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Topological Characterization of Nanosheet Covered by C_3 and C_6

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Abstract: A topological index of a graph is a single numeric quantity which relates the chemical structure with its underlying physical and chemical properties. Topological indices of a nanosheet can help us to understand the properties of the material better. This study deals with computation of degree-dependent topological indices like the Randic index, first Zagreb index, second Zagreb index, geometric arithmetic index, atom bond connectivity index, sum connectivity index and hyper Zagreb index of nanosheet covered by C_3 and C_6. Furthermore, M-polynomial of the nanosheet is also computed, which provides an alternate way to express the topological indices.

Keywords: nanosheet; topological index; M-polynomial; Zagreb index; Randic index

1. Introduction

Nanosheets are two-dimensional polymeric materials which remain among the most actively researched areas of subject chemistry and physics. Generally, nanosheets are inorganic materials which can be created from bulk crystalline layered materials that have fascinating properties and functionalities, excellent electrochemical performance, and high potential for separation applications due to their exceptional molecular transport properties [1]. The nanomaterial has a sheet-like structure with a size larger than 100 nm and thickness less than 5 nm, which is only one or a few atoms thick. Topological indices quantify the physical as well as chemical properties of compounds by associating a unique number to chemical graphs which represent a chemical structure by denoting atoms by vertices and bonds are represented by edges of the graph.

Graphene derived from graphite is a highly attractive two-dimensional lubricating material, wear-resistant with low-friction characteristics [2–4], endowed with high conductivity, tensile strength, and remarkable toughness [5]. Other aspects of nanomaterials like optical properties, applications in human therapeutics, biocompatibility, and stability are established in [6–8]. Boron nitride nanosheets (BNNs) and nanotubes have closely analogous properties to carbon nanotubes. High stiffness and excellent chemical stability make BNNs an ideal material for reinforcement in polymers, ceramics, and metals. BNNs also exhibit excellent thermal conductivity, radiation shielding ability, and high electrical resistance [8,9]. These ultrathin 2D nanomaterials possess utilization for wide ranges of potential applications among the electronics/optoelectronics, electrocatalysis, batteries, supercapacitors, solar cells, photocatalysis, and sensing platforms.

Today, topological indices are extensively applied in computational chemistry methods such as (Q)SARs ((Quantitative) Structure-Activity Relationships) in the area of toxicology and drug design:

computational models are used to predict the behavior and effects of nanomaterials in biological systems. Topological indices (descriptors) provide a comprehensive understanding of the relationships between the physicochemical properties and the behavior of nanomaterials in biological systems for designing safe and functional nanomaterials. Quantitative Structure-Activity Relationship (QSAR) methods help to establish such relationships and have been widely studied [10–13].

Let us consider $G = (V, E)$ be such a graph having n vertices and m edges. The symbol d_u is the degree of vertex $u \in V(G)$ and is the number of vertices that are adjacent to u.

The first degree based topological index is a Randic index $x(G)$, invented by Milan Randic [14] in 1975 and is defined as:

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

Bollobás and Erdös [15] introduced the idea of the general Randic index in 1998.

The general Randic index of graph G is defined as:

$$R_\alpha(G) = \sum_{uv \in E} (d_u d_v)^\alpha \tag{1}$$

The first and second Zagreb index $M_1(G)$, $M_2(G)$, termed by Gutman and Trinajstić [16], are also among the oldest known topological indices and are defined as:

$$M_1(G) = \sum_{uv \in E} [d_u + d_v] \tag{2}$$

$$M_2(G) = \sum_{uv \in E} [d_u d_v] \tag{3}$$

The atom-bond connectivity index, or ABC index, is a degree based topological index which was introduced by Estrada et al. [17]. It is represented as:

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

Sum connectivity index ($SCI(G)$) was invented by Zhou and Trinajstić [18], expressed by Equation (5).

$$SCI(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u + d_v}} \tag{5}$$

The Geometric-arithmetic index or $GA(G)$ is a topological index of a molecular graph G which was introduced by Vukičević and Furtula [19].

The geometric-arithmetic topological index is defined as:

$$\mathrm{GA}(G) = \sum_{uv \in E} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \tag{6}$$

A new degree based topological index called the hyper-Zagreb index was introduced by Shirdel et al. [20], and is given as:

$$HM(G) = \sum_{uv \in E} (d_u + d_v)^2 \tag{7}$$

The first and second multiple Zagreb indices, denoted by $PM_1(G)$ and $PM_2(G)$, were introduced in 2012 [21].

$$PM_1(G) = \prod_{uv \in E} [d_u + d_v] \tag{8}$$

$$PM_2(G) = \prod_{uv \in E} [d_u \times d_v] \tag{9}$$

Degree-based topological indices and M-polynomials of different types of nanotubes are being studied by many researchers. Jagadeesh et al. computed degree based topological indices of graphene [22]. Chen et al. [23] analyzed topological indices of nanotubes covered by C_4. Hayat et al. computed topological indices of nanotubes covered by C_5 and C_7 [24]. Aslam et al. [25] worked for topological characterization of triangular boron nanotubes. Idrees et al. provided results for topological indices of an H-Naphthalenic nanosheet [26]. We refer readers to [27–30] for further studies in this area.

Degree based topological indices of nanosheets tessellated by C_3 and C_6, described in Figure 1, are computed in this paper. These computations can give further insight into the underlying information of the material. Moreover, M-polynomial of the nanosheet is also computed in the paper, which is an eloquent way to describe topological invariants in a single expression. These types of nanosheets appear as a type of coordination nanosheet; for further details of coordination nanosheet, see [31].

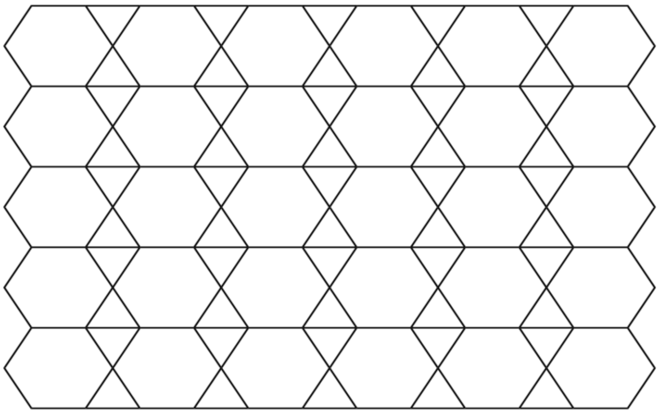

Figure 1. Chemical graph of nanosheet C[6,5] with five rows and six hexagons in each row.

2. Methods

The degree-based topological indices can be computed by using the degrees of end vertices of the coordination nanosheet. We denote it by $C[m,n]$, where m denotes the number of hexagons in each row and n denotes the number of hexagons in each column. Chemical graph of $C[m,n]$ has successive columns of hexagons (C_6) and triangles (C_3). We partition the edges of the graph according to the degrees of the end vertices. All vertices having degrees according to edges connected with the respective vertex are computed as 2, 3, and 4. Here we have five different types of edges whose end vertices have a degree (2,2), (2,3), (3,3), (3,4), and (4,4), symbolically denoted by $E_{(2,2)}$, $E_{(2,3)}$, $E_{(3,3)}$, $E_{(3,4)}$ and $E_{(4,4)}$, respectively. Total number of edges computed of the type $E_{(2,2)}$, $E_{(2,3)}$, $E_{(3,3)}$, $E_{(3,4)}$ and $E_{(4,4)}$ are 4, $4n$, $4m-6$, $4m+2n-6$ and $6mn-6m-7n+7$, respectively. All of these results are summarized in Table 1.

Table 1. Edge partition of coordination nanosheet $C[m,n]$.

Type of Edges	$E_{(2,2)}$	$E_{(2,3)}$	$E_{(3,3)}$	$E_{(3,4)}$	$E_{(4,4)}$
(d_u, d_v) uv $\in E(C[m,n])$	(2,2)	(2,3)	(3,3)	(3,4)	(4,4)
Number of edges	4	$4n$	$4m-6$	$4m+2n-6$	$6mn-6m-7n+7$

3. Results

Theorem 1. *Randic index of coordination nanosheet, denoted by $R_\alpha(C[m,n])$ is given as:*

$$R_\alpha(C[m,n]) = \begin{cases} 24mn + \left(8\sqrt{3} - 12\right)m + \left(4\sqrt{3} + 4\sqrt{6} - 28\right)n + 18 - 12\sqrt{13} & if\ \alpha = \frac{1}{2} \\ \frac{3}{2}mn + \left(\frac{-1+4\sqrt{3}}{6}\right)m + 0.46n + 0.0179 & if\ \alpha = -\frac{1}{2} \end{cases}$$

Proof. General Randic index of the coordination nanosheet is given by Equation (1) and can be computed as:

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

$$R_{\frac{1}{2}}(C[m,n]) = \sum_{uv \in E} \sqrt{d_u d_v}$$
$$= \sum_{uv \in E(2,2)} \sqrt{d_u d_v} + \sum_{uv \in E(2,3)} \sqrt{d_u d_v} + \sum_{uv \in E(3,3)} \sqrt{d_u d_v} + \sum_{uv \in E(3,4)} \sqrt{d_u d_v} + \sum_{uv \in E(4,4)} \sqrt{d_u d_v}$$

Using values from Table 1, we get

$$R_{\frac{1}{2}}(C[m,n]) = 4{+}4n\sqrt{2 \times 2} + (4m-6)\sqrt{3 \times 3} + (4m+2n-6)\sqrt{3 \times 4}$$
$$(6mn - 6m - 7n + 7)\sqrt{4 \times 4}$$

which is simplified to

$$R_{\frac{1}{2}}(C[m,n]) = 24mn + \left(8\sqrt{3} - 12\right)m + \left(4\sqrt{3} + 4\sqrt{6} - 28\right)n + 18 - 12\sqrt{13}$$

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

$$R_{\frac{-1}{2}}(C[m,n]) = \sum_{uv \in E} \frac{1}{\sqrt{d_u d_v}}$$
$$= \sum_{uv \in E(2,2)} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E(2,3)} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E(3,3)} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E(3,4)} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E(4,4)} \frac{1}{\sqrt{d_u d_v}}$$

Again using Table 1, we get

$$R_{\frac{-1}{2}}(C[m,n]) = 4\frac{1}{\sqrt{2\times2}} + 4n\frac{1}{\sqrt{2\times3}} + (4m-6)\frac{1}{\sqrt{3\times3}} + (4m+2n-6)\frac{1}{\sqrt{3\times4}}$$
$$+(6mn - 6m - 7n + 7)\frac{1}{\sqrt{4\times4}}$$

By simplification, we get

$$R_{\frac{-1}{2}}(C[m,n]) = \frac{3}{2}mn + \left(\frac{-1+4\sqrt{3}}{6}\right)m + 0.46n + 0.0179$$

□

Theorem 2. *First Zagreb index of nanosheet $C[m,n]$ is given as:*

$$M_1(C[m,n]) = 48mn + 4m - 22n - 6$$

Proof. We can compute the first Zagreb index of the nanosheet as defined in Equation (2) as:

$$M_1(C[m,n]) = \sum_{uv \in E} [d_u + d_v]$$
$$= \sum_{uv \in E(2,2)} [d_u + d_v] + \sum_{uv \in E(2,3)} [d_u + d_v] + \sum_{uv \in E(3,3)} [d_u + d_v]$$
$$+ \sum_{uv \in E(3,4)} [d_u + d_v] + \sum_{uv \in E(4,4)} [d_u + d_v]$$

Now, from Table 1, we get

$$\begin{aligned} M_1(C[m,n]) = \;& 4(2+2) + 4n(2+3) + (4m-6)(3+3) + (4m+2n-6)(3+4) \\ & +(6mn-6m-7n+7)(4+4) \end{aligned}$$

which can be simplified to

$$M_1(C[m,n]) = 48mn + 4m - 22n - 6$$

□

Theorem 3. *For nanosheet $C[m,n]$, the second Zagreb index is given as:*

$$M_2(C[m,n]) = 96mn - 12m - 64n + 2$$

Proof. To compute the second Zagreb index of the coordination nanosheet, we use edge partition from Table 1 to split the relation in Equation (3) as:

$$M_2(C[m,n]) = \sum_{uv\in E} c[d_u d_v]$$
$$= \sum_{uv\in E(2,2)} [d_u d_v] + \sum_{uv\in E(2,3)} [d_u d_v] + \sum_{uv\in E(3,3)} [d_u d_v] + \sum_{uv\in E(3,4)} [d_u d_v] + \sum_{uv\in E(4,4)} [d_u d_v]$$

After using values from Table 1, we have

$$\begin{aligned} M_2(C[m,n]) = \;& 4(2\times 2) + 4n(2\times 3) + (4m-6)(3\times 3) + (4m+2n-6)(3\times 4) \\ & +(6mn-6m-7n+7)(4\times 4) \end{aligned}$$

which yields

$$M_2(C[m,n]) = 96mn - 12m - 64n + 2$$

□

Theorem 4. *The ABC index of the nanosheet $C[m,n]$ is given as:*

$$ABC(C[m,n]) = 3.67mn + 1.57m - 0.167n - 9.33$$

Proof. We can find the ABC index of coordination nanosheet as defined in Equation (4), which can be further expanded by the edge partition of Table 1:

$$\begin{aligned} ABC(C[m,n]) = \;& \sum_{uv\in E} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\ & = \sum_{uv\in E(2,2)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\ & + \sum_{uv\in E(2,3)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} + \sum_{uv\in E(3,3)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\ & + \sum_{uv\in E(3,4)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} + \sum_{uv\in E(4,4)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \end{aligned}$$

Using values from Table 1, we get

$$\begin{aligned} BC\;(C[m,n] = \;& 4\sqrt{\frac{2+2-2}{2.2}} + 4n\sqrt{\frac{2+3-2}{2.3}} + (4m-6)\sqrt{\frac{3+3-2}{3.3}} \\ & +(4m+2n-6)\sqrt{\frac{3+4-2}{3.4}} + (6mn-6m-7n+7)\sqrt{\frac{4+4-2}{4.4}} \end{aligned}$$

which further reduces to

$$ABC\ C[m,n] = 3.67mn + 1.57m - 0.167n - 9.33$$

□

Theorem 5. *Sum connectivity index SCI of $C[m,n]$ is given as:*

$$SCI(C[m,n]) = 2.12mn + 1.02m + 0.069n - 0.242$$

Proof. After using values from Table 1, we can calculate the sum connectivity index of a coordination nanosheet as defined in Equation (5):

$$\begin{aligned} SCI\ (C[m,n]) = & \sum_{uv\in E} \frac{1}{\sqrt{d_u + d_v}} \\ & = \sum_{uv\in E(2,2)} \frac{1}{\sqrt{d_u + d_v}} + \sum_{uv\in E(2,3)} \frac{1}{\sqrt{d_{u+}d_v}} + \sum_{uv\in E(3,3)} \frac{1}{\sqrt{d_u + d_v}} \\ & + \sum_{uv\in E(3,4)} \frac{1}{\sqrt{d_u + d_v}} + \sum_{uv\in E(4,4)} \frac{1}{\sqrt{d_u + d_v}} \end{aligned}$$

Using the values from Table 1, we have

$$\begin{aligned} SCI\ (C[m,n]) = & \ 4\frac{1}{\sqrt{2+2}} + 4n\frac{1}{\sqrt{2+3}} + (4m-6)\frac{1}{\sqrt{3+3}} + (4m+2n-6)\frac{1}{\sqrt{3+4}} \\ & + (6mn - 6m - 7n + 7)\frac{1}{\sqrt{4+4}} \end{aligned}$$

Now, by simplifying,

$$SCI\ (C[m,n]) = 2.12mn + 1.02m + 0.069n - 0.242$$

□

Theorem 6. *Geometric arithmetic index $GA(C[m,n])$ of such a coordination nanosheet, is given as:*

$$GA(C[m,n]) = 6mn + 1.95m - 0.101n - 0.94$$

Proof. Table 1 contains edge partition values; with these values the geometric arithmetic index of coordination nanosheet as defined in Equation (6) can be calculated as:

$$\begin{aligned} A(C[m,n]) = & \sum_{uv\in E} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\ & = \sum_{uv\in E(2,2)} \left(\frac{2\sqrt{d_u d_v}}{d_u + d_v}\right) + \sum_{uv\in E(2,3)} \left(\frac{2\sqrt{d_u d_v}}{d_u + d_v}\right) + \sum_{uv\in E(3,3)} \left(\frac{2\sqrt{d_u d_v}}{d_u + d_v}\right) \\ & + \sum_{uv\in E(3,4)} \left(\frac{2\sqrt{d_u d_v}}{d_u + d_v}\right) + \sum_{uv\in E(4,4)} \left(\frac{2\sqrt{d_u d_v}}{d_u + d_v}\right) \end{aligned}$$

Now, from Table 1, we have

$$\begin{aligned} GA(C[m,n]) = & \ 4\left(\frac{2\sqrt{2\times 2}}{2+2}\right) + 4n\left(\frac{2\sqrt{2\times 3}}{2+3}\right) + (4m-6)\left(\frac{2\sqrt{3\times 3}}{3+3}\right) \\ & + (4m+2n-6)\left(\frac{2\sqrt{3\times 4}}{3+4}\right) + (6mn - 6m - 7n + 7)\left(\frac{2\sqrt{4\times 4}}{4+4}\right) \end{aligned}$$

Now, the simplified form is,

$$GA(C[m,n]) = 6mn + 1.95m - 0.101n - 0.94$$

□

Theorem 7. *Hyper Zagreb index of the coordination nanosheet $C[m,n]$ is given as:*

$$HM(C[m,n]) = 348mn - 44m - 250n + 2$$

Proof. Hyper Zagreb index of coordination nanosheet as defined in Equation (7) can be computed by using values from Table 1:

$$\begin{aligned} HM(C[m,n]) = & \sum_{uv \in E} (d_u + d_v)^2 \\ & = \sum_{uv \in E(2,2)} (d_u + d_v)^2 + \sum_{uv \in E(2,3)} (d_u + d_v)^2 + \sum_{uv \in E(3,3)} (d_u + d_v)^2 \\ & + \sum_{uv \in E(3,4)} (d_u + d_v)^2 + \sum_{uv \in E(4,4)} (d_u + d_v)^2 \end{aligned}$$

From Table 1, we get

$$\begin{aligned} HM(C[m,n]) = & \; 4(2+2)^2 + 4n(2+3)^2 + (4m-6)(3+3)^2 \\ & + (4m+2n-6)(3+4)^2 + (6mn-6m-7n+7)(4+4)^2 \end{aligned}$$

Now we have

$$HM(C[m,n]) = 384mn - 446n - 44m + 2$$

□

Theorem 8. *Let us consider the coordination nanosheet $C[m,n]$, then first multiple Zagreb index is given as:*

$$PM_1(C[m,n]) = 256 \times (5)^{4n} \times (6)^{(4m-6)} \times (7)^{(4m+2n-6)} \times (8)^{(6mn-6m-7n+7)}$$

Proof. Using the edge partition from Table 1, we can find the first multiple Zagreb index of the nanosheet as defined in Equation (9):

$$\begin{aligned} PM_1(C[m,n]) = & \prod_{uv \in E} [d_u + d_v] \\ & = \prod_{uv \in E(2,2)} [d_u + d_v] + \prod_{uv \in E(2,3)} [d_u + d_v] + \prod_{uv \in E(3,3)} [d_u + d_v] \\ & + \prod_{uv \in E(3,4)} [d_u + d_v] + \prod_{uv \in E(4,4)} [d_u + d_v] \end{aligned}$$

Now from Table 1,

$$PM_1(C[m,n]) = (2+2)^4 \times (2+3)^{4n} \times (3+3)^{(4m-6)} \times (3+4)^{(4m+2n-6)} \times (4+4)^{(6mn-6m-7n+7)}$$
$$PM_1(C[m,n]) = 256 \times 5^{4n} \times 6^{(4m-6)} \times 7^{(4m+2n-6)} \times 8^{(6mn-6m-7n+7)}$$

□

Theorem 9. *The second multiple Zagreb index of $C[m,n]$ is given as:*

$$PM_2C[m,n] = 256 \times (6)^{4n} \times (9)^{(4m-6)} \times (12)^{(4m+2n-6)} \times (16)^{(6mn-6m-7n+7)}$$

Proof. Edge partitions are given in Table 1, and with these values we can calculate the second multiple Zagreb index of coordination nanosheet as defined in Equation (9):

$$\begin{aligned} PM_2C[m,n] = & \prod_{uv\in E}[d_u \times d_v] \\ & = \prod_{uv\in E(2,2)}[d_u d_v] + \prod_{uv\in E(2,3)}[d_u d_v] + \prod_{uv\in E(3,3)}[d_u d_v] \\ & + \prod_{uv\in E(3,4)}[d_u d_v] + \prod_{uv\in E(4,4)}[d_u d_v] \end{aligned}$$

Using the values from Table 1, we get

$$PM_2(C[m,n]) = 256 \times (6)^{4n} \times (9)^{(4m-6)} \times (12)^{(4m+2n-6)} \times (16)^{(6mn-6m-7n+7)}$$

□

4. The M-Polynomial of Nanosheet

Let us consider a molecular graph $G = (V, E)$ having n vertices and m edges. Then the degree of vertex $u \in V(G)$ is denoted by d_u and is the number of vertices that are adjacent to u.

The M-polynomial [32] of a graph, G is defined as

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

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

Theorem 10. *Let G be the graph nanosheet $C[m,n]$, then M-polynomial of G is*

$$M(G,x,y) = 4x^2y^2 + 4nx^2y^3 + (4m-6)x^3y^3 + (4m+2n-6)x^3y^4 + (6mn-6m-7n+7)x^4y^4$$

Proof. By definition, M-polynomial is expressed as

$$\begin{aligned} M(G,x,y) = & \sum_{i\leq y} m_{ij}(G)x^i y^j \\ & = \sum_{2=2} m_{22}(G)x^2y^2 + \sum_{2\leq 3} m_{ij}(G)x^2y^3 \\ & + \sum_{3=3} m_{33}(G)x^3y^3 + \sum_{3\leq 4} m_{34}(G)x^3y^4 + \sum_{4=4} m_{44}(G)x^4y^4 \\ & = \sum_{uv\in E(2,2)} m_{22}(G)x^2y^2 + \sum_{uv\in E(2,3)} m_{ij}(G)x^2y^3 + \sum_{uv\in E(3,3)} m_{33}(G)x^3y^3 \\ & + \sum_{uv\in E(3,4)} m_{34}(G)x^3y^4 + \sum_{uv\in E(4,4)} m_{44}(G)x^4y^4 \end{aligned}$$

$$M(G,x,y) = 4x^2y^2 + 4nx^2y^3 + (4m-6)x^3y^3 + (4m+2n-6)x^3y^4 + (6mn-6m-7n+7)x^4y^4$$

By differentiating M-polynomial with respect to x, we get

$$\begin{aligned} D_x &= 8xy^2 + 8nxy^3 + 3(4m-6)x^2y^3 + 3(4m+2n-6)x^2y^4 + 4(6mn-6m-7n+7)x^3y^4 \\ D_{x\ x=1,y=1} &= 8 + 8n + 3(4m-6) + 3(4m+2n-6) + 4(6mn-6m-7n+7) \\ D_y &= 8x^2y + 12nx^2y^2 + 3(4m-6)x^3y^2 + 4(4m+2n-6)x^3y^3 + 4(6mn-6m-7n+7)\ x^4y^3 \\ D_{y\ x=1,\ y=1} &= 8 + 12n + 3(4\mathrm{m}-6) + 4(4m+2n-6) + 4(6mn-6m-7n+7) \end{aligned}$$

S_x and S_y are obtained by integrating M-polynomial with respect to x and y, respectively.

$$S_x = \frac{4x^2y^2}{2} + \frac{4nx^2y^3}{2} + \frac{(4m-6)x^3y^3}{3} + \frac{(4m+2n-6)x^3y^4}{3} + \frac{(6mn-6m-7n+7)\,x^4y^4}{4}$$

$$S_{x\ \mathrm{x=1,\,y=1}} = 2+2n + \frac{(4m-6)}{3} + \frac{(4m+2n-6)}{3} + \frac{(6mn-6m-7n+7)}{4}$$

$$S_y = \frac{4x^2y^2}{2} + \frac{4nx^2y^3}{3} + \frac{(4m-6)\,x^3y^3}{3} + \frac{(4m+2n-6)x^3y^4}{4} + \frac{(6mn-6m-7n+7)x^4y^4}{4}$$

$$S_{y\ \mathrm{x=1,\,y=1}} = 2 + \frac{4n}{3} + \frac{(4m-6)}{3} + \frac{(4m+2n-6)}{4} + \frac{(6mn-6m-7n+7)}{4}$$

□

Figure 2 shows graphical interpretation of the M-polynomial of the nanosheet. Some topological indices, derived from M-polynomial, are described in Table 2 below.

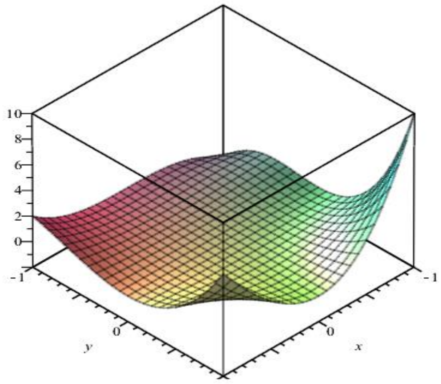

Figure 2. The graph of M-polynomial of coordination nanosheet.

Table 2. The relation between topological indices and M-polynomial.

Topological Index	*f*(*x*,*y*)	Derivation from *M*(*G*,*x*,*y*)
1st Zagreb index	$x+y$	$\left(D_x+D_y\right)M(G,x,y)x=1, y=1$
2nd Zagreb index	xy	$\left(D_xD_y\right)M(G,x,y)x=1, y=1$
Randic index	$\frac{1}{xy}$	$\left(S_xS_y\right)M(G,x,y)x=1, y=1$

$D_x = \frac{\partial(f(x,y))}{\partial x}$, $D_y = \frac{\partial(f(x,y))}{\partial y}$, $S_x = \int_0^x \frac{f(t,y)}{t}\,dt$, and $S_y = \int_0^y \frac{f(x,t)}{t}dt$, $J = f(x,x)$.

5. Conclusions

For the nanosheets covered by C_3 and C_6, various types of degree-based topological indices like Randic index variants of Zagreb indices, atom bond connectivity index, Geometric Arithmetic index, and sum connectivity index etc. are computed analytically. These results depend upon the structural connectivity of the chemical graph of the nanosheet. M-polynomial of the nanosheet is also computed, which provides an eloquent way to express and compute the degree-based topological indices. These findings are extremely helpful in the theoretical study of physical features, chemical reactivity, and biological activities of nanosheets. Topological indices computed in the study can be employed in quantitative structure activity relations and quantitative structure property relations of the nanosheets, and in turn, can be further helpful in understanding the physiochemical properties of the nanosheet.

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