb{G})} \frac{2}{d_u + d_v} \quad (5)$$

For a molecular graph \mathbb{G} the forgotten index or F index [11] is;

$$F(\mathbb{G}) = \sum_{uv \in E(\mathbb{G})} [d_u^2 + d_v^2]. \quad (6)$$

Symmetric Division index or SDD for a molecular Graph \mathbb{G} is defined [12] as;

$$SDD(\mathbb{G}) = \sum_{uv \in E(\mathbb{G})} \left[\frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)} \right]. \quad (7)$$

The reader is encouraged to study [7, 13, 14] for more information on degree-based topological indices.

Deutsch, E.; Deutsch, [15] gave the $c[(\min(d_u, d_v)/\max(d_u, d_v)) + (\max(d_u, d_v)/\min(d_u, d_v))]$ concept of M polynomial of a chemical graph defined as;

$$M(\mathbb{G}, x, y) = \sum_{i \leq j} e_{ij}(\mathbb{G}) \alpha^i \beta^j, \quad (8)$$

where $e_{ij}(\mathbb{G})$, ($i, j \geq 1$) denotes the number of the edges $e = uv$ of molecular graph G such that $(d_u, d_v) = (i, j)$.

For further studies about M -polynomial please read [16–28].

Table 1 gives the relation between the degree base topological indices with M polynomial. Where,

$$\begin{aligned} D_\alpha(f(\alpha, \beta)) &= \alpha \cdot \frac{\partial(f(\alpha, \beta))}{\partial \alpha}, \\ D_\beta(f(\alpha, \beta)) &= \beta \cdot \frac{\partial(f(\alpha, \beta))}{\partial \beta}, \\ J(f) &= f(\alpha, \alpha), \end{aligned} \quad (9)$$

$$S_\alpha(f(\alpha, \beta)) = \int_0^\alpha \frac{f(t, \beta)}{t} dt,$$

$$S_\beta(f(\alpha, \beta)) = \int_0^\beta \frac{f(\alpha, t)}{t} dt.$$

2. Main Results

2.1 Let $O_1\mathbb{G}_{m \times n}$ be the Octa-Graphyne Nano sheet with m hexagons with each row and n hexagons in each column. From the graphical representation of Octa-Graphyne nano sheet, we can observe that each row of $O_1\mathbb{G}_{m \times n}$ consists of m hexagons and $m+1$ squares. The Graph of $O_1\mathbb{G}_{m \times n}$ can be found in Figure 1. Each successive column of $O_1\mathbb{G}_{m \times n}$ also consists of n hexagons and $n+1$ squares. Degrees of end vertices for all edges are used to calculate degree-based topological indices. $O_1\mathbb{G}_{m \times n}$ has $4mn + 2m + 2n$ number of vertices, whereas number of edges for $O_1\mathbb{G}_{m \times n}$ is $6mn + m + n$. By observing graph of $O_1\mathbb{G}_{m \times n}$ one can find that all vertices of $O_1\mathbb{G}_{m \times n}$ has either degree 2 or 3. Depending on the degree of vertices edge partition of $O_1\mathbb{G}_{m \times n}$ is given in Table 2.

Partition of edge sets is defined as,

$$E_{(i,j)} = \{uv \in E(O_1\mathbb{G}_{m \times n}) : d_u = i \text{ and } d_v = j, \quad 2 \leq i \leq j \leq 3\}. \quad (10)$$

Based on edge partition given in Table 2, we can find M polynomial of Octa-Graphyne Nanosheet $O_1\mathbb{G}_{m \times n}$, Whereas Graphical representation of M polynomial of $O_1\mathbb{G}_{m \times n}$ is given in Figure 2.

Theorem 1. Let $O_1\mathbb{G}_{m \times n}$ be the graph of Octa-Graphyne Nanosheet, M polynomial for $O_1\mathbb{G}_{m \times n}$ is given by,

$$\begin{aligned} M(O_1\mathbb{G}_{m \times n}) &= 2(m+n+2)\alpha^2\beta^2 + 4(m+n-2)\alpha^2\beta^3 \\ &\quad + (6mn - 5m - 5n + 4)\alpha^3\beta^3. \end{aligned} \quad (11)$$

Proof. Let $O_1\mathbb{G}_{m \times n}$ be the graph of Octa-Graphyne Nanosheet, By using Table 2, combined with equation 9, we get

$$\begin{aligned} M(O_1\mathbb{G}_{m \times n}) &= \sum_{i \leq j} e_{ij}(O_1\mathbb{G}_{m \times n}) \alpha^i \beta^j \\ &= \sum e_{22}(O_1\mathbb{G}_{m \times n}) \alpha^2 \beta^2 + \sum e_{23}(O_1\mathbb{G}_{m \times n}) \alpha^2 \beta^3 \\ &\quad + \sum e_{33}(O_1\mathbb{G}_{m \times n}) \alpha^3 \beta^3 \\ &= 2(m+n+2)\alpha^2\beta^2 + 4(m+n-2)\alpha^2\beta^3 \\ &\quad + (6mn - 5m - 5n + 4)\alpha^3\beta^3. \end{aligned} \quad (12)$$

□

TABLE 1: Derivation of topological indices from the M polynomial.

Degree base topological indices	$f(\alpha, \beta)$	Derivation from $M(\mathbb{G}, \alpha, \beta)$
$M_1(\mathbb{G})$	$\alpha + \beta$	$(D_\alpha + D_\beta)(M(\mathbb{G}, \alpha, \beta)) _{\alpha=\beta=1}$
$M_2(\mathbb{G})$	$\alpha\beta$	$(D_\alpha D_\beta)(M(\mathbb{G}, \alpha, \beta)) _{\alpha=\beta=1}$
$R_\alpha(\mathbb{G})$	$(\alpha\beta)^\alpha, \alpha \in N$	$D_\alpha^\alpha D_\beta^\alpha (M(\mathbb{G}, \alpha, \beta)) _{\alpha=\beta=1}$
$I(\mathbb{G})$	$\alpha\beta/(\alpha + \beta)$	$2S_\alpha J D_\alpha D_\beta (M(\mathbb{G}, \alpha, \beta)) _{\alpha=\beta=1}$
$H(\mathbb{G})$	$2/(\alpha + \beta)$	$2S_\alpha J (M(\mathbb{G}, \alpha, \beta)) _{\alpha=\beta=1}$
$F(\mathbb{G})$	$\alpha^2 + \beta^2$	$(D_\alpha^2 + D_\beta^2)M(\mathbb{G}, \alpha, \beta) _{\alpha=\beta=1}$
$SDD(\mathbb{G})$	$(\alpha^2 + \beta^2)/\alpha\beta$	$(D_\alpha S_\beta + S_\alpha D_\beta)M(\mathbb{G}, \alpha, \beta) _{\alpha=\beta=1}$

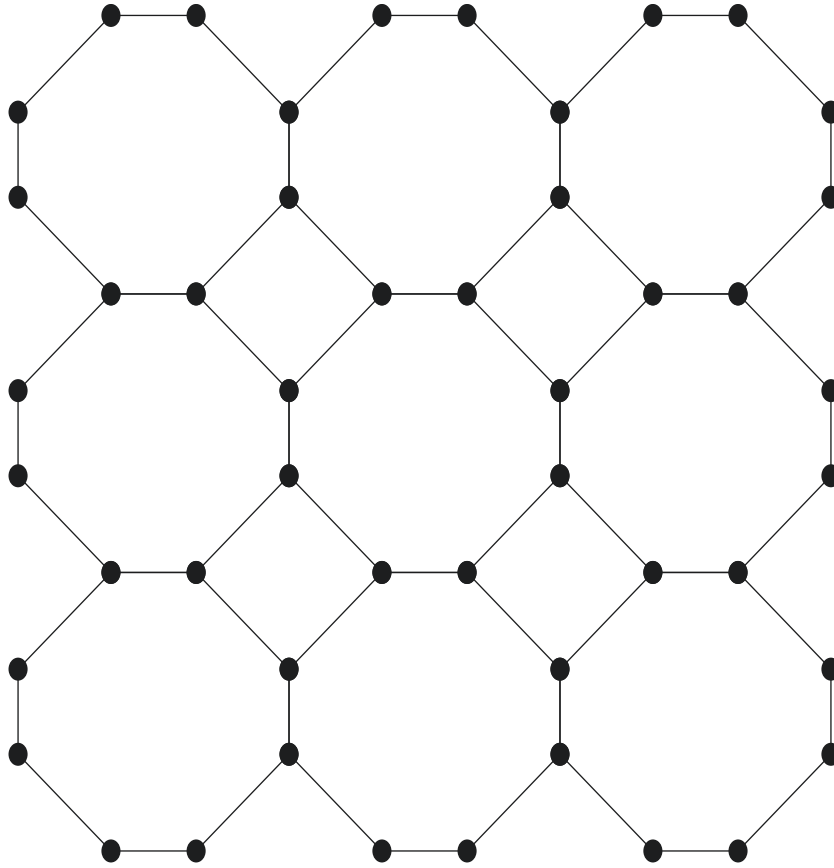


FIGURE 1: Graph of octa-graphyne nanosheet $O_1\mathbb{G}_{3 \times 3}$.

TABLE 2: Edge Partition of $O_1\mathbb{G}_{m \times n}$ Nano sheet.

Edge types	(d_u, d_v)	Frequency
$E_{(2,2)}$	(2, 2)	$2(m + n + 2)$
$E_{(2,3)}$	(2, 3)	$4(m + n - 2)$
$E_{(3,3)}$	(3, 3)	$6mn - 5m - 5n + 4$

Theorem 2. Let $O_1\mathbb{G}_{m \times n}$ be the graph of Octa- Graphyne Nanosheet Let $M(O_1\mathbb{G}_{m \times n}) = 2(m + n + 2)\alpha^2\beta^2 + 4(m + n - 2)\alpha^2\beta^3 + (6mn - 5m - 5n + 4)\alpha^3\beta^3$ be M polynomial of $O_1\mathbb{G}_{m \times n}$ then we have,

$$\begin{aligned}
 M_1(O_1\mathbb{G}_{m \times n}) &= 36mn - 2m - 2n, \\
 M_2(O_1\mathbb{G}_{m \times n}) &= 54mn - 13m - 13n + 4, \\
 R_\alpha(O_1\mathbb{G}_{m \times n}) &= 2(3^{2\alpha+1})mn \\
 &\quad + (2^{2\alpha+1} + 2^{\alpha+2}3^\alpha - 5\mathbb{G}3^{2\alpha})m \\
 &\quad + (2^{2\alpha+1} + 2^{\alpha+2}3^\alpha - 5\mathbb{G}3^{2\alpha})n \\
 &\quad + 4(2^{2\alpha} + 3^{2\alpha} - 2\mathbb{G}2^\alpha\mathbb{G}3^\alpha), \\
 I(O_1\mathbb{G}_{m \times n}) &= 9mn - 0.7m - 0.7n + 0.4.
 \end{aligned} \tag{13}$$

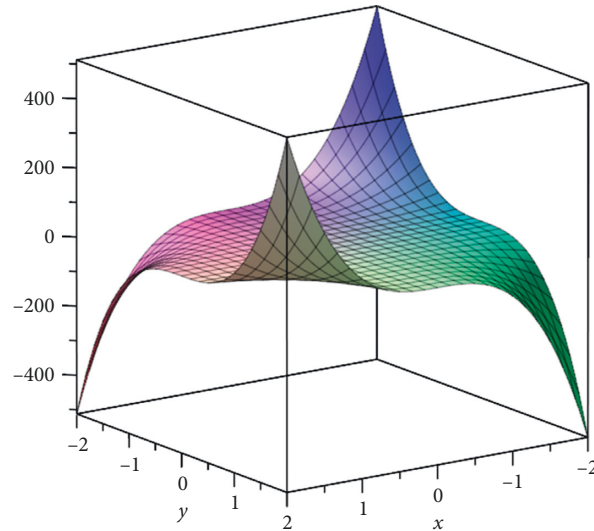


FIGURE 2: The graph of the M-polynomial of $O_1\mathbf{G}_{m \times n}$ Nanosheet.

Proof. Let $M(O_1\mathbf{G}_{m \times n}, \alpha, \beta) = 2(m+n+2)\alpha^2\beta^2 + 4(m+n-2)\alpha^2\beta^3 + (6mn-5m-5n+4)\alpha^3\beta^3$ be M polynomial of Octa- Graphyne Nanosheet then,

$$(i) M_1(O_1\mathbf{G}_{m \times n}) = (D_\alpha + D_\beta)M(O_1\mathbf{G}, \alpha, \beta)|_{\alpha=\beta=1},$$

$$D_\alpha M(O_1\mathbf{G}_{m \times n}, \alpha, \beta) = 4(m+n+2)\alpha^2\beta^2 + 8(m+n-2)\alpha^2\beta^3 + 3(6mn-5m-5n+4)\alpha^3\beta^3,$$

$$D_\beta M(O_1\mathbf{G}_{m \times n}, \alpha, \beta) = 4(m+n+2)\alpha^2\beta^2 + 12(m+n-2)\alpha^2\beta^3 + 3(6mn-5m-5n+4)\alpha^3\beta^3,$$

$$(D_\alpha + D_\beta)M(O_1\mathbf{G}_{m \times n}, \alpha, \beta) = 8(m+n+2)\alpha^2\beta^2 + 20(m+n-2)\alpha^2\beta^3 + 6(6mn-5m-5n+4)\alpha^3\beta^3,$$

$$\begin{aligned} (D_\alpha + D_\beta)M(O_1\mathbf{G}, \alpha, \beta)|_{\alpha=\beta=1} &= 8(m+n+2) + 20(m+n-2) + 6(6mn-5m-5n+4) \\ &= 36mn - 2m - 2n. \end{aligned}$$

$$(ii) M_2(O_1\mathbf{G}_{m \times n}) = (D_\alpha D_\beta)M(O_1\mathbf{G}_{m \times n}, \alpha, \beta)|_{\alpha=\beta=1},$$

$$(D_\alpha D_\beta)M(O_1\mathbf{G}_{m \times n}, \alpha, \beta) = 8(m+n+2)\alpha^2\beta^2 + 24(m+n-2)\alpha^2\beta^3 + 9(6mn-5m-5n+4)\alpha^3\beta^3,$$

$$\begin{aligned} (D_\alpha D_\beta)M(O_1\mathbf{G}_{m \times n}, \alpha, \beta)|_{\alpha=\beta=1} &= 8(m+n+2) + 24(m+n-2) + 9(6mn-5m-5n+4) \\ &= 54mn - 13m - 13n + 4. \end{aligned}$$

$$(iii) R_{\alpha\alpha}(O_1\mathbf{G}_{m \times n}) = D_\alpha^\alpha D_\beta^\alpha M(O_1\mathbf{G}_{m \times n}, \alpha, \beta)|_{\alpha=\beta=1},$$

$$D_\alpha^\alpha D_\beta^\alpha M(O_1\mathbf{G}_{m \times n}, \alpha, \beta) = 2\mathbf{G}2^\alpha 2^\beta (m+n+2)\alpha^2\beta^2 + 4\mathbf{G}2^\alpha 3^\alpha (m+n-2)\alpha^2\beta^3 + 3^\alpha 3^\alpha (6mn-2^\alpha \mathbf{G}5m-5n+4)\alpha^3\beta^3,$$

$$\begin{aligned} D_\alpha^\alpha D_\beta^\alpha M(O_1\mathbf{G}_{m \times n}, \alpha, \beta)|_{\alpha=\beta=1} &= 2\mathbf{G}2^\alpha 2^\alpha (m+n+2)\alpha^2\beta^2 \\ &\quad + 4\mathbf{G}2^\alpha 3^\alpha (m+n-2)\alpha^2\beta^3 + 3^\alpha 3^\alpha (6mn-5m-5n+4)\alpha^3\beta^3 \\ &= 2(3^{2\alpha+1})mn + (2^{2\alpha+1} + 2^{\alpha+2}3^\alpha - 5\mathbf{G}3^{2\alpha})m + (2^{2\alpha+1} + 2^{\alpha+2}3^\alpha - 5\mathbf{G}3^{2\alpha})n + 4(2^{2\alpha} + 3^{2\alpha}). \end{aligned}$$

$$\begin{aligned}
 \text{(iv)} \quad I(O_1\mathbf{G}_{m \times n}) &= S_\alpha J(D_\alpha D_\beta M(O_1\mathbf{G}_{m \times n}, \alpha))|_{\alpha=\beta=1}, \\
 J(D_\alpha D_\beta M(O_1\mathbf{G}_{m \times n}, \alpha)) &= 8(m+n+2)\alpha^4 + 24(m+n-2)\alpha^5 + 9(6mn-5m-5n+4)\alpha^6, \\
 S_\alpha J(D_\alpha D_\beta M(O_1\mathbf{G}_{m \times n}, \alpha)) &= 2(m+n+2)\alpha^4 + \frac{24}{5}(m+n-2)\alpha^5 \\
 &\quad + \frac{3}{2}(6mn-5m-5n+4)\alpha^6, \\
 S_\alpha J(D_\alpha D_\beta M(O_1\mathbf{G}_{m \times n}, \alpha))|_{\alpha=\beta=1} &= 2(m+n+2) + \frac{24}{5}(m+n-2) \\
 &\quad + \frac{3}{2}(6mn-5m-5n+4), \\
 I(O_1\mathbf{G}_{m \times n}) &= 9mn - 0 \cdot 7m - 0 \cdot 7n + 0 \cdot 4. \tag{14}
 \end{aligned}$$

Theorem 3. Let $O_1\mathbf{G}_{m \times n}$ be the graph of Octa- Graphyne Nanosheet Let

- (i) $M(O_1\mathbf{G}_{m \times n}) = 2(m+n+2)\alpha^2\beta^2 + 4(m+n-2)\alpha^2\beta^3 + (6mn-5m-5n+4)\alpha^3\beta^3$ be M polynomial of $O_1\mathbf{G}_{m \times n}$ then we have,
- (ii) $H(O_1\mathbf{G}_{m \times n}) = 2mn + 0 \cdot 933m + 0 \cdot 933n + 0 \cdot 133$

- (iii) $F(O_1\mathbf{G}_{m \times n}) = 108mn - 22m - 22n$
- (iv) $SDD(O_1\mathbf{G}_{m \times n}) = 12mn + 2 \cdot 67m + 2 \cdot 67n - 1 \cdot 33$

Proof. Let $M(O_1\mathbf{G}_{m \times n}, \alpha, \beta) = 2(m+n+2)\alpha^2\beta^2 + 4(m+n-2)\alpha^2\beta^3 + (6mn-5m-5n+4)\alpha^3\beta^3$ be M polynomial of Octa- Graphyne Nanosheet then ,

$$\begin{aligned}
 \text{(i)} \quad H(O_1\mathbf{G}_{m \times n}) &= 2S_\alpha J(M(O_1\mathbf{G}_{m \times n}, \alpha, \beta))|_{\alpha=\beta=1}, \\
 J(M(O_1\mathbf{G}_{m \times n}, \alpha, \beta)) &= 2(m+n+2)\alpha^4 + 4(m+n-2)\alpha^5 + (6mn-5m-5n+4)\alpha^6, \\
 2S_\alpha J(M(O_1\mathbf{G}_{m \times n}, \alpha, \beta)) &= (2mn+m+n+4)\alpha^4 + \frac{8}{5}(4mn+6m+6n)\alpha^5 + \frac{1}{3}mna^6, \\
 H(O_1\mathbf{G}_{m \times n}) &= 2mn + 0 \cdot 933m + 0 \cdot 933n + 0 \cdot 133. \\
 \text{(ii)} \quad F(O_1\mathbf{G}_{m \times n}) &= (D_\alpha^2 + D_\beta^2)(M(O_1\mathbf{G}_{m \times n}, \alpha, \beta))|_{\alpha=\beta=1}, \\
 D_\alpha^2(M(O_1\mathbf{G}_{m \times n}, \alpha, \beta)) &= 8(m+n+2)\alpha^2\beta^2 + 16(m+n-2)\alpha^2\beta^3 + 9(6mn-5m-5n+4)\alpha^3\beta^3, \\
 D_\beta^2(M(O_1\mathbf{G}_{m \times n}, \alpha, \beta)) &= 8(m+n+2)\alpha^2\beta^2 + 36(m+n-2)\alpha^2\beta^3 + 9(6mn-5m-5n+4)\alpha^3\beta^3, \\
 F(O_1\mathbf{G}_{m \times n}) &= 108mn - 22m - 22n. \\
 \text{(iii)} \quad SDD(O_1\mathbf{G}_{m \times n}) &= (D_\alpha S_\beta + S_\alpha D_\beta)(M(O_1\mathbf{G}_{m \times n}, \alpha, \beta))|_{\alpha=\beta=1}, \\
 D_\alpha S_\beta(M(O_1\mathbf{G}_{m \times n}, \alpha, \beta)) &= 2(m+n+2)\alpha^2\beta^2 + \frac{8}{3}(m+n-2)\alpha^2\beta^3 + \frac{1}{3}(6mn-5m-5n+4)\alpha^3\beta^3, \\
 D_\alpha S_\beta(M(O_1\mathbf{G}_{m \times n}, \alpha, \beta))|_{\alpha=\beta=1} &= 2(m+n+2) + \frac{8}{3}(m+n-2) + \frac{1}{3}(6mn-5m-5n+4), \\
 S_\alpha D_\beta(M(O_1\mathbf{G}_{m \times n}, \alpha, \beta)) &= 2(m+n+2)\alpha^2\beta^2 + 6(m+n-2)\alpha^2\beta^3 \\
 &\quad + (6mn-5m-5n+4)\alpha^3\beta^3, \\
 S_\alpha D_\beta(M(O_1\mathbf{G}_{m \times n}, \alpha, \beta))|_{\alpha=\beta=1} &= 2(m+n+2) + 6(m+n-2) \\
 &\quad + (6mn-5m-5n+4), \\
 SDD(O_1\mathbf{G}_{m \times n}) &= 12mn + 2 \cdot 67m + 2 \cdot 67n - 1.33. \tag{15}
 \end{aligned}$$

2.2. Let $O_2\mathbf{G}_{m \times n}$ be the Octa-Grayphdiyne Nanosheet with m hexadecagones with each row and n hexadecagones in each column. From a graphical representation of the Octa-Grayphdiyne Nano sheet we can observe that each row of $O_2\mathbf{G}_{m \times n}$ consists of m hexadecagones and $m + 1$ squares. The graph of Octa-Grayphdiyne Nanosheet $O_2\mathbf{G}_{m \times n}$ is given in Figure 3. Each successive column of $O_2\mathbf{G}_{m \times n}$ also consists n hexadecagones and $n + 1$ squares. Degrees of end vertices for all edges are used to calculate degree-based topological indices. $O_2\mathbf{G}_{m \times n}$ has $8mn + 6m + 6n + 4$ number of vertices, whereas number of edges for $O_2\mathbf{G}_{m \times n}$ is $10mn + 7m + 7n + 4$. By observing graph of $O_2\mathbf{G}_{m \times n}$ one can find that that all vertices of $O_2\mathbf{G}_{m \times n}$ has either degree 2 or 3. Depending on the degree of vertices edge partition of $O_2\mathbf{G}_{m \times n}$ is given in Table 3.

Partition of edge sets is defined as,

$$E_{(i,j)} = \{uv \in E(O_2\mathbf{G}_{m \times n}): d_u = i \text{ and } d_v = j \quad 2 \leq i \leq j \leq 3\}. \quad (16)$$

$$\begin{aligned} M(O_2\mathbf{G}_{m \times n}) &= \sum_{i \leq j} e_{ij}(O_2\mathbf{G}_{m \times n}) \alpha^i \beta^j \\ &= \sum e_{22}(O_2\mathbf{G}_{m \times n}) \alpha^2 \beta^2 + \sum e_{23}(O_2\mathbf{G}_{m \times n}) \alpha^2 \beta^3 + \sum e_{33}(O_2\mathbf{G}_{m \times n}) \alpha^3 \beta^3 \\ &= (2mn + m + n + 4) \alpha^2 \beta^2 + (4mn + 6m + 6n) \alpha^2 \beta^3 + 4mn \alpha^3 \beta^3. \end{aligned} \quad (18)$$

Theorem 5. Let $O_2\mathbf{G}_{m \times n}$ be the graph of Octa-Grayphdiyne Nanosheet Let

$M(O_2\mathbf{G}_{m \times n}) = (2mn + m + n + 4) \alpha^2 \beta^2 + (4mn + 6m + 6n) \alpha^2 \beta^3 + 4mn \alpha^3 \beta^3$ be M polynomial of $O_2\mathbf{G}_{m \times n}$ then we have

- (i) $M_1(O_2\mathbf{G}_{m \times n}) = 52mn + 34m + 34n + 16$.
- (ii) $M_2(O_2\mathbf{G}_{m \times n}) = 68mn + 40m + 40n + 16$.

Based on edge partition given in Table 3, we can find M polynomial of Octa-Grayphdiyne Nanosheet $O_2\mathbf{G}_{m \times n}$, Whereas Graphical representation of M polynomial of $O_2\mathbf{G}_{m \times n}$ is given in Figure 4. \square

Theorem 4. Let $O_2\mathbf{G}_{m \times n}$ be the graph of Octa-Grayphdiyne Nanosheet, M polynomial for $O_2\mathbf{G}_{m \times n}$ is given by,

$$M(O_2\mathbf{G}_{m \times n}) = (2mn + m + n + 4) \alpha^2 \beta^2 + (4mn + 6m + 6n) \alpha^2 \beta^3 + 4mn \alpha^3 \beta^3. \quad (17)$$

Proof. Let $O_2\mathbf{G}_{m \times n}$ be the graph of Octa-Grayphdiyne Nanosheet, Using Table 3, combined with equation 9, we get

- (iii) $R_\alpha(O_2\mathbf{G}_{m \times n}) = 2(4^\alpha + 2\mathbf{G}6^\alpha + 2\mathbf{G}9^\alpha)mn + (4^\alpha + 6^{\alpha+1})m + (4^\alpha + 6^{\alpha+1})n + 4^{\alpha+1}$.
- (iv) $I(O_2\mathbf{G}_{m \times n}) = 12 \cdot 8mn + 8 \cdot 2m + 8 \cdot 2n + 4$.

Proof. Let $M(O_2\mathbf{G}_{m \times n}, \alpha, \beta) = (2mn + m + n + 4) \alpha^2 \beta^2 + (4mn + 6m + 6n) \alpha^2 \beta^3 + 4mn \alpha^3 \beta^3$ be M polynomial of Octa-Grayphdiyne Nanosheet then,

$$\begin{aligned} (i) \quad M_1(O_2\mathbf{G}_{m \times n}) &= (D_\alpha + D_\beta)M(O_2\mathbf{G}_{m \times n}, \alpha, \beta)|_{\alpha=\beta=1}, \\ D_\alpha M(O_2\mathbf{G}_{m \times n}, \alpha, \beta) &= 2(2mn + m + n + 4) \alpha^2 \beta^2 + 2(4mn + 6m + 6n) \alpha^2 \beta^3 \\ &\quad + 12mn \alpha^3 \beta^3, \\ D_\beta M(O_2\mathbf{G}_{m \times n}, \alpha, \beta) &= 2(2mn + m + n + 4) \alpha^2 \beta^2 + 3(4mn + 6m + 6n) \alpha^2 \beta^3 + 12mn \alpha^3 \beta^3, \\ (D_\alpha + D_\beta)M(O_2\mathbf{G}_{m \times n}, \alpha, \beta) &= 4(2mn + m + n + 4) \alpha^2 \beta^2 + 5(4mn + 6m + 6n) \alpha^2 \beta^3 \\ &\quad + 24mn \alpha^3 \beta^3 \\ (D_\alpha + D_\beta)M(O_2\mathbf{G}_{m \times n}, \alpha, \beta)|_{\alpha=\beta=1} &= 4(2mn + m + n + 4) + 5(4mn + 6m + 6n) + 24mn \\ &= 52mn + 34m + 34n + 16. \quad (ii) \quad M_2(O_2\mathbf{G}_{m \times n}) \\ (D_\alpha D_\beta)M(O_2\mathbf{G}_{m \times n}, \alpha, \beta) &= 4(2mn + m + n + 4) \alpha^2 \beta^2 + 6(4mn + 6m + 6n) \alpha^2 \beta^3 + 36mn \alpha^3 \beta^3, \\ (D_\alpha D_\beta)M(O_2\mathbf{G}_{m \times n}, \alpha, \beta)|_{\alpha=\beta=1} &= 4(2mn + m + n + 4) + 6(4mn + 6m + 6n) + 36mn \\ &= 68mn + 40m + 40n + 16. \end{aligned}$$

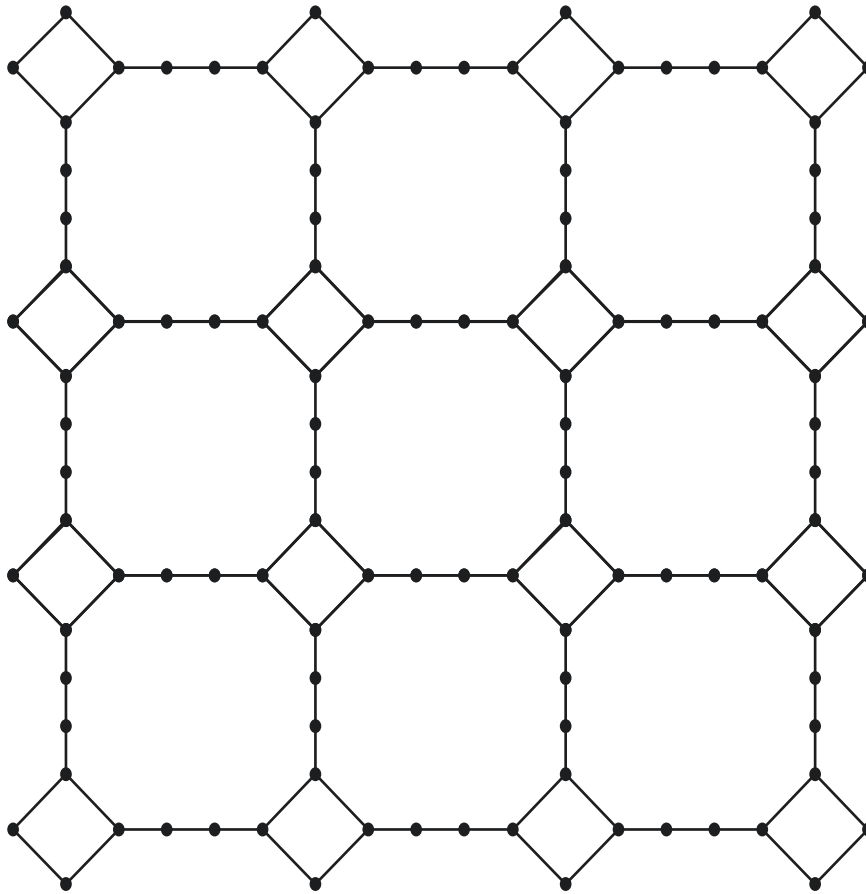


FIGURE 3: Graph of octa-graphdine nanosheet $O_2G_{3 \times 3}$.

TABLE 3: Edge Partition of $O_2G_{m \times n}$ Nano sheet.

Edge types	(d_u, d_v)	Frequency
$E_{(2,2)}$	(2, 2)	$2mn + m + n + 4$
$E_{(2,3)}$	(2, 3)	$4mn + 6m + 6n$
$E_{(3,3)}$	(3, 3)	$4mn$

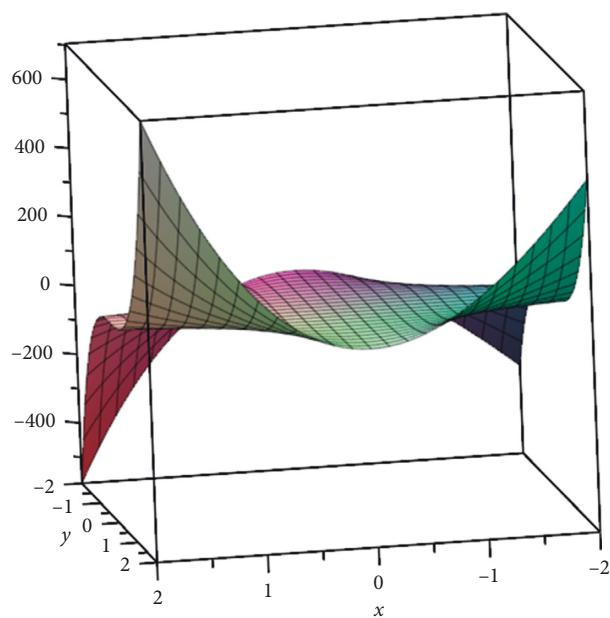


FIGURE 4: The graph of M-polynomial of $O_2G_{m \times n}$ Nanosheet.

$$\begin{aligned}
 (iii) R_{\alpha} (O_2 \mathbf{G}_{m \times n}) &= D_{\alpha}^{\alpha} D_{\beta}^{\alpha} M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta)|_{\alpha=\beta=1}, \\
 D_{\alpha}^{\alpha} D_{\beta}^{\alpha} M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta) &= 2^{\alpha} 2^{\alpha} (2mn + m + n + 4) \alpha^2 \beta^2 \\
 &\quad + 2^{\alpha} 3^{\alpha} (4mn + 6m + 6n) \alpha^2 \beta^3 + 4 \times 3^{\alpha} 3^{\alpha} mn \alpha^3 \beta^3, \\
 D_{\beta}^{\alpha} (M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta))|_{\alpha=\beta=1} &= 2^{\alpha} 2^{\alpha} (2mn + m + n + 4) + 2^{\alpha} 3^{\alpha} (4mn + 6m + 6n) \\
 &\quad + 4 \times 3^{\alpha} 3^{\alpha} mn, \\
 &= 2(4^{\alpha} + 2 \times 6^{\alpha} + 2 \times 9^{\alpha})mn + (4^{\alpha} + 6^{\alpha+1})m + (4^{\alpha} + 6^{\alpha+1})n + 4^{\alpha+1}. \\
 I(O_2 \mathbf{G}_{m \times n}) &= S_{\alpha} J(D_{\alpha} D_{\beta} (M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta)))|_{\alpha=\beta=1}, \\
 J(D_{\alpha} D_{\beta} (M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta))) &= 4(2mn + m + n + 4) \alpha^4 + 6(4mn + 6m + 6n) \alpha^5 + 36mn \alpha^6, \\
 S_{\alpha} J(D_{\alpha} D_{\beta} (M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta))) &= (2mn + m + n + 4) \alpha^4 + \frac{6}{5} (4mn + 6m + 6n) \alpha^5 + 6mn \alpha^6, \\
 S_{\alpha} J(D_{\alpha} D_{\beta} (M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta)))|_{\alpha=1} &= (2mn + m + n + 4) + \frac{6}{5} (4mn + 6m + 6n) + 6mn, \\
 I(O_2 \mathbf{G}_{m \times n}) &= \frac{64mn + 41m + 41n}{5} + 4.
 \end{aligned} \tag{19}$$

Theorem 6. Let $O_2 \mathbf{G}_{m \times n}$ be the graph of Octa-Grayphdine Nanosheet Let

$M(O_2 \mathbf{G}_{m \times n}) = (2mn + m + n + 4) \alpha^2 \beta^2 + (4mn + 6m + 6n) \alpha^2 \beta^3 + 4mn \alpha^3 \beta^3$ be M polynomial of $O_2 \mathbf{G}_{m \times n}$ then we have

- (i) $H(O_2 \mathbf{G}_{m \times n}) = 3.933mn + 2.9m + 2.9n + 2.$
- (ii) $F(O_2 \mathbf{G}_{m \times n}) = 140mn + 86m + 86n + 32.$

$$(iii) SDD(O_2 \mathbf{G}_{m \times n}) = 20.67mn + 15m + 15n + 8.$$

Proof. Let $M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta) = (2mn + m + n + 4) \alpha^2 \beta^2 + (4mn + 6m + 6n) \alpha^2 \beta^3 + 4mn \alpha^3 \beta^3$ be M polynomial of Octa-Grayphdine Nanosheet then,

$$\begin{aligned}
 (i) H(O_2 \mathbf{G}_{m \times n}) &= 2S_{\alpha} J(M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta))|_{\alpha=\beta=1}, \\
 J(M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta)) &= (2mn + m + n + 4) \alpha^4 + (4mn + 6m + 6n) \alpha^5 + 4mn \alpha^6, \\
 S_{\alpha} J(M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta)) &= \frac{1}{4} (2mn + m + n + 4) \alpha^4 + \frac{1}{5} (4mn + 6m + 6n) \alpha^5 + \frac{2}{3} mn \alpha^6, \\
 H(O_2 \mathbf{G}_{m \times n}) &= 3 \cdot 933mn + 2 \cdot 9m + 2 \cdot 9n + 2. \\
 (ii) F(O_2 \mathbf{G}_{m \times n}) &= (D_{\alpha}^2 + D_{\beta}^2)(M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta))|_{\alpha=\beta=1}, \\
 D_{\alpha}^2 (M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta)) &= 4(2mn + m + n + 4) \alpha^2 \beta^2 + 4(4mn + 6m + 6n) \alpha^2 \beta^3 + 36mn \alpha^3 \beta^3, \\
 D_{\beta}^2 (M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta)) &= 4(2mn + m + n + 4) \alpha^2 \beta^2 \\
 &\quad + 9(4mn + 6m + 6n) \alpha^2 \beta^3 + 36mn \alpha^3 \beta^3, \\
 F(O_2 \mathbf{G}_{m \times n}) &= 140mn + 86m + 86n + 32. \\
 (iii) SDD(O_2 \mathbf{G}_{m \times n}) &= (D_{\alpha} S_{\beta} + S_{\alpha} D_{\beta})(M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta))|_{\alpha=\beta=1}, \\
 D_{\alpha} S_{\beta} (M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta))|_{\alpha=\beta=1} &= (2mn + m + n + 4) + \frac{2}{3} (4mn + 6m + 6n) + 4mn, \\
 S_{\alpha} D_{\beta} (M(O_2 \mathbf{G}_{m \times n}, \alpha, \beta))|_{\alpha=\beta=1} &= (2mn + m + n + 4) + \frac{3}{2} (4mn + 6m + 6n) + 4mn, \\
 SDD(O_2 \mathbf{G}_{m \times n}) &= 20.67mn + 15m + 15n + 8.
 \end{aligned} \tag{20}$$

□

3. Conclusion

Various forms of degree-based topological indices, such as Randić index variations of Zagreb indices, atom bond connectivity index, Harmonic index, and Forgotten index and Symmetric Division index are computed using M polynomial for nanosheets based on octa graphene. These discoveries are particularly useful in the theoretical research of nanosheet physical properties, chemical reactivity, and biological activities. The topological indices calculated in this study can be used in quantitative structure activity relations and quantitative structure property relations of nanosheets, which can assist further comprehend the nanosheet's physicochemical properties.

Data Availability

All data is included in Article. There is not hidden data.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

References

- [1] W. u. Jing, Y.-s. Wang, X.-y. Yang et al., "Graphene oxide used as a carrier for adriamycin can reverse drug resistance in breast cancer cells," *Nanotechnology*, vol. 23, no. 35, Article ID 355101, 2012.
- [2] D. Golberg, Y. Bando, O. Stephan, and K. Kurashima, "Octahedral boron nitride fullerenes formed by electron beam irradiation," *Applied Physics Letters*, vol. 73, pp. 2441–2443, 1998.
- [3] M. V. Diudea, "Nanostructures," *Novel Architecture*, NOVA, New York, NY, USA, 2005.
- [4] G. S. L. Fabris, C. A. Paskocimas, J. R. Sambrano, and R. Paupitz, "New 2D nanosheets based on the octa-graphene," *Journal of Solid State Chemistry*, vol. 290, Article ID 121534, 2020.
- [5] H. Weiner, "Structural determination of paraffin boiling point," *Journal of the American Chemical Society*, vol. 69, no. 1, pp. 17–20, 1947.
- [6] M. Randić, "On Characterization of molecular branching," *Journal of the American Chemical Society*, vol. 97, pp. 6609–6615, 1975.
- [7] B. Bollobás and P. Erdős, "Graphs of external weights," *Ars Combinatoria*, vol. 50, pp. 225–233, 1998.
- [8] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total ϕ -electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, pp. 535–538, 1972.
- [9] E. Estrada, L. Torres, L. Rodríguez, and I. Gutman, "An atom-bond connectivity index: modelling the enthalpy of formation of alkanes," *Indian Journal of Chemistry Section A: Inorganic, Physics, Theoretical and Analytical*, vol. 37, pp. 849–855, 1998.
- [10] S. Fajtlowicz, "On conjectures of grafitti II," *Congressus Numerantium*, vol. 60, pp. 189–197, 1987.
- [11] B. Furtula and I. Gutman, "A forgotten topological index," *Journal of Mathematical Chemistry*, vol. 53, 2015.
- [12] D. Vukičević and M. Gašperov, "Bond additive modeling 1. Adriatic indices," *Croatica Chemica Acta*, vol. 83, pp. 243–260, 2010.
- [13] M. Munir, W. Nazeer, S. Shahzadi, and S. M. Kang, "Some invariants of circulant graphs," *Symmetry*, vol. 8, no. 11, p. 134, 2016.
- [14] Y. Hu, X. Li, Y. Shi, T. Xu, and I. Gutman, "On molecular graphs with smallest and greatest zeroth-order general Randić index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 54, pp. 425–434, 2005.
- [15] E. Deutsch and S. Klavžar, "M-Polynomial, and degree-based topological indices, Iran," *Journal of Mathematical Chemistry*, vol. 6, pp. 93–102, 2015.
- [16] V. Alamian, A. Bahrami, and B. Edalatzaadeh, "PI Polynomial of V-Phenylenic nanotubes and nanotori," *International Journal of Molecular Science*, vol. 9, pp. 229–234, 2008.
- [17] M. R. Farahani, "Computing theta polynomial, and theta index of V-phenylenic planar, nanotubes and nanotoris," *International Journal of Theoretical Chemistry*, vol. 1, pp. 01–09, 2013.
- [18] A. Ahmad, "On the degree based topological indices of benzene ring embedded in P-type-surface in 2D network," *Hacetatepe Journal of Mathematics and Statistics*, vol. 47, pp. 9–18, 2018.
- [19] Y. C. Kwun, M. Munir, W. Nazeer, S. Rafique, and S. M. Kang, "M-Polynomials and topological indices of V-Phenylenic Nanotubes and Nanotori," *Scientific Reports*, vol. 7, 2017.
- [20] S. Mondal, N. De, and A. Pal, "The m-polynomial of line graph of subdivision graphs," *Communications*, vol. 68, pp. 2104–2116, 2019.
- [21] M. S. Ahmad, W. Nazeer, S. M. Kang, and C. Y. Jung, "M-polynomials and degree based topological indices for the line graph of firecracker graph," *Global Journal Of Pure And Applied Mathematics*, vol. 13, pp. 2749–2776, 2017.
- [22] M. Munir, W. Nazeer, S. Rafique, and S. M. Kang, "M-polynomial and degree-based topological indices of polyhedral nanotubes," *Symmetry*, vol. 8, 2016.
- [23] M. Munir, W. Nazeer, S. M. Kang, M. I. Qureshi, A. R. Nizami, and Y. C. Kwun, "Some invariants of jahangir graphs," *Symmetry*, vol. 9, 2017.
- [24] S. Kanwal, A. Riyasat, M. K. Siddiqui et al., "On topological indices on total graphs and its line graph for kragujevac tree networks," *Complexity*, vol. 2021, Article ID 8695121, 32 pages, 2021.
- [25] S. Kanwal, S. Shang, M. K. Siddiqui, T. S. Shaikh, A. Afzal, and A.-T. Anton, "On analysis of topological aspects of subdivision of kragujevac tree networks," *Mathematic Problems In Engineering*, vol. 2021, Article ID 9082320, 15 pages, 2021.
- [26] S. Kanwal, R. Safdar, A. Rouf et al., "On chemical invariants of semitotal-point graph and its line structure of acyclic kragujevac network: a novel mathematical analysis," *Journal Of Chemistry*, vol. 2022, Article ID 7995704, 20 pages, 2022.
- [27] S. Nasir, F. Farooq, N. Idrees, M. J. Saif, and F. Saeed, "Topological characterization of nanosheet covered by C3 and C6," *Processes*, vol. 7, no. 7, 2019.
- [28] A. Verma, S. Mondal, N. De, and A. Pal, "Topological Properties of Bismuth Tri-iodide Using Neighborhood M-Polynomial," *International Journal Of Mathematics Trends And Technology*, vol. 65, pp. 83–90, 2019.