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ON M-POLYNOMIAL OF THE TWO-DIMENSIONAL SILICON-CARBONS

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Abstract Topological indices of a molecular structure are numerical variables that significantly correlate various biological activity, physico-chemical properties and chemical reactivity. Representing molecular structure with M-Polynomial and computing the degree-based topological indices via M-polynomial of a graph network is a recent trade. In this article, we determine a closed-form of M-Polynomial for 2-dimensional Silicon-Carbons namely Si_2C_3-*I*$[p,q]$, Si_2C_3-*II*$[p,q]$ and Si_2C_3-*III*$[p,q]$, and hence compute various degree-based topological indices. Additionally, we visualize the graphical representation of M-Polynomials and all the related degree-based topological indices of the above-mentioned Silicon-Carbons.

1 Introduction

Let us consider an undirected simple connected graph $G = (V, E)$, where $V = V(G)$ represents the set of vertex of G and $E = E(G)$ represents the set of edges of G. In a graph G, the degree of a vertex $u \in V(G)$, denoted by $d(u)$, is the total number of vertices adjacent to the vertex u [40].

A combination of chemistry and graph theory produces an interesting branch of mathematical chemistry which is known as Chemical Graph Theory (CGT). Mathematical modeling and physical properties of chemical structures are being studied in CGT. Here, the atoms and chemical bonds between them of a chemical compound are represented by vertices and edges of a graph, respectively. In [2,9,13,19], the utilization of graph theory with chemistry and a variety of chemical applications has been discussed. A *topological index* (also known as a graph-theoretic index or connectivity index) is essentially a numerical parameter that correlates the physical properties of a molecular structure. It is a mathematical representation of a chemical compound, which plays a vital role in the investigation of Quantitative Structure Activity Relationships (QSARs) and Quantitative Structure Property Relationships (QSPRs)[1]. For more details see [14, 38].

Literature Review of Topological Indices and M-polynomial

There is a standard classification of the topological indices such as degree-based topological indices [17], distance-based topological indices [3], degree and distance-based topological indices [35] and counting related topological indices [23] which are associated with many biological and physico-chemical properties of chemical structure like melting point, boiling point, strain energy, etc. Instead of evaluating numerical values of above mentioned topological indices by using definition separately, the concept of polynomials [15] is being introduced which is a general approach to evaluate topological indices at once. By differentiating or integrating (or combination of both) the polynomial of a given structure, we can drive its topological indices.

Several chemical relevant polynomials are described in past, some of which are: matching polynomial [10], the Clar covering polynomial (also known as the Zhang-Zhang polynomial) [41], the Schultz polynomial [16], the Tutte polynomial [22], the Hosoya polynomial [20], etc. Recently, Deutsch and Klavžar in [8] introduced the M-polynomial to calculate several

[1]In the area of mathematical chemistry, QSAR and QSPR are used to forecast the physico-chemical and biological properties of a chemical compound.

degree-based topological indices. The M-Polynomials and related degree-based topological indices of several chemical structures are calculated in [5, 6, 24, 29, 30].

Definition 1.1 ([8]). For a simple connected directed graph G, the expression

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

is known as the M-polynomial of a graph G, where $\delta = min\{d(u)|u \in V(G)\}$, $\Delta = \max\{d(u)|u \in V(G)\}$ and $m_{i,j}(G)$ $(i,j \geq 1)$ is the number of edges $uv \in E(G)$ such that $d(u) = i$, $d(v) = j$.

As mentioned in [7], a degree-based topological index of a graph G is a kind of graph invariant, which is denoted as $I(G)$ and can be written as

$$I(G) = \sum_{i \leq j} m_{i,j}(G) f(i,j).$$

Theorem 1.2 ([8], Theorems 2.1, 2.2). *Let G be a simple connected graph.*

(1) If $I(G) = \sum_{e=uv \in E(G)} f(d(u), d(v))$, where $f(x,y)$ is a polynomial in x and y, then

$$I(G) = f(D_x, D_y)(M(G;x,y))|_{x=y=1}.$$

(2) If $I(G) = \sum_{e=uv \in E(G)} f(d(u), d(v))$, where $f(x,y) = \sum_{i,j \in \mathbb{Z}} \alpha_{i,j} x^i y^j$, then $I(G)$ can be obtained from $M(G;x,y)$ using the operators D_x, D_y, S_x, and S_y.

(3) If $I(G) = \sum_{e=uv \in E(G)} f(d(u), d(v))$, where $f(x,y) = \frac{x^r y^s}{(x+y+\alpha)^t}$, where $r, s \geq 0$, $t \geq 1$ and $\alpha \in \mathbb{Z}$, then

$$I(G) = S_x^t Q_\alpha J D_x^r D_y^s (M(G;x,y))|_{x=1}.$$

Survey of Degree-based Topological Indices

In this section, we discuss some degree-based topological indices which are related to the context of this paper. The *Zagreb indices* were proposed by Gutman and Trinajstić [18] in 1972. The Zagreb indices are helpful in determining the total π-electron energy of molecules which is correlated to their thermodynamic stability. The *Zagreb indices* give higher weight to the interior edges and vertices rather than the terminal edges and vertices. Conversely, being inspired by the idea of the Zagreb indices, *modified Zagreb indices* [28] are introduced. The *Randić index* was introduced by Milan Randić [36] in 1975 which is also recognized as *branching index* or *connectivity index*. The Randić index has immense applications in the field of pharmacology and drug design. After a couple of decades, seeing the success of Randić index, the generalized version of Randić index[2] (for an arbitrary real number α) was introduced by the mathematicians Bollobás and Erdös [4], and Amić et al. [1] in 1998, which is known as *general Randić index*. In a recent investigation, the *symmetric division (deg) index* is introduced in [39] which is used to calculate the total surface area of polychlorobiphenyls. The *inverse sum (indeg) index* [37, 39] forecasts the total surface area of octane isomers. The *augmented Zagreb index* [12] is useful in the study of heat of formation of alkanes. In Table 1, the formulas of different degree-based topological indices are listed for a graph G.

On Silicon-Carbons

Silicon has superiority over other semiconductor objects. It is of minimal effort, nontoxic, essentially its accessibility is boundless, decades of research carried out about its purification, development and device manufacturing. It is utilized in most cutting-edge electronic gadgets.

[2]For $\alpha = -\frac{1}{2}$, R_α becomes Randić or (connectivity) index; for $\alpha = 1$, R_α becomes second Zagreb index; and for $\alpha = -1$, R_α becomes modified second Zagreb index

Table 1. Formulas for degree-based topological indices

Sl. No.	Topological Index	Notation	Formula of Topological Indices
1.	First Zagreb Index [18]	$M_1(G)$	$M_1(G) = \sum_{uv\in E(G)} (d(u)+d(v))$
2.	Second Zagreb Index [18]	$M_2(G)$	$M_2(G) = \sum_{uv\in E(G)} (d(u)d(v))$
3.	Modified Second Zagreb Index [28]	${}^mM_2(G)$	${}^mM_2(G) = \sum_{uv\in E(G)} \frac{1}{d(u)d(v)}$
4.	General Randić Index [4]	$R_\alpha(G)$	$R_\alpha(G) = \sum_{uv\in E(G)} (d(u)d(v))^\alpha$
5.	Inverse Randić Index [1]	$RR_\alpha(G)$	$RR_\alpha(G) = \sum_{uv\in E(G)} \frac{1}{(d(u)d(v))^\alpha}$
6.	Symmetric Division (Deg) Index [39]	$SDD(G)$	$SDD(G) = \sum_{uv\in E(G)} \left\{\frac{\min(d(u),d(v))}{\max(d(u),d(v))} + \frac{\max(d(u),d(v))}{\min(d(u),d(v))}\right\}$
7.	Harmonic Index [11]	$H(G)$	$H(G) = \sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}$
8.	Inverse Sum (Indeg) Index [39]	$ISI(G)$	$ISI(G) = \sum_{uv\in E(G)} \frac{d(u)d(v)}{d(u)+d(v)}$
9.	Augmented Zagreb Index [12]	$AZ(G)$	$AZ(G) = \sum_{uv\in E(G)} \left\{\frac{d(u)d(v)}{d(u)+d(v)-2}\right\}^3$

The most stable structures of two-dimensional Silicon-Carbon monolayer mixes with different stoichiometric blends as mentioned in [26].

The graphene sheets were constructively confined in 2004 [33]. From that point onward honeycomb $2D$ material has stimulated and inspired serious research interests to a great scope because of its exceptional electronic, mechanical, and optical properties, including its anomalous quantum Hall impact, overwhelming electronic conductivity, and high mechanical quality [34].

The carbon and silicon have a 2 allotrope with a honeycomb structure in a particular Silicene. Till this study, bunches of exertion have been given to open a bandgap in Silicene sheets. In addition, $2D$ Silicon-Carbon $(Si\text{-}C)$ monolayers can be seen as piece tunable materials between the ultra-clean $2D$ carbon monolayer-graphene and the untainted $2D$ silicon monolayer-silicene. Several attempts have been directed towards forecasting the most stable structure of the $Si\text{-}C$ sheet, read [21, 27, 42] for more information.

We consider three types of $Si\text{-}C$ structure (commonly known as Silicon-Carbides) namely $Si_2C_3\text{-}I$, $Si_2C_3\text{-}II$ and $Si_2C_3\text{-}III$ based on the low-energy metastable structure for each Si. These structures represent the lowest-energy, second lowest-energy and the third-lowest energy structure respectively.

Our Contribution and Road-map

In [21, 25, 31, 32], several degree-based topological indices of Silicon-Carbons are calculated by using formulas of topological indices mentioned in Table 1. Instead of calculating them (degree-based topological indices) separately, in this paper, we evaluate a closed-form of M-polynomial for Silicon-Carbons namely $Si_2C_3\text{-}I[p,q]$, $Si_2C_3\text{-}II[p,q]$ and $Si_2C_3\text{-}III[p,q]$ in Sections 2, 3 and 4. We establish M-polynomial for Silicon-Carbons and henceforward compute the nine related degree-based topological indices of Silicon-Carbons for different values of p and q. Moreover, the graphical representation of the M-polynomials and related degree-based topological indices of all the three molecular structures are shown in respective sections for different values of p and q. Finally, we draw a conclusion in Section 5.

2 Silicon-Carbide $Si_2C_3\text{-}I[p,q]$ $2D$ Structure

In the structure of the molecular graph of Silicon-Carbide $Si_2C_3\text{-}I[p,q]$, p denotes the number of connected unit cells in a single row (chain) and q denotes the number of connected rows each with p number of cells. The $2D$ molecular graph of Silicon-Carbide $Si_2C_3\text{-}I[p,q]$ is given in Figure 1(b) for $p = 4$ and $q = 3$. In Figure 2 we have signified how the cells are connected in a row (chain) and how one row is connected to another row. Observe that, in the graph of Si_2C_3-$I[p,q]$, the total number of vertices is $10pq$ and the number of edges is $15pq-2p-3q$.

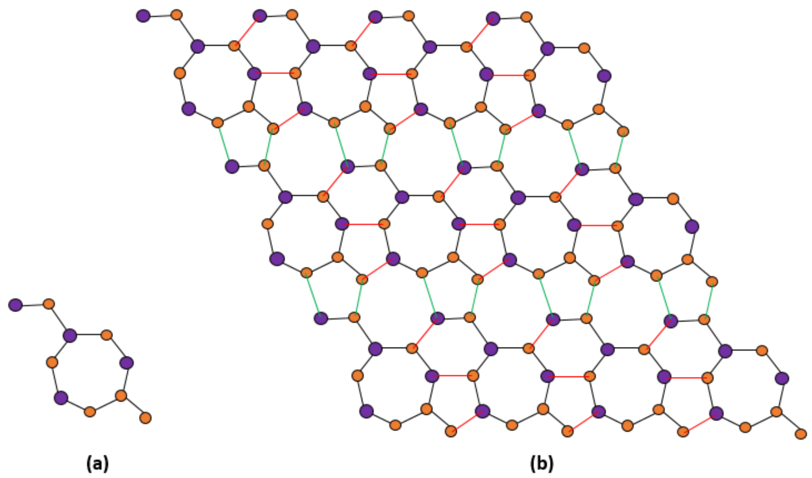

Figure 1. (a) A chemical unit cell of Si_2C_3-$I[p,q]$, (b) Molecular structure of Si_2C_3-$I[p,q]$ for $p=4$ and $q=3$. In the figure, the Carbon atoms Cs are colored brown and the Silicon atoms Sis are marked blue.

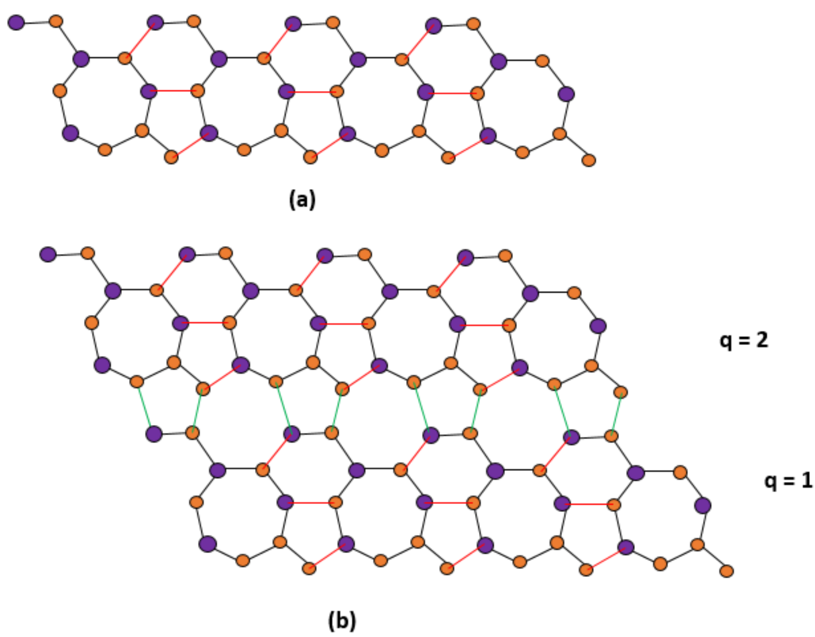

Figure 2. (a) In Si_2C_3-$I[4,1]$, we have one row with $p=4$ and $q=1$ (b) In Si_2C_3-$I[4,2]$, two rows are combined. Green lines (edges) connect the upper and lower rows.

2.1 Computing M-polynomial for Si_2C_3-$I[p,q]$

Theorem 2.1. *Let Si_2C_3-$I[p,q]$ be the Silicon-Carbide. Then the M-polynomial of Si_2C_3-$I[p,q]$ for $p,q\geq 1$ is*

$$M(Si_2C_3\text{-}I[p,q];x,y)=xy^2+xy^3+(p+2q)x^2y^2+(6p+8q-9)x^2y^3+(15pq-9p-13q+7)x^3y^3.$$

Proof. As mentioned earlier that for the structure of Silicon-Carbide Si_2C_3-$I[p,q]$, we have:

$$|V(Si_2C_3\text{-}I[p,q])|=10pq \quad \text{and} \quad |E(Si_2C_3\text{-}I[p,q])|=15pq-2p-3q.$$

And moreover, we can see that there are three partitions according to the degree of vertices, namely,

$$\begin{aligned} & V_1(Si_2C_3\text{-}I[p,q]) = \{u \in V(Si_2C_3\text{-}I[p,q]) : d(u) = 1\}, \\ & V_2(Si_2C_3\text{-}I[p,q]) = \{u \in V(Si_2C_3\text{-}I[p,q]) : d(u) = 2\}, \\ \text{and} \quad & V_3(Si_2C_3\text{-}I[p,q]) = \{u \in V(Si_2C_3\text{-}I[p,q]) : d(u) = 3\}. \end{aligned}$$

Table 2. Vertex partition of Si_2C_3-$I[p,q]$ for different values of p and q.

$[p,q]$	$[1,1]$	$[1,2]$	$[1,3]$	$[2,1]$	$[2,2]$	$[2,3]$	$[3,1]$	$[3,2]$	$[3,3]$	$[4,1]$	$[4,2]$	$[4,3]$
V_1	2	2	2	2	2	2	2	2	2	2	2	2
V_2	6	12	18	10	16	22	14	20	26	18	24	30
V_3	2	6	10	8	22	36	14	38	62	20	54	88

Now we use the computed values in Table 2 and MATLAB software for generalizing the formulas for the number of such vertices, given as: $|V_1(Si_2C_3\text{-}I[p,q])| = 2$, $|V_2(Si_2C_3\text{-}I[p,q])| = 4p + 2 + 6(q-1)$ and $V_3(Si_2C_3\text{-}I[p,q]) = 10pq - 4p - 6q + 2$. Also, we divide the edge set of Si_2C_3-$I[p,q]$ into five disjoint parts based on the degrees of end vertices of each edge, as follows:

$$\begin{aligned} & E_1 = E_{\{1,2\}} = \{e = uv \in E(Si_2C_3\text{-}I[p,q]) : d(u) = 1, d(v) = 2\}, \\ & E_2 = E_{\{1,3\}} = \{e = uv \in E(Si_2C_3\text{-}I[p,q]) : d(u) = 1, d(v) = 3\}, \\ & E_3 = E_{\{2,2\}} = \{e = uv \in E(Si_2C_3\text{-}I[p,q]) : d(u) = 2, d(v) = 2\}, \\ & E_4 = E_{\{2,3\}} = \{e = uv \in E(Si_2C_3\text{-}I[p,q]) : d(u) = 2, d(v) = 3\}, \\ \text{and} \quad & E_5 = E_{\{3,3\}} = \{e = uv \in E(Si_2C_3\text{-}I[p,q]) : d(u) = 3, d(v) = 3\}. \end{aligned}$$

From the molecular graph [3] of Si_2C_3-$I[p,q]$, we can observe that $|E_1| = 1$, $|E_2| = 1$, $|E_3| = p + 2q$, $|E_4| = 6p - 1 + 8(q-1)$, and $|E_5| = 15pq - 9p - 13q + 7$.

Therefore by definition, the M-polynomial of Si_2C_3-$I[p,q]$ is

$$\begin{aligned} & M(Si_2C_3\text{-}I[p,q]; x, y) \\ & = \sum_{i \le j} m_{i,j} x^i y^j, \quad \text{where } i, j \in \{1,2,3\} \\ & = \sum_{1 \le 2} m_{1,2} x^1 y^2 + \sum_{1 \le 3} m_{1,3} x^1 y^3 + \sum_{2 \le 2} m_{2,2} x^2 y^2 + \sum_{2 \le 3} m_{2,3} x^2 y^3 + \sum_{3 \le 3} m_{3,3} x^3 y^3 \\ & = \sum_{uv \in E_1(Si_2C_3\text{-}I[p,q])} m_{1,2} x^1 y^2 + \sum_{uv \in E_2(Si_2C_3\text{-}I[p,q])} m_{1,3} x^1 y^3 + \sum_{uv \in E_3(Si_2C_3\text{-}I[p,q])} m_{2,2} x^2 y^2 + \\ & \quad \sum_{uv \in E_4(Si_2C_3\text{-}I[p,q])} m_{2,3} x^2 y^3 + \sum_{uv \in E_5(Si_2C_3\text{-}I[p,q])} m_{3,3} x^3 y^3 \\ & = |E_{\{1,2\}}| x^1 y^2 + |E_{\{1,3\}}| x^1 y^3 + |E_{\{2,2\}}| x^2 y^2 + |E_{\{2,3\}}| x^2 y^3 + |E_{\{3,3\}}| x^3 y^3 \\ & = xy^2 + xy^3 + (p + 2q) x^2 y^2 + (6p - 1 + 8(q-1)) x^2 y^3 + (15pq - 9p - 13q + 7) x^3 y^3. \end{aligned}$$

□

To compute the degree-based topological indices of a given graph G (mentioned in Table 1) from M-polynomial, we use the derivation formulas in terms of integral or derivative (or both) as given in Table 3 [8].

From the M-polynomial produced in Theorem 2.1, below we derive the values of the related degree-based topological indices of the Si_2C_3-$I[p,q]$ for variables p and q.

[3] Also, the molecular graph of Si_2C_3-$I[p,q]$ does not have any edge uv such that $d(u) = 1$ and $d(v) = 1$ and as a consequence $|E_{\{1,1\}}| = 0$.

Table 3. Formulas for degree-based topological indices derived from M-polynomial.

S. No.	Topological Index	Notation	f(x,y)	Derivation from $(M(G;x,y))$
1.	First Zagreb Index	$M_1(G)$	$x+y$	$(D_x+D_y)(M(G;x,y))\|_{x=y=1}$
2.	Second Zagreb Index	$M_2(G)$	xy	$(D_xD_y)(M(G;x,y))\|_{x=y=1}$
3.	Modified Second Zagreb Index	${}^mM_2(G)$	$\frac{1}{xy}$	$(S_xS_y)(M(G;x,y))\|_{x=y=1}$
4.	General Randić Index	$R_\alpha(G)$	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)(M(G;x,y))\|_{x=y=1}$
5.	Inverse Randić Index	$RR_\alpha(G)$	$\frac{1}{(xy)^\alpha}$	$(S_x^\alpha S_y^\alpha)(M(G;x,y))\|_{x=y=1}$
6.	Symmetric Division (Deg) Index	$SDD(G)$	$\frac{x^2+y^2}{xy}$	$(D_xS_y+D_yS_x)(M(G;x,y))\|_{x=y=1}$
7.	Harmonic Index	$H(G)$	$\frac{2}{x+y}$	$2S_xJ(M(G;x,y))\|_{x=1}$
8.	Inverse Sum (Indeg) Index	$ISI(G)$	$\frac{xy}{x+y}$	$S_xJD_xD_y(M(G;x,y))\|_{x=1}$
9.	Augmented Zagreb Index	$AZ(G)$	$\left(\frac{xy}{x+y-2}\right)^3$	$S_x^3Q_{-2}JD_x^3D_y^3(M(G;x,y))\|_{x=1}$

In the Table 3, the notations $D_x = x\frac{\partial(f(x,y))}{\partial x}$, $D_y = y\frac{\partial(f(x,y))}{\partial y}$,

$$S_x = \int_0^x \frac{f(t,y)}{t}dt, \qquad S_y = \int_0^y \frac{f(x,t)}{t}dt,$$

$$J(f(x,y)) = f(x,x), \quad Q_\alpha(f(x,y)) = x^\alpha f(x,y),\ \alpha \neq 0.$$

Theorem 2.2. *Let Si_2C_3-$I[p,q]$ be the Silicon-Carbide. Then*

1. $M_1(Si_2C_3\text{-}I[p,q]) = 90pq - 20p - 30q + 4.$
2. $M_2(Si_2C_3\text{-}I[p,q]) = 135pq - 41p - 61q + 14.$
3. ${}^mM_2(Si_2C_3\text{-}I[p,q]) = \frac{5}{3}pq + \frac{1}{4}p + \frac{7}{18}q + \frac{1}{9}.$
4. $R_\alpha(Si_2C_3\text{-}I[p,q]) = 2^\alpha + 3^\alpha + 2^{2\alpha}(p+2q) + 2^\alpha 3^\alpha(6p-1+8(q-1)) + 3^{2\alpha}(15pq-9p-13q+7).$
5. $RR_\alpha(Si_2C_3\text{-}I[p,q]) = \frac{1}{2^\alpha} + \frac{1}{3^\alpha} + \frac{1}{2^{2\alpha}}(p+2q) + \frac{1}{2^\alpha 3^\alpha}(6p-1+8(q-1)) + \frac{1}{3^{2\alpha}}(15pq-9p-13q+7).$
6. $SDD(Si_2C_3\text{-}I[p,q]) = 30pq - 3p - \frac{14}{3}q + \frac{1}{3}.$
7. $H(Si_2C_3\text{-}I[p,q]) = 5pq - \frac{1}{10}p - \frac{2}{15}q - \frac{1}{10}.$
8. $ISI(Si_2C_3\text{-}I[p,q]) = \frac{45}{2}pq - \frac{53}{10}p - \frac{79}{10}q + \frac{67}{60}.$
9. $AZ(Si_2C_3\text{-}I[p,q]) = \frac{10935}{64}pq - \frac{2977}{64}p - \frac{4357}{64}q + \frac{1223}{64}.$

Proof. As computed in Theorem 2.1, the M-polynomial for Si_2C_3-$I[p,q]$ is

$$M(Si_2C_3\text{-}I[p,q];x,y) = xy^2 + xy^3 + (p+2q)x^2y^2 + (6p-1+8(q-1))x^2y^3 + (15pq-9p-13q+7)x^3y^3.$$

For notational ease, we write $f(x,y) = M(Si_2C_3\text{-}I[p,q];x,y)$. Therefore,

- $D_x(f(x,y)) = xy^2 + xy^3 + 2(p+2q)x^2y^2 + 2(6p-1+8(q-1))x^2y^3 + 3(15pq-9p-13q+7)x^3y^3,$
- $D_y(f(x,y)) = 2xy^2 + 3xy^3 + 2(p+2q)x^2y^2 + 3(6p-1+8(q-1))x^2y^3 + 3(15pq-9p-13q+7)x^3y^3,$
- $D_yD_x(f(x,y)) = 2xy^2 + 3xy^3 + 4(p+2q)x^2y^2 + 6(6p-1+8(q-1))x^2y^3 + 9(15pq-9p-13q+7)x^3y^3,$
- $S_x(f(x,y)) = xy^2 + xy^3 + \frac{1}{2}(p+2q)x^2y^2 + \frac{1}{2}(6p-1+8(q-1))x^2y^3 + \frac{1}{3}(15pq-9p-13q+7)x^3y^3,$
- $S_y(f(x,y)) = \frac{1}{2}xy^2 + \frac{1}{3}xy^3 + \frac{1}{2}(p+2q)x^2y^2 + \frac{1}{3}(6p-1+8(q-1))x^2y^3 + \frac{1}{3}(15pq-9p-13q+7)x^3y^3,$

- $S_xS_y(f(x,y)) = \frac{1}{2}xy^2 + \frac{1}{3}xy^3 + \frac{1}{4}(p+2q)x^2y^2 + \frac{1}{6}(6p-1+8(q-1))x^2y^3 + \frac{1}{9}(15pq-9p-13q+7)x^3y^3$,
- $D_x^\alpha D_y^\alpha(f(x,y)) = 2^\alpha xy^2 + 3^\alpha xy^3 + 2^{2\alpha}(p+2q)x^2y^2 + 2^\alpha 3^\alpha(6p-1+8(q-1))x^2y^3 + 3^{2\alpha}(15pq-9p-13q+7)x^3y^3$,
- $D_xS_y(f(x,y)) = \frac{1}{2}xy^2 + \frac{1}{3}xy^3 + (p+2q)x^2y^2 + \frac{2}{3}(6p-1+8(q-1))x^2y^3 + (15pq-9p-13q+7)x^3y^3$,
- $D_yS_x(f(x,y)) = 2xy^2 + 3xy^3 + (p+2q)x^2y^2 + \frac{3}{2}(6p-1+8(q-1))x^2y^3 + (15pq-9p-13q+7)x^3y^3$,
- $S_x^\alpha S_y^\alpha(f(x,y)) = \frac{1}{2^\alpha}xy^2 + \frac{1}{3^\alpha}xy^3 + \frac{1}{2^{2\alpha}}(p+2q)x^2y^2 + \frac{1}{2^\alpha 3^\alpha}(6p-1+8(q-1))x^2y^3 + \frac{1}{3^{2\alpha}}(15pq-9p-13q+7)x^3y^3$,
- $S_xJ(f(x,y)) = \frac{1}{3}x^3 + \frac{1}{4}x^4 + \frac{1}{4}(p+2q)x^4 + \frac{1}{5}(6p-1+8(q-1))x^5 + \frac{1}{6}(15pq-9p-13q+7)x^6$,
- $S_xJD_xD_y(f(x,y)) = \frac{2}{3}x^3 + \frac{3}{4}x^4 + (p+2q)x^4 + \frac{6}{5}(6p-1+8(q-1))x^5 + \frac{9}{6}(15pq-9p-13q+7)x^6$,
- $S_x^3Q_{-2}JD_x^3D_y^3(f(x,y)) = 2^3x + \frac{3^3}{2^3}x^2 + 2^3(p+2q)x^2 + 2^3(6p-1+8(q-1))x^3 + \frac{3^6}{4^3}(15pq-9p-13q+7)x^6$.

Hence, the degree-based topological indices of the Si_2C_3-$I[p,q]$ based on the derivation formulas mentioned in Table 3 are as follows:

1. First Zagreb Index:
$M_1(Si_2C_3\text{-}I[p,q]) = (D_x+D_y)(f(x,y))|_{x=y=1} = 90pq-20p-30q+4$.
2. Second Zagreb Index:
$M_2(Si_2C_3\text{-}I[p,q]) = (D_xD_y)(f(x,y))|_{x=y=1} = 135pq-41p-61q+14$.
3. Modified Second Zagreb Index:
${}^mM_2(Si_2C_3\text{-}I[p,q]) = (S_xS_y)(f(x,y))|_{x=y=1} = \frac{5}{3}pq + \frac{1}{4}p + \frac{7}{18}q + \frac{1}{9}$.
4. General Randić Index:
$R_\alpha(Si_2C_3\text{-}I[p,q]) = (D_x^\alpha D_y^\alpha)(f(x,y))|_{x=y=1} = 2^\alpha + 3^\alpha + 2^{2\alpha}(p+2q) + 2^\alpha 3^\alpha(6p-1+8(q-1)) + 3^{2\alpha}(15pq-9p-13q+7)$.
5. Inverse Randić Index:
$RR_\alpha(Si_2C_3\text{-}I[p,q]) = (S_x^\alpha S_y^\alpha)(f(x,y))|_{x=y=1} = \frac{1}{2^\alpha} + \frac{1}{3^\alpha} + \frac{1}{2^{2\alpha}}(p+2q) + \frac{1}{2^\alpha 3^\alpha}(6p-1+8(q-1)) + \frac{1}{3^{2\alpha}}(15pq-9p-13q+7)$.
6. Symmetric Division (Deg) Index:
$SDD(Si_2C_3\text{-}I[p,q]) = (D_xS_y+D_yS_x)(f(x,y))|_{x=y=1} = 30pq-3p-\frac{14}{3}q+\frac{1}{3}$.
7. Harmonic Index:
$H(Si_2C_3\text{-}I[p,q]) = 2S_xJ(f(x,y))|_{x=1} = 5pq-\frac{1}{10}p-\frac{2}{15}q-\frac{1}{10}$.
8. Inverse Sum (Indeg) Index:
$ISI(Si_2C_3\text{-}I[p,q]) = S_xJD_xD_y(f(x,y))|_{x=1} = \frac{45}{2}pq-\frac{53}{10}p-\frac{79}{10}q+\frac{67}{60}$.
9. Augmented Zagreb Index:
$AZ(Si_2C_3\text{-}I[p,q]) = S_x^3Q_{-2}JD_x^3D_y^3(f(x,y))|_{x=1} = \frac{10935}{64}pq-\frac{2977}{64}p-\frac{4357}{64}q+\frac{1223}{64}$.

□

2.2 Plotting the M-polynomial and Associated Indices of Si_2C_3-$I[p,q]$

For different values of p and q of the Si_2C_3-$I[p,q]$, the respective M-polynomials and several related degree-based topological indices are tabulated in Table 4. To see the related topological indices and the nature of M-polynomials, we vary the values of p and q from $p=2$ to $p=4$ and $q=1$ to $q=3$. The values of p and q in the table may be extended as and when required based on Theorem 2. From the table, we can observe that the values of each of the topological indices are increasing with the values of p and q increasing.

Table 4. Computation of degree-based topological indices of Si_2C_3-$I[p, q]$ at different values of p and q and the respective M-polynomials.

Sl.	$[p, q]$	$[2, 1]$	$[2, 2]$	$[2, 3]$	$[3, 1]$	$[3, 2]$	$[3, 3]$	$[4, 1]$	$[4, 2]$	$[4, 3]$
	M-Polynomial / Topological Index	$xy^2 + xy^3 + 4x^2y^2 + 11x^2y^3 + 6x^3y^3$	$xy^2 + xy^3 + 6x^2y^2 + 19x^2y^3 + 23x^3y^3$	$xy^2 + xy^3 + 8x^2y^2 + 27x^2y^3 + 40x^3y^3$	$xy^2 + xy^3 + 5x^2y^2 + 17x^2y^3 + 12x^3y^3$	$xy^2 + xy^3 + 7x^2y^2 + 25x^2y^3 + 44x^3y^3$	$xy^2 + xy^3 + 9x^2y^2 + 33x^2y^3 + 76x^3y^3$	$xy^2 + xy^3 + 6x^2y^2 + 23x^2y^3 + 18x^3y^3$	$xy^2 + xy^3 + 8x^2y^2 + 31x^2y^3 + 68x^3y^3$	$xy^2 + xy^3 + 10x^2y^2 + 39x^2y^3 + 112x^3y^3$
1.	First Zagreb Index	114	264	414	184	424	664	254	584	914
2.	Second Zagreb Index	141	350	559	235	579	923	329	808	1287
3.	Modified Second Zagreb Index	4.333	8.055	11.777	6.25	11.638	17.027	8.166	15.222	22.277
4.	General Randić Index ($\alpha = 1/2$)	56.0906	130.6865	205.282	90.7875	210.3835	329.979	125.484	290.0804	454.676
5.	Inverse Randić Index ($\alpha = 1/2$)	9.7751	19.7078	29.6404	14.7246	29.6573	44.5899	19.6741	39.6068	59.5394
6.	Symmetric Division (Deg) Index	49.66	105	160.33	76.66	162	247.33	103.66	219	334.33
7.	Harmonic Index	9.566	19.433	29.3	14.466	29.333	44.2	19.366	39.233	59.1
8.	Inverse Sum (Indeg) Index	33.2	70.3	107.4	50.4	110	169.6	67.6	149.7	231.8
9.	Augmented Zagreb Index	199.7187	473.3593	747	324.062	768.5625	1213.062	448.406	1063.7656	1679.125

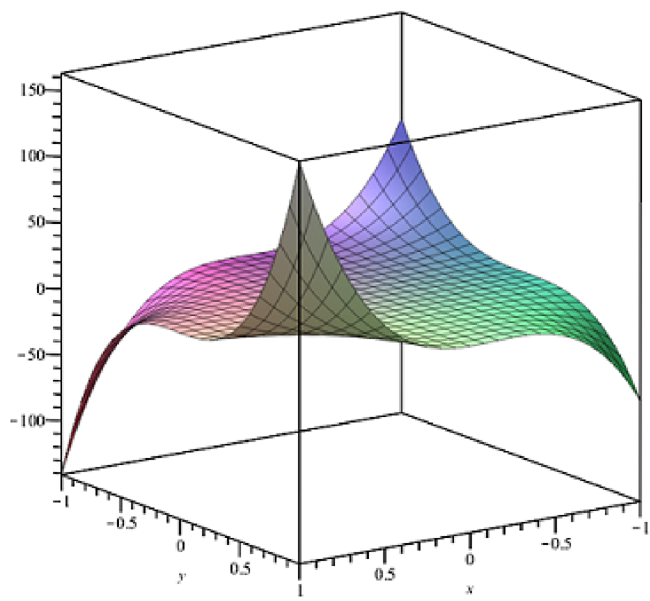

Figure 3. The plot of the M-polynomial of Si_2C_3-$I[4, 3]$, where $-1 \leq x, y \leq 1$.

We have drawn the M-polynomial in Maple-2020 software. Figure 3 gives the graphical representation of the M-polynomial (as proposed in Theorem 2) of the Silicon-Carbide Si_2C_3-$I[4, 3]$ in range $-1 \leq x, y \leq 1$.

Moreover, observing the wide range of values (in Table 4) of the different degree-based topological indices of Si_2C_3-$I[p, q]$ for different values of p and q, we plot the values of first Zagreb, second Zagreb, general Randić ($\alpha = 1/2$), inverse Randić ($\alpha = 1/2$), symmetric division (deg) and augmented Zagreb indices in Figure 4, and the values of modified second Zagreb, harmonic and inverse sum (indeg) indices in Figure 5.

3 Silicon-Carbide Si_2C_3-$II[p, q]$ $2D$ Structure

In the $2D$ molecular graph of Silicon-Carbide Si_2C_3-$II[p, q]$, p denotes the number of connected unit cells (as shown in Figure 6(a)) in a single row (chain) and q denotes the number of connected rows each with p number of cells. Please refer to Figure 6(b) for Silicon-Carbide Si_2C_3-$II[3, 3]$.

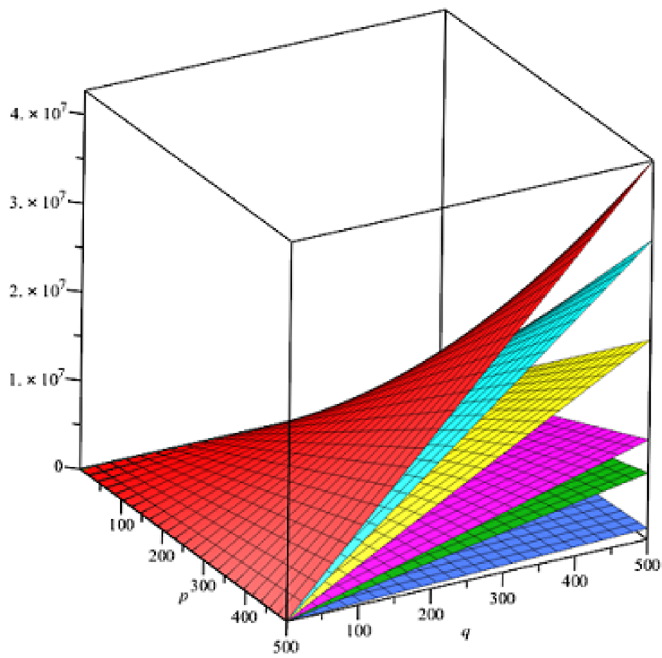

Figure 4. Red, Cyan, Yellow, Pink, Green and Royal Blue represent augmented Zagreb index $AZ(G)$, second Zagreb index $M_2(G)$, first Zagreb index $M_1(G)$, general Randić index $R_{1/2}(G)$, symmetric division (deg) index $SDD(G)$ and inverse Randić index $RR_{1/2}(G)$ of Si_2C_3-*I*$[p, q]$ for different values of p and q ($1 \leq p, q \leq 500$) respectively.

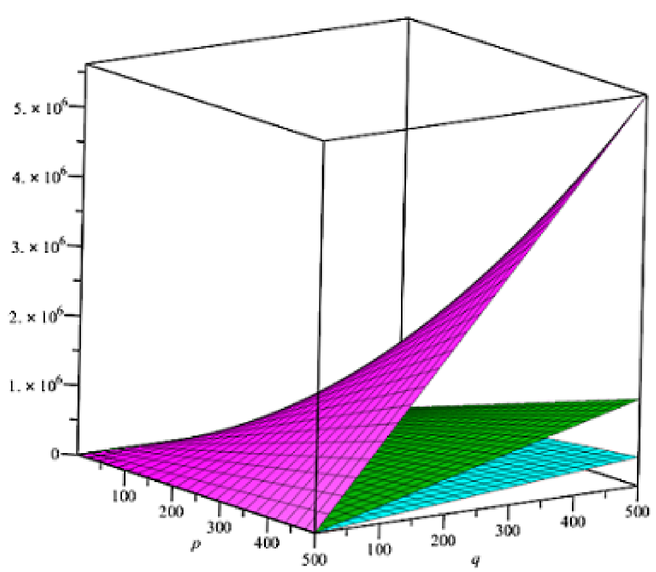

Figure 5. Pink, Green and Cyan represent inverse sum (indeg) index $ISI(G)$, harmonic index $H(G)$ and modified second Zagreb index ${}^{m}M_2(G)$ of Si_2C_3-*I*$[p, q]$ for different values of p and q ($1 \leq p, q \leq 500$) respectively.

In Figure 7, we have signified how the cells are connected in a row (chain) and how one row is connected to another row. One can easily calculate that the total number of vertices is $10pq$ and the number of edges is $15pq - 3p - 3q$ in Si_2C_3-*II*$[p, q]$ graph.

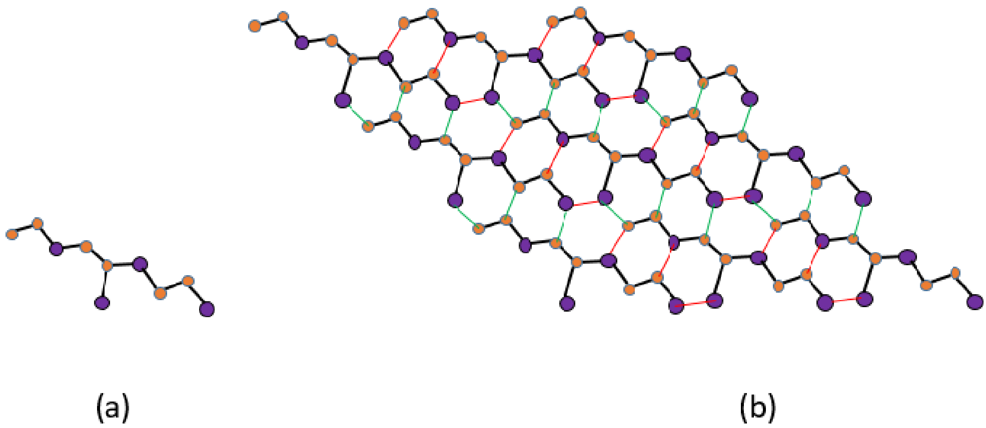

Figure 6. (a) A chemical unit cell of Si_2C_3-$II[p,q]$, (b) Si_2C_3-$II[p,q]$ where $p = 3$ and $q = 3$. Here, the Carbon atoms Cs are marked brown and the Silicon atoms Sis are marked blue.

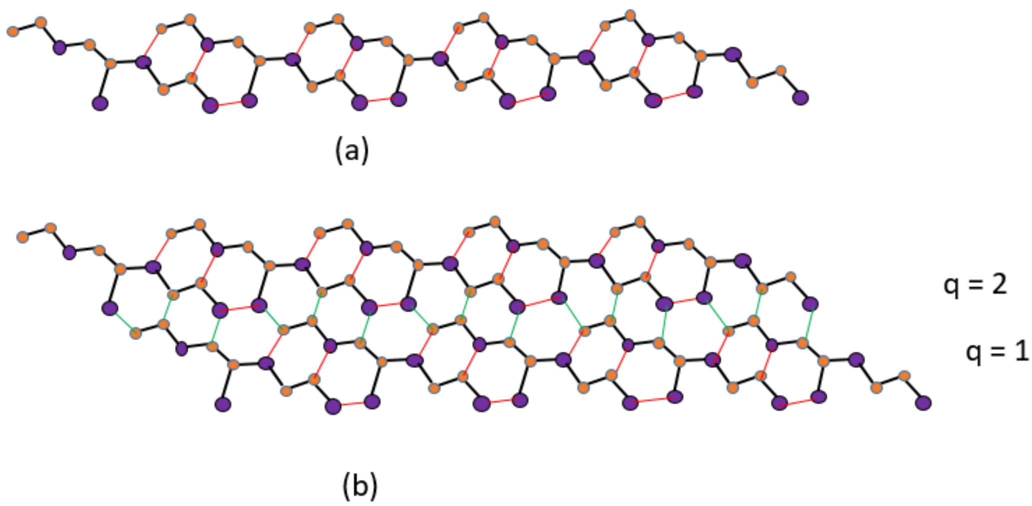

Figure 7. (a) Graphical view of Si_2C_3-$II[5,1]$, (b) Structure of Si_2C_3-$II[5,2]$, where the upper and lower rows are connected by green lines (edges).

3.1 Computing M-polynomial for Si_2C_3-$II[p,q]$

The M-polynomial for Si_2C_3-$II[p,q]$ is given by Theorem 3.1. Whereas in Theorem 3.2, we have derived the degree-based topological indices of Si_2C_3-$II[p,q]$ from the M-polynomial. The proofs of Theorems 3.1 and 3.2 are left as an exercise to the interested readers. Although, we have kept them in the Appendix section (Section 6, page 153) for more clarification.

Theorem 3.1. *Let us consider the Silicon-Carbide Si_2C_3-$II[p,q]$. The M-polynomial of Si_2C_3-$II[p,q]$ for $p, q \geq 1$ is given by*

$$M(Si_2C_3\text{-}II[p,q]; x, y) = 2xy^2 + xy^3 + (2p+2q)x^2y^2 + (8p+8q-14)x^2y^3 + (15pq-13p-13q+11)x^3y^3.$$

Theorem 3.2. *Let Si_2C_3-$II[p,q]$ be the Silicon-Carbide. Then*

1. $M_1(Si_2C_3\text{-}II[p,q]) = 90pq - 30p - 30q + 6$.
2. $M_2(Si_2C_3\text{-}II[p,q]) = 135pq - 61p - 61q + 22$.
3. ${}^mM_2(Si_2C_3\text{-}II[p,q]) = \frac{5}{3}pq + \frac{7}{18}p + \frac{7}{18}q + \frac{2}{9}$.

4. $R_\alpha(Si_2C_3\text{-}II[p,q]) = 2^{\alpha+1} + 3^\alpha + 2^{2\alpha}(2p+2q) + 2^\alpha 3^\alpha(8p+8q-14) + 3^{2\alpha}(15pq-13p-13q+11)$.
5. $RR_\alpha(Si_2C_3\text{-}II[p,q]) = \frac{1}{2^{\alpha-1}} + \frac{1}{3^\alpha} + \frac{1}{2^{2\alpha}}(2p+2q) + \frac{1}{2^\alpha 3^\alpha}(8p+8q-14) + \frac{1}{3^{2\alpha}}(15pq-13p-13q+11)$.
6. $SDD(Si_2C_3\text{-}II[p,q]) = 30pq - \frac{14}{3}p - \frac{14}{3}q$.
7. $H(Si_2C_3\text{-}II[p,q]) = 5pq - \frac{2}{15}p - \frac{2}{15}q - \frac{1}{10}$.
8. $ISI(Si_2C_3\text{-}II[p,q]) = \frac{45}{2}pq - \frac{79}{10}p - \frac{79}{10}q + \frac{107}{60}$.
9. $AZ(Si_2C_3\text{-}II[p,q]) = \frac{10935}{64}pq - \frac{4357}{64}p - \frac{4357}{64}q + \frac{2091}{64}$.

3.2 Plotting the M-polynomial and Associated Indices of Si_2C_3-$II[p,q]$

For different values of p and q of the Si_2C_3-$II[p,q]$, the respective M-polynomials and associated degree-based topological indices are mentioned in Table 5. To see the related topological indices and the nature of M-polynomials, we vary the values of p and q of the Si_2C_3-$II[p,q]$ from $p=2$ to $p=4$ and $q=1$ to $q=3$. The values of p and q in the table may be extended as and when required based on Theorem 3.1. From the table we can observe, the values of each of the topological indices are increasing with the values of p and q increasing.

Table 5. Computation of degree-based topological indices of Si_2C_3-$II[p,q]$ at different values of p and q and the respective M-polynomials.

Sl.	$[p,q]$	$[2,1]$	$[2,2]$	$[2,3]$	$[3,1]$	$[3,2]$	$[3,3]$	$[4,1]$	$[4,2]$	$[4,3]$
	M-polynomial / Topological Index	$2xy^2+xy^3+6x^2y^2+10x^2y^3+2x^3y^3$	$2xy^2+xy^3+8x^2y^2+18x^2y^3+19x^3y^3$	$2xy^2+xy^3+10x^2y^2+26x^2y^3+36x^3y^3$	$2xy^2+xy^3+8x^2y^2+18x^2y^3+4x^3y^3$	$2xy^2+xy^3+10x^2y^2+26x^2y^3+36x^3y^3$	$2xy^2+xy^3+12x^2y^2+34x^2y^3+68x^3y^3$	$2xy^2+xy^3+10x^2y^2+26x^2y^3+6x^3y^3$	$2xy^2+xy^3+12x^2y^2+34x^2y^3+53x^3y^3$	$2xy^2+xy^3+14x^2y^2+42x^2y^3+100x^3y^3$
1.	First Zagreb Index	96	246	396	156	396	636	216	546	876
2.	Second Zagreb Index	109	318	527	183	527	871	257	736	1215
3.	Modified Second Zagreb Index	4.722	8.444	12.166	6.777	12.1666	17.555	8.833	15.888	22.944
4.	General Randić Index ($\alpha = 1/2$)	47.0553	121.6512	196.2472	76.6512	196.247	315.843	106.247	270.843	435.439
5.	Inverse Randić Index ($\alpha = 1/2$)	9.7407	19.6733	29.6060	14.6733	29.6060	44.5386	19.6060	39.5386	59.4713
6.	Symmetric Division (Deg) Index	47	101.33	156.666	71.333	156.666	242	96.666	212	327.333
7.	Harmonic Index	9.5	19.3666	29.233	14.366	29.233	44.1	19.233	39.1	58.966
8.	Inverse Sum (Indeg) Index	23.0833	60.183	97.283	37.683	97.2833	156.883	52.283	134.383	216.483
9.	Augmented Zagreb Index	170.1562	443.7968	717.4375	272.9375	717.4375	1161.937	375.7187	991.0781	1606.437

The graphical representation of the M-polynomial of Silicon-Carbide Si_2C_3-$II[4,3]$ is given by Figure 8 in the range $0.5 \le x, y \le 0.5$. Moreover, observing the wide range of values (in Table 5) of the different degree-based topological indices of Si_2C_3-$II[p,q]$ for different values of p $(2 \le p \le 4)$ and q $(1 \le q \le 3)$, we plot the values of first Zagreb, second Zagreb, general Randić $(\alpha = 1/2)$, inverse Randić $(\alpha = 1/2)$, symmetric division (deg) and augmented Zagreb indices in Figure 9, and the values of modified second Zagreb, harmonic and inverse sum (indeg) indices in Figure 10.

4 Silicon-Carbide Si_2C_3-$III[p,q]$ $2D$ Structure

In the $2D$ molecular graph of Silicon-Carbide Si_2C_3-$III[p,q]$, p denotes the number of connected unit cells (as shown in Figure 11(a)) in a single row (chain) and q denotes the number of connected rows each with p number of cells. Figure 11(b) is a pictorial view of the Si_2C_3-$III[5,4]$. Figure 12 shows how the cells are connected in a row (chain) and how one row is connected to another row in a structure of Silicon-Carbide Si_2C_3-$III[p,q]$. Note that the graph of Si_2C_3-$III[p,q]$ consists of $10pq$ vertices and $15pq - 2p - 3q$ edges.

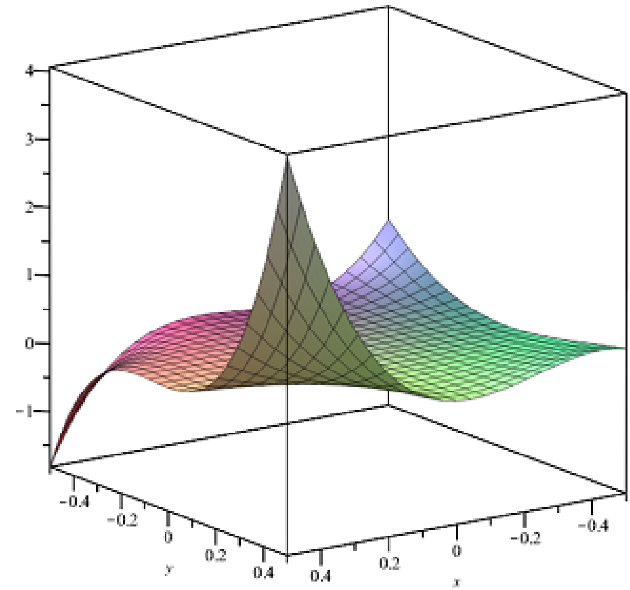

Figure 8. The geometrical representation of the M-polynomial of Si_2C_3-*II*$[4, 3]$, where $0.5 \leq x, y \leq 0.5$.

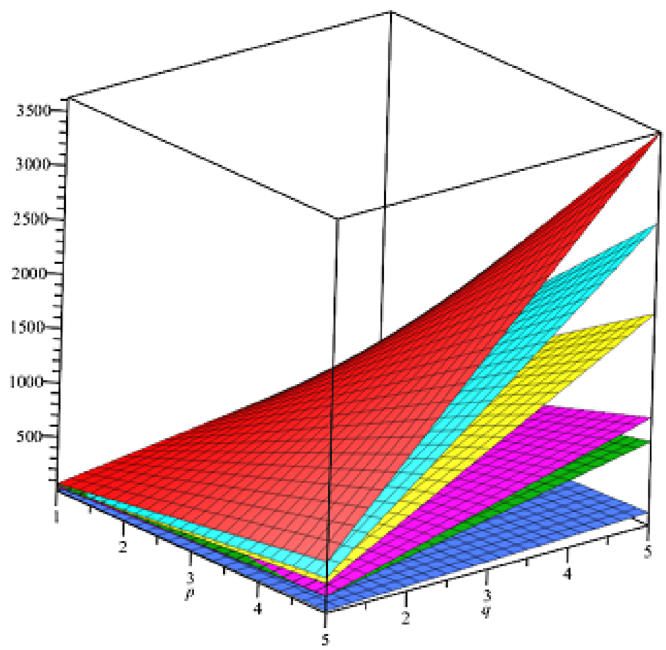

Figure 9. Red, Cyan, Yellow, Pink, Green and Royal Blue represent augmented Zagreb $AZ(G)$, second Zagreb $M_2(G)$, first Zagreb $M_1(G)$, general Randić $R_{1/2}(G)$, symmetric division (deg) $SDD(G)$ and inverse Randić $RR_{1/2}(G)$ indices of Si_2C_3-*II*$[p, q]$ for different values of p and q ($1 \leq p, q \leq 5$), respectively.

4.1 Evaluating M-polynomial for Si_2C_3-*III*$[p, q]$

The M-polynomial of Si_2C_3-*III*$[p, q]$ is given by Theorem 4.1 and in Theorem 4.2, we have derived the degree-based topological indices of Si_2C_3-*III*$[p, q]$ from the M-polynomial. Readers may prove Theorems 4.1 and 4.2 in a similar way as done in Section 2. Although, one can refer to Section 6 (Appendix, in page 153) for the proofs.

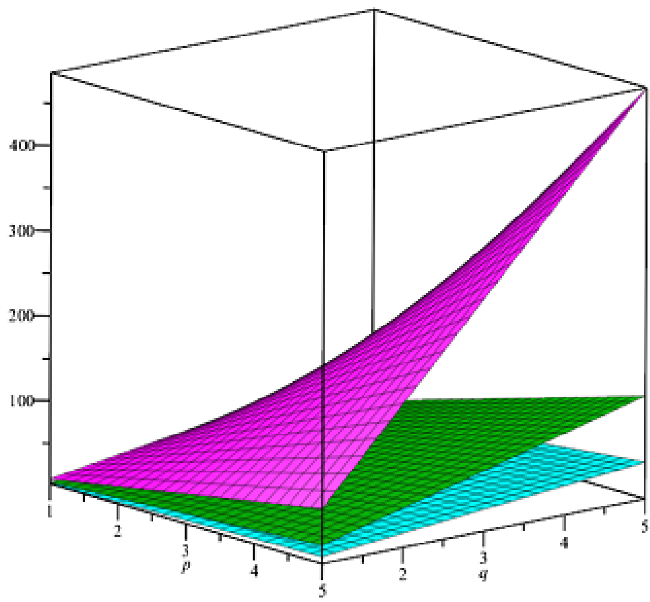

Figure 10. Pink, Green and Cyan represent inverse sum index $ISI(G)$, harmonic index $H(G)$ and modified second Zagreb index ${}^{m}M_2(G)$ of Si_2C_3-$II[p,q]$ for different values of p and q $(1 \leq p, q \leq 5)$, respectively.

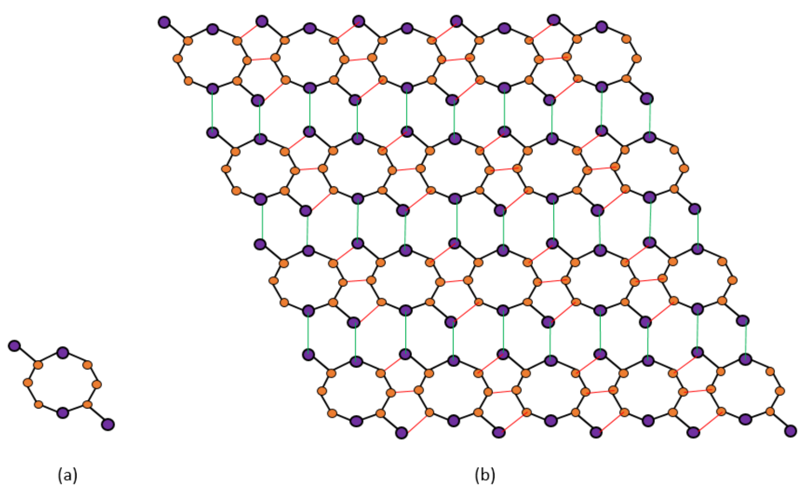

Figure 11. (a) A chemical unit cell of Si_2C_3-$III[p,q]$, (b) Graph of Si_2C_3-$III[p,q]$ where $p = 5$ and $q = 4$. Here, the Carbon atoms Cs are marked brown and the Silicon atoms Sis are marked blue.

Theorem 4.1. *Let us consider the Silicon-Carbide Si_2C_3-$III[p,q]$. The M-polynomial of Si_2C_3-$III[p,q]$ for $p, q \geq 1$ is given by*

$$M(Si_2C_3\text{-}III[p,q]; x, y) = 2xy^3 + (2q+2)x^2y^2 + (8p+8q-12)x^2y^3 + (15pq-10p-13q+8)x^3y^3.$$

Theorem 4.2. *For the Silicon-Carbide Si_2C_3-$III[p,q]$, we have the following results.*

1. $M_1(Si_2C_3\text{-}III[p,q]) = 90pq - 20p - 30q + 4$.
2. $M_2(Si_2C_3\text{-}III[p,q]) = 135pq - 42p - 61q + 14$.
3. ${}^{m}M_2(Si_2C_3\text{-}III[p,q]) = \frac{5}{3}pq + \frac{2}{9}p - \frac{5}{18}q + \frac{1}{18}$.
4. $R_\alpha(Si_2C_3\text{-}III[p,q]) = 2\,3^\alpha + 2^{2\alpha}(2q+2) + 2^\alpha 3^\alpha(8p+8q-12) + 3^{2\alpha}(15pq-10p-13q+8)$.

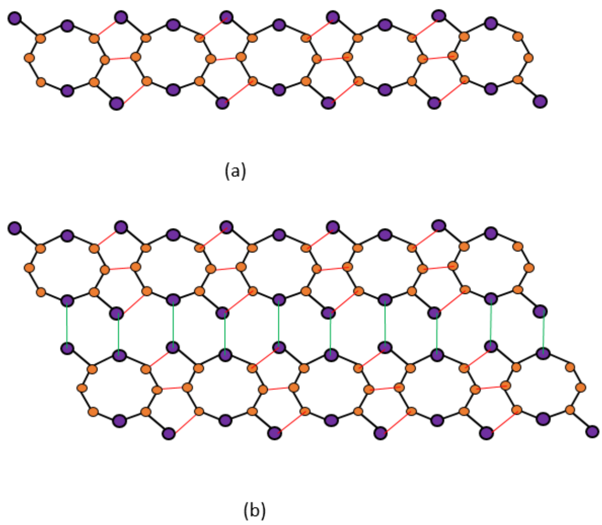

Figure 12. (a) Graph of Si_2C_3-$III[5,1]$, (b) Structure of Si_2C_3-$III[5,2]$, where the upper and lower rows are connected by green lines (edges).

5. $RR_\alpha(Si_2C_3\text{-}III[p,q]) = \frac{2}{3^\alpha} + \frac{1}{2^{2\alpha}}(2q+2) + \frac{1}{2^\alpha 3^\alpha}(8p+8q-12) + \frac{1}{3^{2\alpha}}(15pq-10p-13q+8)$.
6. $SDD(Si_2C_3\text{-}III[p,q]) = 30pq - \frac{8}{3}p - \frac{14}{3}q + \frac{2}{3}$.
7. $H(Si_2C_3\text{-}III[p,q]) = 5pq - \frac{2}{15}p - \frac{2}{15}q - \frac{2}{15}$.
8. $ISI(Si_2C_3\text{-}III[p,q]) = \frac{45}{2}pq - \frac{27}{5}p - \frac{79}{10}q + \frac{11}{5}$.
9. $AZ(Si_2C_3\text{-}III[p,q]) = \frac{10935}{64}pq - \frac{1597}{32}p - \frac{4357}{64}q + \frac{143}{8}$.

4.2 Plotting the M-polynomial and Associated Indices of Si_2C_3-$III[p,q]$

For different values of p and q of the Si_2C_3-$III[p,q]$, the respective M-polynomials and several related degree-based topological indices are tabulated in Table 6. To see the related topological indices and the nature of M-polynomials, we have varies the values of p and q of the Si_2C_3-$III[p,q]$ from $p=2$ to $p=4$ and $q=1$ to $q=3$. The values of p and q in the table may be extended as and when required based on Theorem 4.1. From the table, we can observe that the values of each of the topological indices are increasing with the values of p and q increasing.

Table 6. Computation of degree-based topological indices of Si_2C_3-$III[p,q]$ at different values of p and q and the respective M-polynomials.

Sl.	$[p,q]$	$[2,1]$	$[2,2]$	$[2,3]$	$[3,1]$	$[3,2]$	$[3,3]$	$[4,1]$	$[4,2]$	$[4,3]$
	M-polynomial / Topological Index	$xy^3+4x^2y^2+12x^2y^3+5x^3y^3$	$xy^3+6x^2y^2+20x^2y^3+22x^3y^3$	$xy^3+8x^2y^2+28x^2y^3+39x^3y^3$	$xy^3+4x^2y^2+20x^2y^3+10x^3y^3$	$xy^3+6x^2y^2+28x^2y^3+42x^3y^3$	$xy^3+8x^2y^2+36x^2y^3+74x^3y^3$	$xy^3+4x^2y^2+28x^2y^3+15x^3y^3$	$xy^3+6x^2y^2+36x^2y^3+62x^3y^3$	$xy^3+8x^2y^2+44x^2y^3+109x^3y^3$
1.	First Zagreb Index	114	264	414	184	424	664	254	584	914
2.	Second Zagreb Index	139	348	557	232	576	920	325	804	1283
3.	Modified Second Zagreb Index	3.5555	6.611	9.666	5.444	10.1666	14.888	7.333	13.722	20.111
4.	General Randić Index ($\alpha=1/2$)	55.8579	130.4538	205.0498	90.4538	210.0498	329.6451	125.049	289.64	454.2416
5.	Inverse Randić Index ($\alpha=1/2$)	9.7203	19.6529	29.5856	14.6529	29.5856	44.5183	19.5856	39.5183	59.4509
6.	Symmetric Division (Deg) Index	50.666	106	161.333	78	163.333	248.666	105.333	220.666	336
7.	Harmonic Index	9.466	19.33	29.2	14.33	29.2	44.066	19.2	39.066	58.933
8.	Inverse Sum (Indeg) Index	28.5	65.6	102.7	45.6	105.2	164.8	62.7	144.8	226.9
9.	Augmented Zagreb Index	191.7031	465.343	738.9843	312.6562	757.156	1201.656	433.6093	1048.968	1664.328

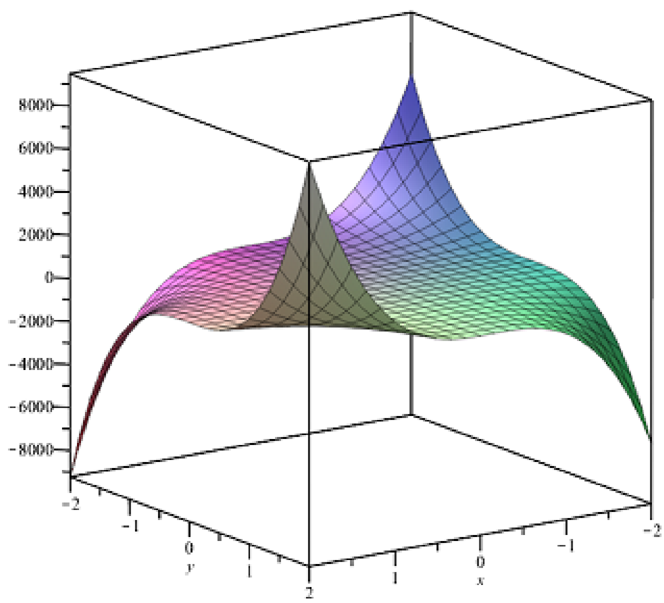

Figure 13. The plot of the M-polynomial of Si_2C_3-*III*$[4,3]$, where $-2 \leq x, y \leq 2$.

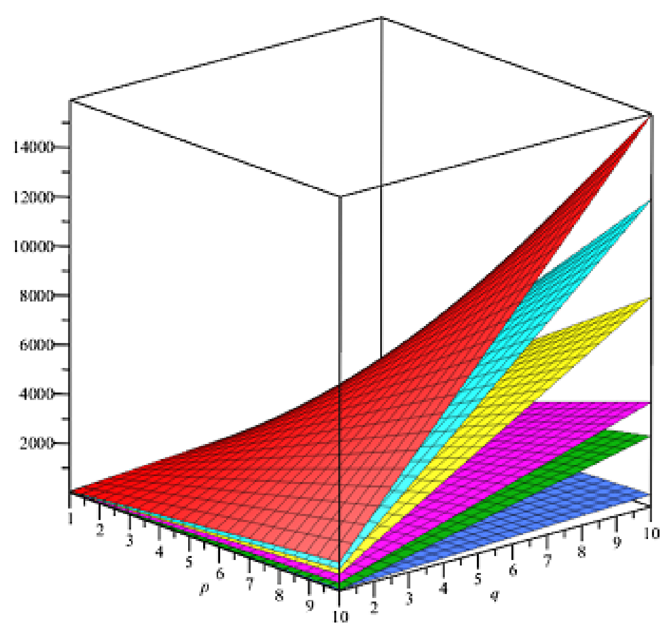

Figure 14. Red, Cyan, Yellow, Pink, Green and Royal Blue represent augmented Zagreb $AZ(G)$, second Zagreb $M_2(G)$, first Zagreb $M_1(G)$, general Randić $R_{1/2}(G)$, symmetric division (deg) $SDD(G)$ and inverse Randić $RR_{1/2}(G)$ indices of Si_2C_3-*III*$[p,q]$ for different values of p and q $(1 \leq p, q \leq 10)$ respectively.

The graphical representation of the M-polynomial of Silicon-Carbide Si_2C_3-*III*$[4,3]$ is given by Figure 13 in range $-2 \leq x, y \leq 2$. Moreover, observing the wide range of values (in Table 6) of the different degree-based topological indices of Si_2C_3-*III*$[p,q]$ for different values of p $(2 \leq p \leq 4)$ and q $(1 \leq q \leq 3)$, we plot the values of first Zagreb, second Zagreb, general Randić $(\alpha = 1/2)$, inverse Randić $(\alpha = 1/2)$, symmetric division (deg) and augmented Zagreb indices in Figure 14, and the values of modified second Zagreb, harmonic and inverse sum (indeg) indices in Figure 15.

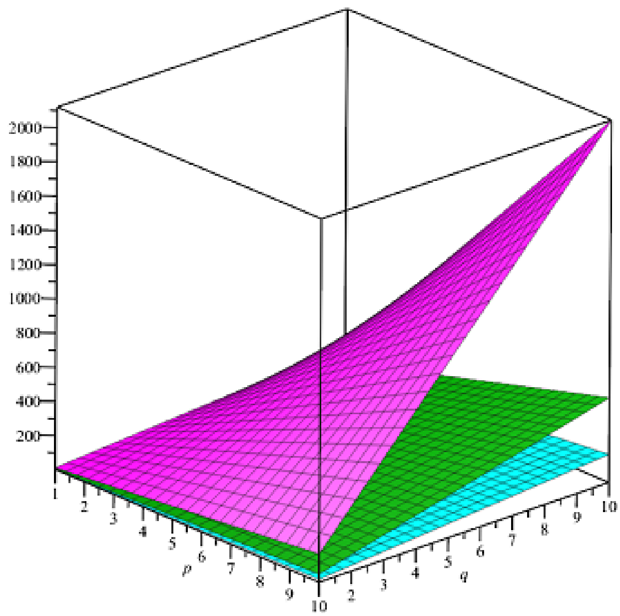

Figure 15. Pink, Green and Cyan represent inverse sum (indeg) index $ISI(G)$, harmonic $H(G)$ and modified second Zagreb ${}^mM_2(G)$ indices of Si_2C_3-*III*$[p, q]$ for different values of p and q $(1 \leq p, q \leq 10)$ respectively.

5 Conclusion

In this paper, we have considered the molecular graph of Silicon-Carbons. Instead of calculating the various degree-based topological indices separately, we derived a closed-form of M-polynomial to calculate directly the nine related degree-based topological indices for each of the Si_2C_3-*I*$[p, q]$, Si_2C_3-*II*$[p, q]$ and Si_2C_3-*III*$[p, q]$ for different values of p and q. We can easily see that all topological indices are in increasing order as the values of p and q increase. In addition, we have plotted the M-polynomials and all the topological indices for different values of p and q for each of the Si_2C_3-*I*$[p, q]$, Si_2C_3-*II*$[p, q]$ and Si_2C_3-*III*$[p, q]$ structures for different values of p and q.

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6 Appendix: Proofs of Some of the Theorems

Proof of Theorem 3.1. As mentioned earlier that for the structure of Si_2C_3-$II[p,q]$, we have:

$$|V(Si_2C_3\text{-}II[p,q])| = 10pq \quad \text{and} \quad |E(Si_2C_3\text{-}II[p,q])| = 15pq - 3p - 3q.$$

And moreover, we can see that there are three partitions according to the degree of vertices, namely,

$$\begin{aligned} & V_1(Si_2C_3\text{-}II[p,q]) = \{u \in V(Si_2C_3\text{-}II[p,q]) : d(u) = 1\}, \\ & V_2(Si_2C_3\text{-}II[p,q]) = \{u \in V(Si_2C_3\text{-}II[p,q]) : d(u) = 2\}, \\ \text{and} \quad & V_3(Si_2C_3\text{-}II[p,q]) = \{u \in V(Si_2C_3\text{-}II[p,q]) : d(u) = 3\}. \end{aligned}$$

Table 7. Vertex partition of Si_2C_3-$II[p,q]$.

$[p,q]$	$[1,1]$	$[1,2]$	$[1,3]$	$[2,1]$	$[2,2]$	$[2,3]$	$[3,1]$	$[3,2]$	$[3,3]$	$[4,1]$	$[4,2]$	$[4,3]$
V_1	3	3	3	3	3	3	3	3	3	3	3	3
V_2	6	12	18	12	18	24	18	24	30	24	30	36
V_3	1	5	9	5	19	33	9	33	57	13	47	81

Now we use the computed values Table 7 and MATLAB software for generalizing the formulas for the number of such vertices, given as: $|V_1(Si_2C_3\text{-}II[p,q])| = 3$, $|V_2(Si_2C_3\text{-}II[p,q])| = 6(p+q-1)$ and $V_3(Si_2C_3\text{-}II[p,q]) = 10pq - 6p - 6q + 3$ Also, we divide the edge set of Si_2C_3-$II[p,q]$ into five disjoint parts based on the degrees of end vertices of each edge, as follows:

$$\begin{aligned} & E_1 = E_{\{1,2\}} = \{e = uv \in E(Si_2C_3\text{-}II[p,q]) : d(u) = 1, d(v) = 2\}, \\ & E_2 = E_{\{1,3\}} = \{e = uv \in E(Si_2C_3\text{-}II[p,q]) : d(u) = 1, d(v) = 3\}, \\ & E_3 = E_{\{2,2\}} = \{e = uv \in E(Si_2C_3\text{-}II[p,q]) : d(u) = 2, d(v) = 2\}, \\ & E_4 = E_{\{2,3\}} = \{e = uv \in E(Si_2C_3\text{-}II[p,q]) : d(u) = 2, d(v) = 3\}, \\ \text{and} \quad & E_5 = E_{\{3,3\}} = \{e = uv \in E(Si_2C_3\text{-}II[p,q]) : d(u) = 3, d(v) = 3\}. \end{aligned}$$

From the molecular graph of Si_2C_3-$II[p,q]$, we can observe that $|E_1| = 2$, $|E_2| = 1$, $|E_3| = 2p + 2q$, $|E_4| = 8p + 8q - 14$, and $|E_5| = 15pq - 13p - 13q + 11$. Therefore by definition, the

M-polynomial of Si_2C_3-*II*$[p,q]$ is

$$\begin{aligned}
&M(Si_2C_3\text{-}II[p,q];x,y)\\
&=\sum_{i\leq j} m_{i,j}x^iy^j, \quad \text{where } \ i,j\in\{1,2,3\}\\
&=\sum_{1\leq 2} m_{1,2}x^1y^2+\sum_{1\leq 3} m_{1,3}x^1y^3+\sum_{2\leq 2} m_{2,2}x^2y^2+\sum_{2\leq 3} m_{2,3}x^2y^3+\sum_{3\leq 3} m_{3,3}x^3y^3\\
&=\sum_{uv\in E_1(Si_2C_3\text{-}II[p,q])} m_{1,2}x^1y^2+\sum_{uv\in E_2(Si_2C_3\text{-}II[p,q])} m_{1,3}x^1y^3+\sum_{uv\in E_3(Si_2C_3\text{-}II[p,q])} m_{2,2}x^2y^2+\\
&\quad\sum_{uv\in E_4(Si_2C_3\text{-}II[p,q])} m_{2,3}x^2y^3+\sum_{uv\in E_5(Si_2C_3\text{-}II[p,q])} m_{3,3}x^3y^3\\
&=|E_{\{1,2\}}|x^1y^2+|E_{\{1,3\}}|x^1y^3+|E_{\{2,2\}}|x^2y^2+|E_{\{2,3\}}|x^2y^3+|E_{\{3,3\}}|x^3y^3\\
&=2xy^2+xy^3+(2p+2q)x^2y^2+(8p+8q-14)x^2y^3+(15pq-13p-13q+11)x^3y^3.
\end{aligned}$$

□

Proof of Theorem 3.2. As computed in Theorem 3.1, the M-polynomial for Si_2C_3-*II*$[p,q]$ is $M(Si_2C_3\text{-}II[p,q];x,y)=2xy^2+xy^3+(2p+2q)x^2y^2+(8p+8q-14)x^2y^3+(15pq-13p-13q+11)x^3y^3$.
For notational simplicity, we write $f(x,y)=M(Si_2C_3\text{-}II[p,q];x,y)$. Therefore,

- $D_x(f(x,y))=2xy^2+xy^3+2(2p+2q)x^2y^2+2(8p+8q-14)x^2y^3+3(15pq-13p-13q+11)x^3y^3$,
- $D_y(f(x,y))=4xy^2+3xy^3+2(2p+2q)x^2y^2+3(8p+8q-14)x^2y^3+3(15pq-13p-13q+11)x^3y^3$,
- $D_yD_x(f(x,y))=4xy^2+3xy^3+4(2p+2q)x^2y^2+6(8p+8q-14)x^2y^3+9(15pq-13p-13q+11)x^3y^3$,
- $S_x(f(x,y))=2xy^2+xy^3+\frac{1}{2}(2p+2q)x^2y^2+\frac{1}{2}(8p+8q-14)x^2y^3+\frac{1}{3}(15pq-13p-13q+11)x^3y^3$,
- $S_y(f(x,y))=xy^2+\frac{1}{3}xy^3+\frac{1}{2}(2p+2q)x^2y^2+\frac{1}{3}(8p+8q-14)x^2y^3+\frac{1}{3}(15pq-13p-13q+11)x^3y^3$,
- $S_xS_y(f(x,y))=xy^2+\frac{1}{3}xy^3+\frac{1}{4}(2p+2q)x^2y^2+\frac{1}{6}(8p+8q-14)x^2y^3+\frac{1}{9}(15pq-13p-13q+11)x^3y^3$,
- $D_x^\alpha D_y^\alpha(f(x,y))=2^{\alpha+1}xy^2+3^\alpha xy^3+2^{2\alpha}(2p+2q)x^2y^2+2^\alpha 3^\alpha(8p+8q-14)x^2y^3+3^{2\alpha}(15pq-13p-13q+11)x^3y^3$,
- $D_xS_y(f(x,y))=xy^2+\frac{1}{3}xy^3+(2p+2q)x^2y^2+\frac{2}{3}(8p+8q-14)x^2y^3+(15pq-13p-13q+11)x^3y^3$,
- $D_yS_x(f(x,y))=4xy^2+\frac{1}{3}xy^3+(2p+2q)x^2y^2+\frac{3}{2}(8p+8q-14)x^2y^3+(15pq-13p-13q+11)x^3y^3$,
- $S_x^\alpha S_y^\alpha(f(x,y))=\frac{2}{2^\alpha}xy^2+\frac{1}{3^\alpha}xy^3+\frac{1}{2^{2\alpha}}(2p+2q)x^2y^2+\frac{1}{2^\alpha 3^\alpha}(8p+8q-14)x^2y^3+\frac{1}{3^{2\alpha}}(15pq-13p-13q+11)x^3y^3$,
- $S_xJ(f(x,y))=\frac{2}{3}x^3+\frac{1}{4}x^4+\frac{1}{4}(2p+2q)x^4+\frac{1}{5}(8p+8q-14)x^5+\frac{1}{6}(15pq-13p-13q+11)x^6$,
- $S_xJD_xD_y(f(x,y))=\frac{4}{3}x^3+\frac{3}{4}x^4+(2p+2q)x^4+\frac{6}{5}(8p+8q-14)x^5+\frac{9}{6}(15pq-13p-13q+11)x^6$,
- $S_x^3Q_{-2}JD_x^3D_y^3(f(x,y))=2^4x+\frac{3^3}{2^3}x^2+2^3(2p+2q)x^2+2^3(8p+8q-14)x^3+\frac{3^6}{4^3}(15pq-13p-13q+11)x^4$.

Hence, the degree-based topological indices of the $Si_2C_3\text{-}II[p,q]$ based on the derivation formulas mentioned in Table 3 are as follows.

1. First Zagreb Index:
$M_1(Si_2C_3\text{-}II[p,q]) = (D_x + D_y)(f(x,y))|_{x=y=1} = 90pq - 30p - 30q + 6.$
2. Second Zagreb Index:
$M_2(Si_2C_3\text{-}II[p,q]) = (D_x D_y)(f(x,y))|_{x=y=1} = 135pq - 61p - 61q + 22.$
3. Modified Second Zagreb Index:
${}^m M_2(Si_2C_3\text{-}II[p,q]) = (S_x S_y)(f(x,y))|_{x=y=1} = \frac{5}{3}pq + \frac{7}{18}p + \frac{7}{18}q + \frac{2}{9}.$
4. General Randić Index:
$R_\alpha(Si_2C_3\text{-}II[p,q]) = (D_x^\alpha D_y^\alpha)(f(x,y))|_{x=y=1} = 2^{\alpha+1} + 3^\alpha + 2^{2\alpha}(2p+2q) + 2^\alpha 3^\alpha(8p + 8q - 14) + 3^{2\alpha}(15pq - 13p - 13q + 11).$
5. Inverse Randić Index:
$RR_\alpha(Si_2C_3\text{-}II[p,q]) = (S_x^\alpha S_y^\alpha)(f(x,y))|_{x=y=1} = \frac{2}{2^\alpha} + \frac{1}{3^\alpha} + \frac{1}{2^{2\alpha}}(2p+2q) + \frac{1}{2^\alpha 3^\alpha}(8p + 8q - 14) + \frac{1}{3^{2\alpha}}(15pq - 13p - 13q + 11).$
6. Symmetric Division (Deg) Index:
$SDD(Si_2C_3\text{-}II[p,q]) = (D_x S_y + D_y S_x)(f(x,y))|_{x=y=1} = 30pq - \frac{14}{3}p - \frac{14}{3}q.$
7. Harmonic Index:
$H(Si_2C_3\text{-}II[p,q]) = 2S_x J(f(x,y))|_{x=1} = 5pq - \frac{2}{15}p - \frac{2}{15}q - \frac{1}{10}.$
8. Inverse Sum (Indeg) Index:
$ISI(Si_2C_3\text{-}II[p,q]) = S_x J D_x D_y(f(x,y))|_{x=1} = \frac{45}{2}pq - \frac{79}{10}p - \frac{79}{10}q + \frac{107}{60}.$
9. Augmented Zagreb Index:
$AZ(Si_2C_3\text{-}II[p,q]) = S_x^3 Q_{-2} J D_x^3 D_y^3(f(x,y))|_{x=1} = \frac{10935}{64}pq - \frac{4357}{64}p - \frac{4357}{64}q + \frac{2091}{64}.$

□

Proof of Theorem 4.1. As mentioned earlier that for the structure of $Si_2C_3\text{-}III[p,q]$, we have:

$$|V(Si_2C_3\text{-}III[p,q])| = 10pq \quad \text{and} \quad |E(Si_2C_3\text{-}III[p,q])| = 15pq - 2p - 3q$$

And moreover, we can see that there are three partitions according to the degree of vertices, namely,

$$V_1(Si_2C_3\text{-}III[p,q]) = \{u \in V(Si_2C_3\text{-}III[p,q]) : d(u) = 1\},$$
$$V_2(Si_2C_3\text{-}III[p,q]) = \{u \in V(Si_2C_3\text{-}III[p,q]) : d(u) = 2\},$$
$$\text{and} \quad V_3(Si_2C_3\text{-}III[p,q]) = \{u \in V(Si_2C_3\text{-}III[p,q]) : d(u) = 3\}.$$

Table 8. Vertex partition of $Si_2C_3\text{-}III[p,q]$.

$[p,q]$	$[1,1]$	$[1,2]$	$[1,3]$	$[2,1]$	$[2,2]$	$[2,3]$	$[3,1]$	$[3,2]$	$[3,3]$	$[4,1]$	$[4,2]$	$[4,3]$
V_1	2	2	2	2	2	2	2	2	2	2	2	2
V_2	6	9	12	10	13	16	14	17	20	18	21	24
V_3	2	9	16	8	25	42	14	41	68	20	57	94

Now we use the computed values Table 8 and MATLAB software for generalizing the formulas for the number of such vertices given as: $|V_1(Si_2C_3\text{-}III[p,q])| = 2$, $|V_2(Si_2C_3\text{-}III[p,q])| = 4p + 3q - 1$ and $V_3(Si_2C_3\text{-}III[p,q]) = 10pq - 4p - 3q - 1$ Also, we divide the edge set of $Si_2C_3\text{-}III[p,q]$ into four disjoint parts based on the end vertices of each edge, as follows:

$$E_1 = E_{\{1,3\}} = \{e = uv \in E(Si_2C_3\text{-}III[p,q]) : d(u) = 1, d(v) = 3\},$$
$$E_2 = E_{\{2,2\}} = \{e = uv \in E(Si_2C_3\text{-}III[p,q]) : d(u) = 2, d(v) = 2\},$$
$$E_3 = E_{\{2,3\}} = \{e = uv \in E(Si_2C_3\text{-}III[p,q]) : d(u) = 2, d(v) = 3\},$$
$$\text{and} \quad E_4 = E_{\{3,3\}} = \{e = uv \in E(Si_2C_3\text{-}III[p,q]) : d(u) = 3, d(v) = 3\}.$$

From the molecular graph of Si_2C_3-*III*$[p,q]$, we can observe that $|E_1| = 2$, $|E_2| = 2q+2$, $|E_3| = 8p+8q-12$, and $|E_4| = 15pq-10p-13q+8$. Also Molecular graph of Si_2C_3-*III*$[p,q]$ does not have any edge uv such that $d(u) = 1$, $d(v) = 1$ and also $d(u) = 1$,$d(v) = 2$ as a consequence $|E_{\{1,1\}}| = 0$ and $|E_{\{1,2\}}| = 0$.

Therefore by definition, the M-polynomial of Si_2C_3-*III*$[p,q]$ is

$$\begin{aligned}
&M(Si_2C_3\text{-}\mathit{III}[p,q];x,y)\\
&=\sum_{i\le j} m_{i,j}x^iy^j, \quad \text{where } i,j\in\{1,2,3\}\\
&=\sum_{1\le 3} m_{1,3}x^1y^3+\sum_{2\le 2} m_{2,2}x^2y^2+\sum_{2\le 3} m_{2,3}x^2y^3+\sum_{3\le 3} m_{3,3}x^3y^3\\
&=\sum_{uv\in E_1(Si_2C_3\text{-}\mathit{III}[p,q])} m_{1,3}x^1y^3+\sum_{uv\in E_2(Si_2C_3\text{-}\mathit{III}[p,q])} m_{2,2}x^2y^2+\sum_{uv\in E_3(Si_2C_3\text{-}\mathit{III}[p,q])} m_{2,3}x^2y^3+\\
&\quad\sum_{uv\in E_4(Si_2C_3\text{-}\mathit{III}[p,q])} m_{3,3}x^3y^3\\
&=|E_{\{1,3\}}|x^1y^3+|E_{\{2,2\}}|x^2y^2+|E_{\{2,3\}}|x^2y^3+|E_{\{3,3\}}|x^3y^3\\
&=2xy^3+(2q+2)x^2y^2+(8p+8q-12)x^2y^3+(15pq-10p-13q+8)x^3y^3.
\end{aligned}$$

□

Proof of Theorem 4.2. As computed in Theorem 4.1, the M-polynomial for Si_2C_3-*III*$[p,q]$ is $M(Si_2C_3\text{-}\mathit{III}[p,q];x,y) = 2xy^3+(2q+2)x^2y^2+(8p+8q-12)x^2y^3+(15pq-10p-13q+8)x^3y^3$. For notational simplicity, we write $f(x,y) = M(Si_2C_3\text{-}\mathit{III}[p,q];x,y)$. Therefore,

- $D_x(f(x,y)) = 2xy^3+(2(2q+2)x^2y^2+2(8p+8q-12)x^2y^3+3(15pq-10p-13q+8)x^3y^3$,
- $D_y(f(x,y)) = 6xy^3+2(2q+2)x^2y^2+(8p+8q-12)x^2y^3+3(15pq-10p-13q+8)x^3y^3$,
- $D_yD_x(f(x,y)) = 6xy^3+4(2q+2)x^2y^2+6(8p+8q-12)x^2y^3+9(15pq-10p-13q+8)x^3y^3$,
- $S_x(f(x,y)) = 2xy^3+\frac{1}{2}(2q+2)x^2y^2+\frac{1}{2}(8p+8q-12)x^2y^3+\frac{1}{3}(15pq-10p-13q+8)x^3y^3$,
- $S_y(f(x,y)) = \frac{2}{3}xy^3+\frac{1}{2}(2q+2)x^2y^2+\frac{1}{3}(8p+8q-12)x^2y^3+\frac{1}{3}(15pq-10p-13q+8)x^3y^3$,
- $S_xS_y(f(x,y)) = \frac{2}{3}xy^3+\frac{1}{4}(2q+2)x^2y^2+\frac{1}{6}(8p+8q-12)x^2y^3+\frac{1}{9}(15pq-10p-13q+8)x^3y^3$,
- $D_x^\alpha D_y^\alpha(f(x,y)) = 2\,3^\alpha xy^3+2^{2\alpha}(2q+2)x^2y^2+2^\alpha 3^\alpha(8p+8q-12)x^2y^3+3^{2\alpha}(15pq-10p-13q+8)x^3y^3$,
- $D_xS_y(f(x,y)) = \frac{2}{3}xy^3+(2q+2)x^2y^2+\frac{2}{3}(8p+8q-12)x^2y^3+(15pq-10p-13q+8)x^3y^3$,
- $D_yS_x(f(x,y)) = 6xy^3+(2q+2)x^2y^2+\frac{3}{2}(8p+8q-12)x^2y^3+(15pq-10p-13q+8)x^3y^3$,
- $S_x^\alpha S_y^\alpha(f(x,y)) = \frac{2}{3^\alpha}xy^3+\frac{1}{2^{2\alpha}}(2q+2)x^2y^2+\frac{1}{2^\alpha 3^\alpha}(8p+8q-12)x^2y^3+\frac{1}{3^{2\alpha}}(15pq-10p-13q+8)x^3y^3$,
- $S_xJ(f(x,y)) = \frac{1}{2}x^4+\frac{1}{4}(2q+2)x^4+\frac{1}{5}(8p+8q-12)x^5+\frac{1}{6}(15pq-10p-13q+8)x^6$,
- $S_xJD_xD_y(f(x,y)) = \frac{3}{2}x^4+(2q+2)x^4+\frac{6}{5}(8p+8q-12)x^5+\frac{3}{2}(15pq-10p-13q+8)x^6$,
- $S_x^3Q_{-2}JD_x^3D_y^3(f(x,y)) = \frac{2\,3^3}{2^3}x^2+2^3(2q+2)x^2+2^3(8p+8q-12)x^3+\frac{3^6}{4^3}(15pq-10p-13q+8)x^4$.

Hence, the degree-based topological indices of the Si_2C_3-*III*$[p,q]$ based on the derivation formulas mentioned in Table 3 are as follows:

1. First Zagreb Index:
$M_1(Si_2C_3\text{-}\mathit{III}[p,q]) = (D_x+D_y)(f(x,y))|_{x=y=1} = 90pq-20p-30q+4$.
2. Second Zagreb Index:
$M_2(Si_2C_3\text{-}\mathit{III}[p,q]) = (D_xD_y)(f(x,y))|_{x=y=1} = 135pq-42p-61q+14$.

3. Modified Second Zagreb Index:
$^{m}M_2(Si_2C_3\text{-}III[p,q]) = (S_xS_y)(f(x,y))|_{x=y=1} = \frac{5}{3}pq + \frac{2}{9}p - \frac{5}{18}q + \frac{1}{18}$.
4. General Randić Index:
$R_\alpha(Si_2C_3\text{-}III[p,q]) = (D_x^\alpha D_y^\alpha)(f(x,y))|_{x=y=1} = 2\ 3^\alpha + 2^{2\alpha}(2q+2) + 2^\alpha 3^\alpha(8p+8q-12) + 3^{2\alpha}(15pq-10p-13q+8)$.
5. Inverse Randić Index:
$RR_\alpha(Si_2C_3\text{-}III[p,q]) = (S_x^\alpha S_y^\alpha)(f(x,y))|_{x=y=1} = \frac{2}{3^\alpha} + \frac{1}{2^{2\alpha}}(2q+2) + \frac{1}{2^\alpha 3^\alpha}(8p+8q-12) + \frac{1}{3^{2\alpha}}(15pq-10p-13q+8)$.
6. Symmetric Division (Deg) Index:
$SDD(Si_2C_3\text{-}III[p,q) = (D_xS_y + D_yS_x)(f(x,y))|_{x=y=1} = 30pq - \frac{8}{3}p - \frac{14}{3}q + \frac{2}{3}$.
7. Harmonic Index:
$H(Si_2C_3\text{-}III[p,q]) = 2S_xJ(f(x,y))|_{x=1} = 5pq - \frac{2}{15}p - \frac{2}{15}q - \frac{2}{15}$.
8. Inverse Sum (Indeg) Index:
$ISI(Si_2C_3\text{-}III[p,q]) = S_xJD_xD_y(f(x,y))|_{x=1} = \frac{45}{2}pq - \frac{27}{5}p - \frac{79}{10}q + \frac{11}{5}$.
9. Augmented Zagreb Index:
$AZ(Si_2C_3\text{-}III[p,q]) = S_x^3Q_{-2}JD_x^3D_y^3(f(x,y))|_{x=1} = \frac{10935}{64}pq - \frac{1597}{32}p - \frac{4357}{64}q + \frac{143}{8}$.

□

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