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Multiplicative topological descriptors of Silicon carbide

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Abstract

Topological indices helps us to collect information about algebraic graphs and gives us mathematical approach to understand the properties of chemical structures. In this paper, we aim to compute multiplicative degree-based topological indices of Silicon-Carbon $Si_2C_3 - III[p,q]$ and $SiC_3 - III[p,q]$.

Keywords: Topological index, molecular graph, Silicon carbide.
AMS 2010 codes: 68R10, 81Q30, 81T15.

1 Introduction

In mathematics, graph theory is the study of graphs, which are mathematical structures used to model pairwise relations between objects. A graph in this context is made up of vertices, nodes, or points which are connected by edges, arcs, or lines. A graph may be undirected, meaning that there is no distinction between the two vertices associated with each edge, or its edges may be directed from one vertex to another; see Graph (discrete mathematics) for more detailed definitions and for other variations in the types of graph that are commonly considered. Graphs are one of the prime objects of study in discrete mathematics and found many applications in our life [1–4].

In the fields of chemical graph theory, molecular topology, and mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound [5–8]. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used for example in the development

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of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure [9–12].

In mathematical chemistry, precisely speaking, in chemical-graph-theory (CGT), a molecular graph and graph network is a simple and connected graph, in which atoms represents vertices and chemical bonds represents edges. We reserve G for simple connected graph, E for edge set and V for vertex set throughout the thesis. The degree of a vertex u of graph G is the number of vertices that are attached with u and is denoted by d_v. With the help of TIs, many properties of molecular structure can be obtained without going to lab [13]. The reality is, many research paper has been written on computation of degree-based indices and polynomials of different molecular structure and networks but only few work has been done so far on distance based indices and polynomials. In this paper, we aim to compute multiplicative degree-based TIs. Some indices related to Wiener's work are the first and second multiplicative Zagreb indices [14], respectively

$$II_1(G) = \prod_{u \in V(G)} (d_u)^2,$$

$$II_2(G) = \prod_{uv \in E(G)} d_u \cdot d_v.$$

and the Narumi-Katayama index [52]

$$NK(G) = \prod_{u \in V(G)} d_u.$$

Like the Wiener index, these types of indices are the focus of considerable research in computational chemistry [16–18]. For example, in the year 2011, Gutman in [16] characterized the multiplicative Zagreb indices for trees and determined the unique trees that obtained maximum and minimum values for $M_1(G)$ and $M_2(G)$, respectively. Wang *et al.* in [19] extended the results of Gutman to the following index for k-trees,

$$W_1^s(G) = \prod_{u \in V(G)} (d_u)^s.$$

Notice that $s = 1, 2$ is the Narumi-Katayama and Zagreb index, respectively. Based on the successful consideration of multiplicative Zagreb indices, Eliasi *et al.* [20] continued to define a new multiplicative version of the first Zagreb index as

$$II_1^*(G) = \prod_{uv \in E(G)} (d_u + d_v).$$

Furthering the concept of indexing with the edge set, the first author introduced the first and second hyper-Zagreb indices of a graph [21]. They are defined as

$$HII_1(G) = \prod_{uv \in E(G)} (d_u + d_v)^2,$$

$$HII_2(G) = \prod_{uv \in E(G)} (d_u \cdot d_v)^2.$$

In [22] Kulli *et al.* defined the first and second generalized Zagreb indices

$$MZ_1^a(G) = \prod_{uv \in E(G)} (d_u + d_v)^{\alpha},$$

$$MZ_2^a(G) = \prod_{uv \in E(G)} (d_u \cdot d_v)^{\alpha}.$$

Multiplicative sum connectivity and multiplicative product connectivity indices [23] are define as:

$$SCII(G) = \prod_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}},$$

$$PCII(G) = \prod_{uv \in E(G)} \frac{1}{\sqrt{d_u \cdot d_v}}.$$

Multiplicative atomic bond connectivity index and multiplicative Geometric arithmetic index are defined as

$$ABCII(G) = \prod_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}},$$

$$GAII(G) = \prod_{uv \in E(G)} \frac{2\sqrt{d_u \cdot d_v}}{d_u + d_v},$$

$$GA^{a}II(G) = \prod_{uv \in E(G)} \left(\frac{2\sqrt{d_u \cdot d_v}}{d_u + d_v} \right)^{\alpha}.$$

2 Silicon Carbide

In 1891, an American scientist discover Silicon Carbide. But now a days, we can produce silicon carbide artificially by silica and carbon. Till 1929, silicon carbide was known as the hardest material on earth.Its Mohs hardness rating is 9, which makes this similar to diamond. Here, we will find out reverse zagreb, hyper reverse zagreb and its polynomials for silicon carbide $Si_2C_3 - III[p,q]$ and $SiC_3 - III[p,q]$. We consider 2D SiC compounds with two different types of SiC structure based on low-energy metastable structures for each SiC. The types are $Si_2C_3 - III[p,q]$ and $SiC_3 - III[p,q]$ that denotes the lowest-energy and the second lowest energy structure respectively. The unit cell of $Si_2C_3 - III[p,q]$ is given in Figure 1. The 2D lattice graphs of $Si_2C_3 - III[5,1]$, $Si_2C_3 - III[5,2]$ and $Si_2C_3 - III[5,4]$ are shown in Figures 2,3 and 4 respectively.

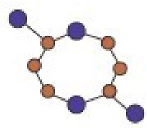

Fig. 1 Unit Cell

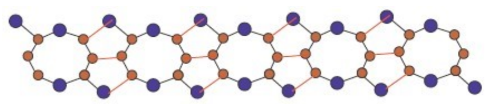

Fig. 2 $Si_2C_3 - III[5,1]$

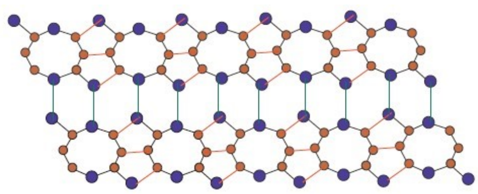

Fig. 3 $Si_2C_3 - III[5,2]$

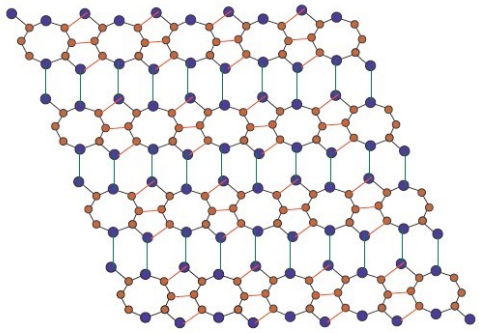

Fig. 4 $Si_2C_3 - III[5,4]$

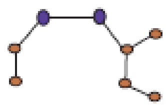

Fig. 5 Unit Cell

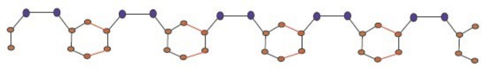

Fig. 6 $SiC_3 - III[5,1]$

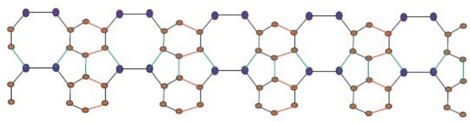

Fig. 7 $SiC_3 - III[5,2]$

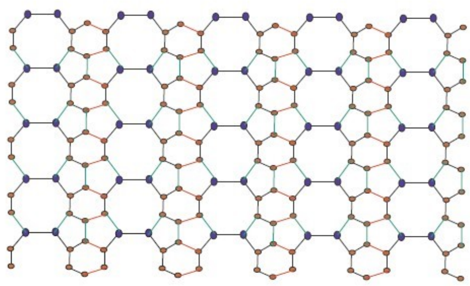

Fig. 8 $SiC_3 - III[5,4]$

3 Methodology

To compute our main results we count the number of edges of $Si_2C_3 - III[p,q]$ and $SiC_3 - III[p,q]$ by using Figures 1-4 and Figures 5-8 respectively. After that, we divide these edge sets into classes based on the degree of vertices. The Edge partition of $Si_2C_3 - III[p,q]$ is given in Table 1 and the edge partition of $SiC_3 - III(G)$ is given in Table 2. By using these edge partitions, we compute our main results.

(d_u, d_v)	Frequency
(1,3)	2
(2,2)	2p+2
(2,3)	8p+8q-12
(3,3)	15pq-10p-13q+8

Table 1 Edge partition of $Si_2C_3 - III[p,q]$

(d_u, d_v)	Frequency
(1,2)	2
(1,3)	1
(2,2)	3p+2q-3
(2,3)	6p+4q-8
(3,3)	12pq-12p-8q+8

Table 2 Edge partition of $SiC_3 - III[p,q]$

4 Main Results

In this article, we will compute some degree-based multiplicative topological indices for $Si_2C_3 - III[p,q]$ and $SiC_3 - III[p,q]$.

4.1 Multiplicative Topological Indices for Silicon Carbides $Si_2C_3 - III[p,q]$

Theorem 4.2. *Let $Si_2C_3 - III[p,q]$ be the Silicon Carbide. Then*

1. $MZ_1^{\alpha}(Si_2C_3 - III[p,q]) = (2)^{\alpha(15pq-10p-5q+16)} \times (3)^{\alpha(15pq-10p-13q+8)} \times (5)^{\alpha(8p+8q-12)}$.

2. $MZ_2^{\alpha}(Si_2C_3 - III[p,q]) = (2)^{4\alpha(2p+3q-2)} \times (3)^{6\alpha(5pq-2p-3q+1)}$.

3. $GA^{\alpha}II(Si_2C_3 - III[p,q]) = (2)^{2\alpha(6p+6q-5)} \times (3)^{\alpha(4p+4q-5)} \times (5)^{\alpha(12-8q-8p)}$.

Proof. Using edge partition given in Table 1, we have

$$\begin{aligned}
MZ_1^{\alpha}(Si_2C_3 - III[p,q]) &= \prod_{uv\varepsilon E(Si_2C_3 - III[p,q])} (d_u + d_v)^{\alpha} \\
&= (1+3)^{2\alpha} \times (2+2)^{\alpha(2q+2)} \times (2+3)^{\alpha(8p+8q-12)} \\
&\quad \times (3+3)^{\alpha(15pq-10p-13q+8)} \\
&= (2)^{\alpha(15pq-10p-5q+16)} \times (3)^{\alpha(15pq-10p-13q+8)} \times (5)^{\alpha(8p+8q-12)}.
\end{aligned}$$

$$\begin{aligned}
MZ_2^{\alpha}(Si_2C_3 - III[p,q]) &= \prod_{uv\varepsilon E(Si_2C_3 - III[p,q])} (d_u \times d_v)^{\alpha} \\
&= (1\times 3)^{2\alpha} \times (2\times 2)^{\alpha(2q+2)} \times (2\times 3)^{\alpha(8p+8q-12)} \\
&\quad \times (3\times 3)^{\alpha(15pq-10p-13q+8)} \\
&= (2)^{4\alpha(2p+3q-2)} \times (3)^{6\alpha(5pq-2p-3q+1)}.
\end{aligned}$$

$$
\begin{aligned}
GA^{\alpha}II(Si_2C_3-III[p,q]) &= \prod_{uv\varepsilon E(Si_2C_3-III[p,q])} (\frac{2\sqrt{d_u\times d_v}}{d_u+d_v})^{\alpha}\\
&= (\frac{2\sqrt{1\times 3}}{1+3})^{2\alpha}\times(\frac{2\sqrt{2\times 2}}{2+2})^{\alpha(2q+2)}\\
&\quad (\frac{2\sqrt{2\times 3}}{2+3})^{\alpha(8p+8q-12)}\times(\frac{2\sqrt{3\times 3}}{3+2})^{\alpha(15pq-10p-13q+8)}\\
&= (2)^{2\alpha(6p+6q-5)}\times(3)^{\alpha(4p+4q-5)}\times(5)^{\alpha(12-8q-8p)}.
\end{aligned}
$$

□

Theorem 4.3. *Let $Si_2C_3-III[p,q]$ be the Silicon Carbide. Then*

1. $MZ_1(Si_2C_3-III[p,q]) = II_1^* = (2)^{(15pq-10p-5q+16)}\times(3)^{(15pq-10p-13q+8)}\times(5)^{(8p+8q-12)}$.
2. $MZ_2(Si_2C_3-III[p,q]) = (2)^{4(2p+3q-2)}\times(3)^{6(5pq-2p-3q+1)}$.
3. $GAII(Si_2C_3-III[p,q]) = (2)^{2(6p+6q-5)}\times(3)^{(4p+4q-5)}\times(5)^{(12-8q-8p)}$.

Proof. Taking $\alpha=1$, in Theorem 4.2, we get our desire results. □

Theorem 4.4. *Let $S_2iC_3-III[p,q]II[p,q]$ be the Silicon Carbide. Then*

1. $HII_1(Si_2C_3-III[p,q]) = (2)^{2(15pq-10p-5q+16)}\times(3)^{2(15pq-10p-13q+8)}\times(5)^{2(8p+8q-12)}$
2. $HII_2(Si_2C_3-III[p,q]) = (2)^{8(2p+3q-2)}\times(3)^{12(5pq-2p-3q+1)}$

Proof. Taking $\alpha=2$ in Theorem 4.2, we get our desire results. □

Theorem 4.5. *Let $Si_2C_3-III[p,q]$ be the Silicon Carbide. Then*

1. $SCII(Si_2C_3-III[p,q]) = (\frac{1}{\sqrt{2}})^{(15pq-10p-5q+16)}\times(\frac{1}{\sqrt{3}})^{(15pq-10p-13q+8)}\times(\frac{1}{\sqrt{5}})^{(8p+8q-12)}$.
2. $PCII(Si_2C_3-III[p,q]) = (\frac{1}{\sqrt{2}})^{4(2p+3q-2)}\times(\frac{1}{\sqrt{3}})^{6(5pq-2p-3q+1)}$.

Proof. Taking $\alpha=-\frac{1}{2}$ in Theorem4.2, we get our desire results. □

Theorem 4.6. *Let $Si_2C_3-III[p,q]$ be the Silicon Carbide. Then*

$$ABCII(Si_2C_3-III[p,q]) = [(\frac{1}{2})^{\frac{1}{2}}]^{4p+5q-5}\times[(\frac{2}{3})]^{15pq-10p-13q+9}.$$

Proof.

$$
\begin{aligned}
GA^{\alpha}II(Si_2C_3-III[p,q]) &= \prod_{uv\varepsilon E(Si_2C_3-III[p,q])} \sqrt{\frac{d_u+d_v-2}{d_u\times d_v}}\\
&= \left(\sqrt{\frac{1+3-2}{1\times 3}}\right)^{2}\times\left(\sqrt{\frac{2+2-2}{2\times 2}}\right)^{2q+2}\\
&\quad\times\left(\sqrt{\frac{2+3-2}{2\times 3}}\right)^{(8p+8q-12)}\times\left(\sqrt{\frac{3+3-2}{3\times 3}}\right)^{(15pq-10p-13q+8)}\\
&= [(\frac{1}{2})^{\frac{1}{2}}]^{4p+5q-5}\times[(\frac{2}{3})]^{15pq-10p-13q+9}.
\end{aligned}
$$

□

4.7 Multiplicative Topological Indices for Silicon Carbides $SiC_3 - III[p,q]$

Theorem 4.8. *Let $SiC_3 - III[p,q]$ be the Silicon Carbide. Then*

1. $MZ_1^{\alpha}(SiC_3 - III[p,q]) = (2)^{\alpha(12pq+6p+4q+4)} \times (3)^{\alpha(12pq-12p-8q+10)} \times (5)^{\alpha(6p+4q-8)}$.
2. $MZ_2^{\alpha}(SiC_3 - III[p,q]) = (2)^{4\alpha(3p+2q-3)} \times (3)^{3\alpha(8pq-6p-4q+3)}$.
3. $GA^{\alpha}II(SiC_3 - III[p,q]) = (2)^{\alpha(9p+6q-10)} \times (3)^{\alpha(3p+2q-\frac{11}{2})} \times (5)^{\alpha(8-6p-4q)}$.

Proof. Using the edge partition given in Table 2, we have

$$\begin{aligned} MZ_1^{\alpha}(SiC_3 - III[p,q]) &= \prod_{uv\varepsilon E(SiC_3-III[p,q])} (d_u + d_v)^{\alpha} \\ &= (1+2)^{2\alpha} \times (1+3)^{\alpha} \times (2+2)^{\alpha(3p+2q-3)} \times (2+3)^{\alpha(6p+4q-8)} \\ &\quad \times (3+3)^{\alpha(12pq-12p-8q+8)} \\ &= (2)^{\alpha(12pq+6p+4q+4)} \times (3)^{\alpha(12pq-12p-8q+10)} \times (5)^{\alpha(6p+4q-8)}. \end{aligned}$$

$$\begin{aligned} 2.MZ_2^{\alpha}(SiC_3 - III[p,q]) &= \prod_{uv\varepsilon E(SiC_3-III[p,q])} (d_u \times d_v)^{\alpha} \\ &= (1\times 2)^{2\alpha} \times (1\times 3)^{\alpha} \times (2\times 2)^{\alpha(3p+2q-3)} \times (2\times 3)^{\alpha(6p+4q-8)} \\ &\quad \times (3\times 3)^{\alpha(12pq-12p-8q+8)} \\ &= (2)^{4\alpha(3p+2q-3)} \times (3)^{3\alpha(8pq-6p-4q+3)}. \end{aligned}$$

$$\begin{aligned} 3.GA^{\alpha}II(SiC_3 - III[p,q]) &= \prod_{uv\varepsilon E(Si_2C_3-III[p,q])} \left(\frac{2\sqrt{d_u \times d_v}}{d_u + d_v}\right)^{\alpha} \\ &= \left(\frac{2\sqrt{1\times 2}}{1+2}\right)^{2\alpha} \times \left(\frac{2\sqrt{1\times 3}}{1+3}\right)^{\alpha} \times \left(\frac{2\sqrt{2\times 2}}{2+2}\right)^{\alpha(3p+2q-3)} \\ &\quad \left(\frac{2\sqrt{2\times 3}}{2+3}\right)^{\alpha(6p+4q-8)} \times \left(\frac{2\sqrt{3\times 3}}{3+2}\right)^{\alpha(12pq-12p-8q-8)} \\ &= (2)^{\alpha(9p+6q-10)} \times (3)^{\alpha(3p+2q-\frac{11}{2})} \times (5)^{\alpha(8-6p-4q)}. \end{aligned}$$

□

Theorem 4.9. *Let $SiC_3 - III[p,q]$ be the Silicon Carbide. Then*

1. $MZ_1(SiC_3 - III[p,q]) = II_1^* = (2)^{(12pq+6p+4q+4)} \times (3)^{(12pq-12p-8q+10)} \times (5)^{(6p+4q-8)}$.
2. $MZ_2(SiC_3 - III[p,q]) = (2)^{4(3p+2q-3)} \times (3)^{3(8pq-6p-4q+3)}$.
3. $GAII(SiC_3 - III[p,q]) = (2)^{(9p+6q-10)} \times (3)^{(3p+2q-\frac{11}{2})} \times (5)^{(8-6p-4q)}$.

Proof. Taking $\alpha = 1$, in Theorem 4.8, we get our desire results. □

Theorem 4.10. *Let $SiC_3 - III[p,q]$ be the Silicon Carbide. Then*

1. $HII_1(SiC_3 - III[p,q]) = (2)^{2(12pq+6p+4q+4)} \times (3)^{2(12pq-12p-8q+10)} \times (5)^{2(6p+4q-8)}$.
2. $HII_2(SiC_3 - III[p,q]) = (2)^{8(3p+2q-3)} \times (3)^{6(8pq-6p-4q+3)}$.

Proof. Taking $\alpha = 2$, in Theoem 4.8, we get our desire results. □

Theorem 4.11. *Let $SiC_3 - III[p,q]$ be the Silicon Carbide. Then*

1. $SCII(SiC_3 - III[p,q]) = (\frac{1}{\sqrt{2}})^{(12pq+6p+4q+4)} \times (\frac{1}{\sqrt{3}})^{\alpha(12pq-12p-8q+10)} \times (\frac{1}{\sqrt{5}})^{\alpha(6p+4q-8)}$.
2. $PCII(SiC_3 - III[p,q]) = (\frac{1}{\sqrt{2}})^{4(3p+2q-3)} \times (\frac{1}{\sqrt{3}})^{3(8pq-6p-4q+3)}$.

Proof. Taking $\alpha = -\frac{1}{2}$, in Theorem 4.8, we get our desire results. □

Theorem 4.12. *Let $SiC_3 - III[p,q]$ be the Silicon Carbide. Then*

$$ABCII(SiC_3 - III[p,q]) = [\frac{1}{\sqrt{6}}][(\frac{1}{2})^{(\frac{1}{2})}]^{9p+6q-11} \times [(\frac{2}{3})]^{(12pq-12p-8q+8)}.$$

Proof.

$$\begin{aligned} GA^{\alpha}II(SiC_3 - III[p,q]) &= \prod_{uv\varepsilon E(Si_2C_3 - III[p,q])} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}} \\ &= \left(\sqrt{\frac{1+2-2}{1\times 2}}\right)^2 \times \left(\sqrt{\frac{1+3-2}{1\times 3}}\right) \times \left(\sqrt{\frac{2+2-2}{2\times 2}}\right)^{3p+2q-3} \\ &\times \left(\sqrt{\frac{2+3-2}{2\times 3}}\right)^{(6p+4q-8)} \times \left(\sqrt{\frac{3+3-2}{3\times 3}}\right)^{(12pq-12p-8q+8)} \\ &= \left[\frac{1}{\sqrt{6}}\right] \times \left[(\frac{1}{2})^{(\frac{1}{2})}\right]^{9p+6q-11} \times \left[(\frac{2}{3})\right]^{(12pq-12p-8q+8)}. \end{aligned}$$

□

Conclusion

Topological indices has many applications in chemistry, physics and other applied sciences. In this paper we have computed multiplicative Zagreb indices, multiplicative geometric arithmetic index, multiplicative atomic bond connectivity index, etc of two Silicon Carbide structures.

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