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On the Vertex Degree Polynomial of Some Classes of Silicon- Carbon

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Abstract
Graph polynomials are helpful in measuring the structural information of networks us- combinatorial graph invariants. Also, the graph polynomials are used for the characterization of graphs. Using graph polynomials, many problems in graph theory and discrete math- ematics can be solved efficiently. These polynomials have been found very useful in disciplines related to engineering, information science, mathematical chemistry, etc. The application of graph theory in chemical and molecular structure research has far exceeded people's expectations, and it has recently grown exponentially. In the molecular graph, atoms are represented by vertices and bonds by edges. Topological indices help us to predict many physicochemical properties of the concerned molecular compound. Hanan Ahmed et al [11] introduced a new graph polynomial known as vertex degree polynomial.In this article, we compute first and second Zagreb indices for silicon-carbon $Si_2C_3 - I[p, q]$ and $Si_2C_3 - II[p, q]$ second via vertex degree polynomial.

Keywords: Vertex Degree Polynomial, Zagreb Indices, Silicon-Carbon, Double Silicon-Carbon, Strong Double of Silicon Carbide

2010 Math. Subject Classification: 05C05, 05C07, 05C35

1. INTRODUCTION

Silicon is a semiconductor material with several advantages over other similar materials, such as its low cost, nontoxicity, and almost limitless availability, as well as many years of ex-practice in its purification, manufacture, and device development. It is used in practice for all of the most recent electrical products. Graph theory can be used to depict a chemical structure, with vertices representing atoms and edges representing chemical bonds. For quite a few years, Chemical Graph theory has been assuming an imperative part in mathematical chemistry, quantitative structure-activity relationships (QSAR) and structure-property re townships (QSPR), and closeness/assorted variety investigation of sub-atomic libraries [28]. Essentially, molecular descriptors utilized as a part of these research fields are obtained from the graph of molecule ule, which speaks to use some method to calculate numbers associated with molecular graph then using these number to describe the molecule. A network is a connected graph that has no multiple edges and loops. The number of vertices that are connected to a fixed vertex f is called the degree of f. The distance between two vertices is the length of the shortest path between them. The concept of valence in chemistry and the concept of degree in a graph is somehow closely related. For details on bases of graph theory, we refer to the book [29]. A graph can be recognized by a connection table, polynomial, sequence of numbers, matrix or numeric number which is also called a topological index that represents the whole graph. A topological index got special attention as it predicts several pieces of information related to the molecular structure of the compounds for more discussion see [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]. Till now, more than 140 topological indices are defined, but none of them is enough to determine all physicochemical properties of the understudy molecule. However, these indices to- together can do this to some extent. Later, in 1975, Milan Randic introduced Randic index [26]. In 2022 Hanan Ahmed et al introduced domination topological indices [12, 25]. Many papers [13, 16, 17, 18, 19, 20, 21, 22, 23, 27] are written on this simple graph invariant. In 1972, Gutman introduced the first and the second Zagreb indices in [24].

$$M_1(G) = \sum_{f \in V(G)} d^2(f).$$

$$M_2(G) = \sum_{fg \in E(G)} d(f)d(g).$$

In 2023 [11], Hanan Ahmed et al. introduced new graph polynomial known as vertex degree polynomial defined as:

$$VD(G, x) = \sum_{fg \in E(G)} d(f)x^{d(g)}.$$

Using this new polynomial one can calculate the first and second Zagreb indices. For more comprehensive and detailed study on vertex degree polynomial of graphs, we mention the fol- lowing articles [14, 15] for readers. The authors obtained that the derivative of $V D(G, x)$ at x = 1 is two times the second Zagreb index $M_2(G)$ and the sum of coefficients of the vertex degree polynomial is equal to first Zagreb index $M\ 1(G)$. This result opens a new gateway to the study of the first and second Zagreb indices and their implications.

Theorem 1.1. *[11] Let G be a graph with vertex degree polynomial $V D(G, x)$. Then*

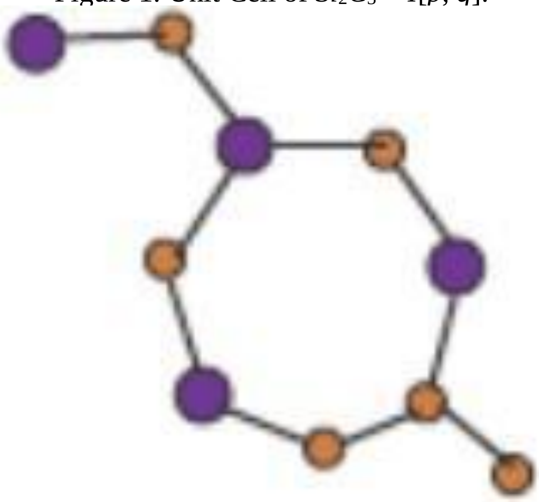
$D_x(V D(G, x))|_{x=1} = 2M_2(G)$,
$(V D(G, x))|_{x=1} = M_1(G)$.

2. COMPUTATIONAL RESULTS

In this section we give our main results.

2.1 Results for Silicon-Carbon $Si_2C_3 - I[p, q]$

Figure 1. Unit Cell of $Si_2C_3 - I[p, q]$.



Theorem 2.1. *Let $Si_2C_3 - I[p, q]$ be the Silicon Carbide. Then*
$V D(Si_2C_3 - I[p, q], x) = x^3 + x^2 + 5x + 4x^2(p + 2q) + (2x^3 + 3x^2)\ 6p - 1 + 8(q - 1)$

$+ 6x^3\, 15pq - 9p - 13q + 7$.

Proof. From the graph of $Si_2C_3 - I[p, q]$ (Figures 1,2 and 3), we can see that the total number of vertices are $10pq$, and total number of edges are $15pq - 2p - 3q$. The edge set of $Si_2C_3 - I[p, q]$ with $p, q \geq 1$ has following five partitions:

$E^2(Si_2C_3 - I[p, q]) = \{e = fg \in E(Si_2C_3 - I[p, q]) : d(f) = 1, d(g) = 2\}$.
$E^3(Si_2C_3 - I[p, q]) = \{e = fg \in E(Si_2C_3 - I[p, q]) : d(f) = 1, d(g) = 3\}$.
$E^2(Si_2C_3 - I[p, q]) = \{e = fg \in E(Si_2C_3 - I[p, q]) : d(f) = 2, d(g) = 2\}$.
2

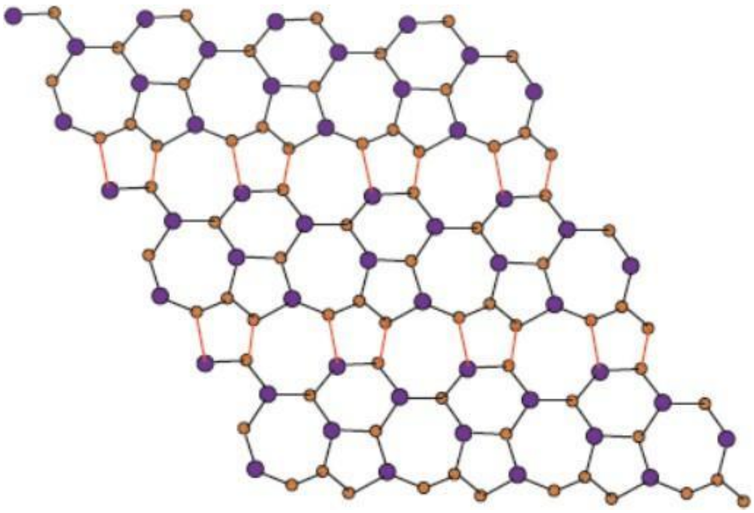


Figure 2. Sheet of $Si_2C_3 - I[p, q]$ for p = 4 and q = 3.

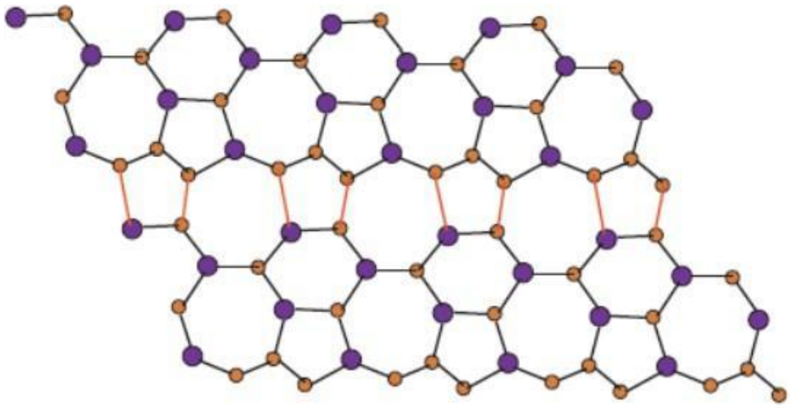


Figure 3. Sheet of $Si_2C_3 - I[p, q]$ for p = 4 and q = 2.

$E^3(Si_2C_3 - I[p, q]) = \{e = fg \in E(Si_2C_3 - I[p, q]) : d(f) = 2, d(g) = 3\}$.
$E^3(Si_2C_3 - I[p, q]) = \{e = fg \in E(Si_2C_3 - I[p, q]) : d(f) = 3, d(g) = 3\}$.
3

Now,

$$|E_1^2(Si_2C_3 - I[p,q])| = 1,$$

$$|E_1^3(Si_2C_3 - I[p,q])| = 1,$$

$$|E_2^2(Si_2C_3 - I[p,q])| = p + 2q,$$

$$Si_2C_3 - I[p,q])| = 6p - 1 + 8(q - 1),$$

Hence,

$$\begin{aligned} VD(Si_2C_3 - I[p,q], x) &= \sum_{fg \in E(G)} d(f)x^{d(g)} \\ &= (1x^2 + 2x)1 + (1x^3 + 3x)1 + (2x^2 + 2x^2)(p + 2q) \\ &+ (2x^3 + 3x^2)(6p - 1 + 8(q - 1)) + (3x^3 + 3x^3)(15pq - 9p - 13q + 7) \\ &= x^3 + x^2 + 5x + 4x^2(p + 2q) + (2x^3 + 3x^2)\big(6p - 1 + 8(q - 1)\big) \\ &+ 6x^3\big(15pq - 9p - 13q + 7\big). \end{aligned}$$

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

$M_1(Si_2C_3 - I[p, q]) = 7 + 4(p + 2q) + 5(6p - 1 + 8(q - 1)) + 6(15pq - 9p - 13q + 7)$. $M_2(Si_2C_3 - I[p, q]) = 5 + 4(p + 2q) + 6(6p - 1 + 8(q - 1)) + 9(15pq - 9p - 13q + 7)$.

Proof. We have, if $Si_2C_3 - I[p, q]$ be the Silicon Carbide, then
$V D(Si_2C_3 - I[p, q], x) = x^3 + x^2 + 5x + 4x^2(p + 2q) + (2x^3 + 3x^2)\ 6p - 1 + 8(q - 1)$
$+ 6x^3\ 15pq - 9p - 13q + 7$.

Hence, from Theorem 1.1, we get

$$\begin{aligned} M_1(Si_2C_3 - I[p, q]) &= V D(Si_2C_3 - I[p, q], x)|_{x=1} \\ &= 7 + 4(p + 2q) + 5(6p - 1 + 8(q - 1)) + 6(15pq - 9p - 13q + 7). \end{aligned}$$

And,

$$\begin{aligned} 2M_2(Si_2C_3 - I[p, q]) &= D_x(V D(G, x))|_{x=1} \\ &= 2x + 3x^2 + 5 + 8x(p + 2q) + (6x^2 + 6x)(6p - 1 + 8(q - 1)) \\ &\quad + 18x^2(15pq - 9p - 13q + 7) \\ &= 10 + 8(p + 2q) + 12(6p - 1 + 8(q - 1)) + 18(15pq - 9p - 13q + 7). \end{aligned}$$

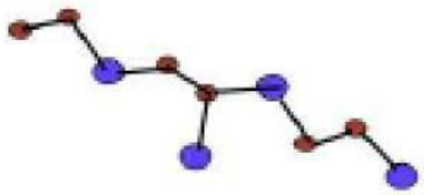


Figure 4. Unit Cell of $Si_2C_3 - II[p, q]$.

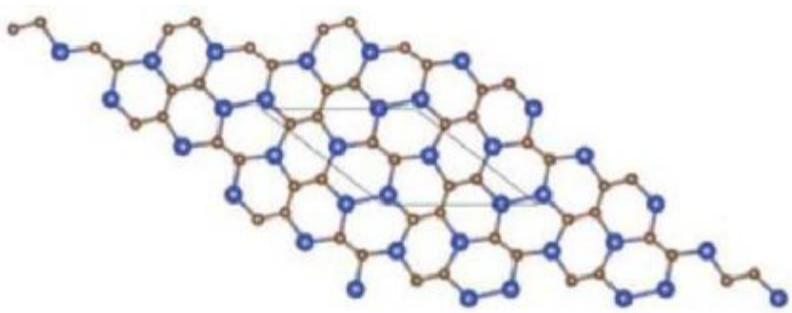


Figure 5. Sheet of $Si_2C_3 - II[p, q]$ for p = 3 and q = 3.

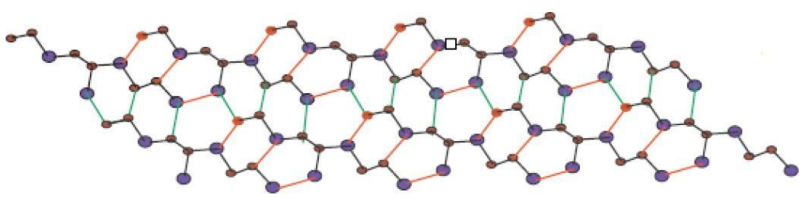


Figure 6. Sheet of $Si_2C_3 - II[p, q]$ for p = 5 and q = 2.

2.2 Results for Silicon-Carbon $Si_2C_3 - II[p, q]$

Theorem 2.3. *Let $Si_2C_3 - II[p, q]$ be the Silicon Carbide. Then*
$V D(Si_2C_3 - II[p, q], x) = x^3 + 2x^2 + 7x + 4x^2(2p + 2q) + (2x^3 + 3x^2)(8p + 8q - 14)$
$+ 6x^3(15pq - 13p - 13q + 11)$.

Proof. Let G be the graph of $Si_2C_3 - II[p, q]$. From the graph of $Si_2C_3 - II[p, q]$ (Figures 4–6), we can see that the total number of vertices are $10pq$ and total number of edges are $15pq-3p-3q$. The edge set of $Si_2C_3 - II[p, q]$ with $p, q \geq 1$ has following five partitions:

$$E_1^2(Si_2C_3 - II[p,q]) = \{e = fg \in E(Si_2C_3 - II[p,q]) : d(f) = 1, d(g) = 2\}.$$

$$E_1^3(Si_2C_3 - II[p,q]) = \{e = fg \in E(Si_2C_3 - II[p,q]) : d(f) = 1, d(g) = 3\}.$$

$$E_2^2(Si_2C_3 - II[p,q]) = \{e = fg \in E(Si_2C_3 - II[p,q]) : d(f) = 2, d(g) = 2\}.$$

$$E_2^3(Si_2C_3 - II[p,q]) = \{e = fg \in E(Si_2C_3 - II[p,q]) : d(f) = 2, d(g) = 3\}.$$

$$E_3^3(Si_2C_3 - II[p,q]) = \{e = fg \in E(Si_2C_3 - II[p,q]) : d(f) = 3, d(g) = 3\}.$$

Now,

$$|E_1^2(Si_2C_3 - II[p,q])| = 2,$$
$$|E_1^3(Si_2C_3 - II[p,q])| = 1,$$
$$|E_2^2(Si_2C_3 - II[p,q])| = 2p + 2q,$$
$$|E_2^3(Si_2C_3 - II[p,q])| = 8p + 8q - 14,$$
$$|E_3^3(Si_2C_3 - II[p,q])| = 15pq - 13p - 13q + 11.$$

Hence,

$$\begin{aligned}
VD(Si_2C_3 - II[p,q], x) &= \sum_{fg \in E(Si_2C_3 - II[p,q])} d(f) x^{d(g)} \\
&= (x^2 + 2x)2 + (x^3 + 3x) \times 1 + (2x^2 + 2x^2)(2p + 2q) \\
&+ (2x^x + 3x^2)(8p + 8q - 14) \\
&+ (3x^3 + 3x^3)(15pq - 13p - 13q + 11) \\
&= x^3 + 2x^2 + 7x + 4x^2(2p + 2q) + (2x^3 + 3x^2)(8p + 8q - 14) \\
&+ 6x^3(15pq - 13p - 13q + 11).
\end{aligned}$$

Theorem 2.4. *Let $Si_2C_3 - II[p,q]$ be the Silicon Carbide. Then*

$$M_1(Si_2C_3 - II[p,q]) = 10 + 4(2p+2q) + 5(8p+8q-14) + 6(15pq-13p-13q+11).$$

$$M_2(Si_2C_3 - II[p,q]) = 7 + 4(2p+2q) + 6(8p+8q-14) + 9(15pq-13p-13q+11).$$

Proof. We have, if $Si_2C_3 - II[p,q]$ be the Silicon Carbide, then

$$VD(Si_2C_3 - II[p,q],x) = x^3 + 2x^2 + 7x + 4x^2(2p+2q) + (2x^3+3x^2)(8p+8q-14) + 6x^3(15pq-13p-13q+11).$$

Hence, from Theorem 1.1, we get

$$\begin{aligned} M_1(Si_2C_3 - II[p,q]) &= VD(Si_2C_3 - II[p,q],x)|_{x=1} \\ &= 10 + 4(2p+2q) + 5(8p+8q-14) + 6(15pq-13p-13q+11). \end{aligned}$$

And,

$2M_2(Si_2C_3 - II[p, q]) = D_x(VD(Si_2C_3 - II[p, q], x))|_{x=1}$
$= 3x^2 + 4x + 7 + 8x(2p + 2q) + (6x^2 + 6x)(8p + 8q - 14)$
$+ 18x^2(15pq - 13p - 13q + 11)$
$= 14 + 8(2p + 2q) + 12(8p + 8q - 14) + 18(15pq - 13p - 13q + 11).$

3. CONCLUSION

Mathematical chemistry provides useful tools like polynomials and functions that rely on information contained in the symmetry of graphs of chemical compounds and very helpful for the prediction of the understudy molecular compound and its characteristics without the usage of quantum mechanics. The findings of this study can help to understand the physical features and biological activities of silicon carbide. In this paper, we investigated the topological indices namely; first and second Zagreb indices for silicon-carbon $Si_2C_3 - I[p, q]$ and $Si_2C_3 - II[p, q]$ second via vertex degree polynomial.

Conflicts of Interest

The authors declare that they have no conflict of interest.

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