Computation of Sombor Indices for Some Classes of Silicon Carbides

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Abstract
An index from which we can predict different properties of the molecule of a molecular graph without doing any experiment is called topological index. Silicon carbide is a semiconductor crystalline compound formed by silicon and carbon. The crystal of Silicon carbide is like a closely attached structure in which atoms have covalent bonds between them. In this paper, the molecular graphs of silicon carbide are discussed and further we calculated the exact formulas of Sombor index for these Silicon carbides. The offered results can help to analyse several chemical or physical properties of the Silicon carbides. These methods will be helpful to save time and money in developing new resources, compounds and medications, which is very useful for the betterment of mankind.

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Introduction

Mathematical chemistry is the branch of mathematics that deals with the combination of mathematics and chemistry. By using these combinations, we apply mathematical rules to solve the problems facing in chemistry [21, 32]. Usually, we use rules of special branch of mathematics which is called graph theory. Graph theory [4] is the branch of mathematics that deals the graphs, networks and used to represent structures. Chemical graph theory is a branch of mathematical chemistry which is concerned with the non-trivial uses of graphs to solve molecular difficulties in chemistry [33]. In general, a graph is used to represent a molecule and a molecule is a group of atoms which has his own identification, chemical properties and unique structure. Normally, we consider atoms of the molecule as the vertices of the graph and the chemical bonds as the edges of the graph. Order of the graph is the total number of vertices in a graph and the size of the graph is total number of edges in a graph. We use another term in chemical graphs which is called degree of a vertex, i.e., the number of edges connected to that vertex is called degree of that vertex.

Topology of the structure of a molecule plays a great role in understanding the structural and chemical properties of a compound like boiling point, melting point, valency etc. For instance, the boiling point of chemical compound that is a physical property that can be estimated using degree and distance between the vertices of the chemical compound. Thus, topology of a molecule represents important properties about the molecule. By seeing this behave, in 1947, Wiener identified first topological index in 1947 when he was doing work on boiling points of alkane, this finding led to the foundation of the idea of topological indices [9].

A topological index is the value of a particular mathematical function which shows important properties of molecular structure and gives us useful information without experiments. This is briefly explained by Diudeab et. al.[6]. Randic presented first degree-based topological index in 1975 [26]. Afterward the work of the Randic, Gutman introduced the first, second and third Zagreb indices continuously in 1970's [12]. After that, hundreds of topological indices were introduced which are used in literature till now [1, 3, 5, 7-8, 10-11, 14-20, 22-25, 27-31, 34-44].

Recently, Gutman [13] proposed a new degree-based topological index called the Sombor index. Sombor introduces the ordinary Sombor index, the reduced Sombor index and the average Sombor index which are defined as following:

The ordinary Sombor index for a graph G [13] is defined as

$$SO(G) = \sum_{i\sim j} \sqrt{{d_i}^2 + {d_j}^2}. \qquad (1)$$

The reduced Sombor index [13] for a graph G is defined as

$$SO_{red}(G) = \sum_{i\sim j} \sqrt{(d_i - 1)^2 + (d_j - 1)^2}. \qquad (2)$$

The average Sombor index for a graph G [13] is defined as

$$SO_{avr}(G) = \sum_{i\sim j} \sqrt{(d_i - \bar{d})^2 + (d_j - \bar{d})^2}. \qquad (3)$$

Silicon carbide is a semiconductor crystalline compound formed by silicon and carbon. The crystal of Silicon carbide is like a closely attached structure in which atoms have covalent bonds between them. The arrangement of atoms is like two primary coordination tetrahedral where four silicon and four carbon atoms are bonded to a central Si and C atoms are formed. These tetrahedral units are packed together through their corners to form polar arrangements and polytypes [2].

The aim of this paper is to calculate the Sombor indices for different structures [2] of Silicon carbides such as $Si_2C_3 - I[p,q]$, $Si_2C_3 - II[p,q]$, $Si_2C_3 - III[p,q]$ and $SiC_3 - III[p,q]$. These silicon carbides are defined in next section.

Computation of $(Si_2C_3 - I[p,q])$

Consider the silicon carbide $(Si_2C_3 - I[p,q])$ as shown in the **Error! Reference source not found.**. In order to understand the structure of molecule of $(Si_2C_3 - I[p,q])$, we consider p shows the number of unit cells connected in a chain and q shows the number of rows in a connection and red lines shows linkage between two chains [2].

Error! Reference source not found.(a) shows the structure of $(Si_2C_3 - I[p,q])$ for p=4 and q=1 and **Error! Reference source not found.**(b) shows the structure of $(Si_2C_3 - I[p,q])$ for p=4 and q=2, while **Error! Reference source not found.**(c) shows the structure of one-dimensional unit cell of $(Si_2C_3 - I[p,q])$ in which brown vertices shows carbon atoms and blue vertices shows the silicon atoms.

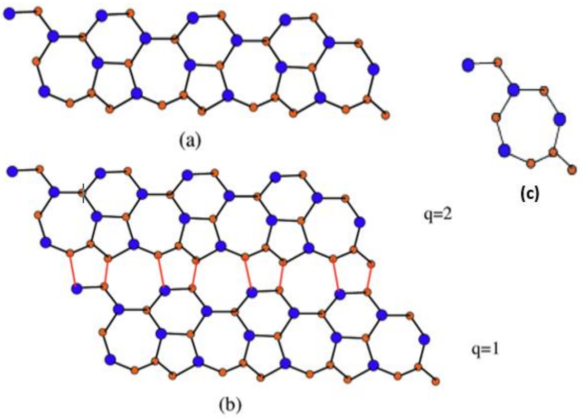

Figure 1. Two Dimensional structure of $(Si_2C_3 - I[p,q])$ with carbon (brown) and silicon (blue). a). $(Si_2C_3 - I[4,1])$ one row with p=4 and q=1. b) $(Si_2C_3 - I[4,2])$. c) $(Si_2C_3 - I[1,1])$.

Table 1. Frequency partition of $E(Si_2C_3 - I[p,q])$

(d_i, d_j)	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Frequency	1	1	$p+2q$	$6p-1+8(q-1)$	$3p(5q-3)-13q+7$

Theorem 2.1. Consider the silicon carbide $(Si_2C_3 - I[p,q])$, then the ordinary Sombor index of the silicon carbide $(Si_2C_3 - I[p,q])$ is

$$SO(Si_2C_3 - I[p,q]) = \begin{bmatrix} (6p-1+8(q-1))\sqrt{13} + (45pq - 5(5p+7q) + 21)\sqrt{2} + \sqrt{5} \\ +\sqrt{10} \end{bmatrix}.$$

Proof: The ordinary Sombor index is defined as $SO(G) = \sum_{i\sim j} \sqrt{{d_i}^2 + {d_j}^2}$.

$$
\begin{aligned}
&SO(Si_2C_3 - I[p,q]) \\
&= \left[(1)\sqrt{1^2+2^2} + (1)\sqrt{1^2+3^2} + (p+2q)\sqrt{2^2+2^2} + \big(6p-1+8(q-1)\big)\sqrt{2^2+3^2} \right. \\
&\left. + (3p(5q-3) - 13q + 7)\sqrt{3^2+3^2}\right]. \\
&= \sqrt{5} + \sqrt{10} + (2p+4q)\sqrt{2} + \big(6p-1+8(q-1)\big)\sqrt{13} + +(3p(5q-3) - 13q + 7)3\sqrt{2}. \\
&= \big(6p-1+8(q-1)\big)\sqrt{13} + (45pq - 5(5p+7q) + 21)\sqrt{2} + \sqrt{5} + \sqrt{10}.
\end{aligned}
$$

Theorem 2.2. Consider the silicon carbide $(Si_2C_3 - I[p,q])$, then the reduced Sombor index of the silicon carbide $(Si_2C_3 - I[p,q])$ is

$$
SO_{red}(Si_2C_3 - I[p,q]) = \begin{bmatrix} \big(6p-1+8(q-1)\big)\sqrt{5} + (6p(5q-3) - 26q + 14)\sqrt{2} + p \\ +2q+3 \end{bmatrix}.
$$

Proof: The reduced Sombor index is defined as $SO_{red}(G) = \sum_{i\sim j}\sqrt{(d_i-1)^2 + (d_j-1)^2}$.

After putting values from the Table 1 as in above equation *(1)*, we acquired the required result, i.e.,

$$
\begin{aligned}
&SO_{red}(Si_2C_3 - I[p,q]) \\
&= (1)\sqrt{(1-1)^2+(2-1)^2} + (1)\sqrt{(1-1)^2+(3-1)^2} + (p+2q)\sqrt{(2-1)^2+(2-1)^2} \\
&+ \big(6p-1+8(q-1)\big)\sqrt{(2-1)^2+(3-1)^2} \\
&+ (3p(5q-3) - 13q + 7)\sqrt{(3-1)^2+(3-1)^2}. \\
&= 1 + 2 + (p+2q) + \big(6p-1+8(q-1)\big)\sqrt{5} + (3p(5q-3) - 13q + 7)2\sqrt{2}. \\
&= \big(6p-1+8(q-1)\big)\sqrt{5} + (6p(5q-3) - 26q + 14)\sqrt{2} + p + 2q + 3.
\end{aligned}
$$

Theorem 2.3. Consider the silicon carbide $(Si_2C_3 - I[p,q])$, then the average Sombor index of the silicon carbide $(Si_2C_3 - I[p,q])$ is

$$
\begin{aligned}
&SO_{avr}(Si_2C_3 - I[p,q]) \\
&= \sqrt{(1-\bar{d})^2+(2-\bar{d})^2} + \sqrt{(1-\bar{d})^2+(3-\bar{d})^2} + (p+2q)\sqrt{(2-\bar{d})^2+(2-\bar{d})^2} \\
&+ \big(6p-1+8(q-1)\big)\sqrt{(2-\bar{d})^2+(3-\bar{d})^2} \\
&+ (3p(5q-3) - 13q + 7)\sqrt{(3-\bar{d})^2+(3-\bar{d})^2}.
\end{aligned}
$$

Proof: The average Sombor index is defined as $SO_{avr}(G) = \sum_{i\sim j}\sqrt{(d_i-\bar{d})^2 + (d_j-\bar{d})^2}$, where, $\bar{d} = \frac{2|E(G)|}{|V(G)|}$

But for $(Si_2C_3 - I[p,q])$, we havev$|E(G)| = 15pq - 2p - 3q, |V(G)| = 10pq$ and

$\bar{d} = \frac{15pq-2p-3q}{5pq}$.

Now putting values from Table 1 in above equation (2), we acquired the required result, i.e.,

$$SO_{avr}(Si_2C_3 - I[p,q])$$
$$= \sqrt{(1-\bar{d})^2 + (2-\bar{d})^2} + \sqrt{(1-\bar{d})^2 + (3-\bar{d})^2} + (p+2q)\sqrt{(2-\bar{d})^2 + (2-\bar{d})^2}$$
$$+ \big(6p - 1 + 8(q-1)\big)\sqrt{(2-\bar{d})^2 + (3-\bar{d})^2}$$
$$+ (3p(5q-3) - 13q + 7)\sqrt{(3-\bar{d})^2 + (3-\bar{d})^2}.$$

Here, $\bar{d} = \frac{15pq-2p-3q}{5pq}$.

Comparison

Here, we present a numerical and graphical comparison of ordinary Sombor index, reduced Sombor index and average Sombor index for the Silicon carbide $Si_2C_3 - I[p,q]$, where (p,q)=1, 2, 3,..., 8 (see *Figure 2* and Table 2).

Table 2. Computation of Sombor Indices for Silicon Carbides $Si_2C_3 - I[p,q]$.

(p,q)	(1,1)	(2,2)	(3,3)	(4,4)	(5,5)	(6,6)	(7,7)	(8,8)
$SO(Si_2C_3 - I[p,q])$	31.911	188.46	472.27	883.37	1421.7	2087.4	2880.3	3800.6
$SO_{red}(Si_2C_3 - I[p,q])$	8.6948	14.717	20.738	26.763	32.78	38.80	44.82	50.85
$SO_{avr}(Si_2C_3 - I[p,q])$	3.1716	11.648	25.735	41.889	58.891	76.314	93.973	111.78

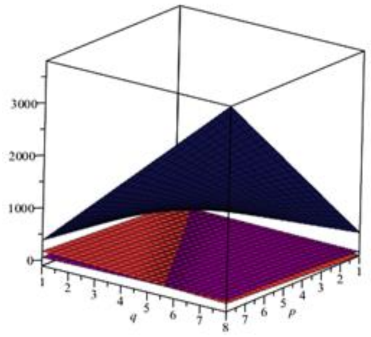

Figure 2. Graphically representation of computing Sombor index for the Silicon Carbides $Si_2C_3 - I[p,q]$.

Computation of $(Si_2C_3 - II[p,q])$

Consider the silicon carbide $(Si_2C_3 - II[p,q])$ as shown in the *Figure 3*. In order to understand the structure [20] of molecule of $(Si_2C_3 - II[p,q])$, we consider p represents the number of unit cells connected in a chain and q represents the number of rows in a connection and red lines shows linkage between two chains. *Figure 3* (a) shows the structure of one dimensional unit cell of $(Si_2C_3 - II[p,q])$ in which brown vertices shows carbon atoms and blue vertices shows silicon atoms, *Figure 3* (b) shows the structure of $(Si_2C_3 - II[p,q])$ for p=3 and q=3 and *Figure 3* (c) shows the structure of $(Si_2C_3 - II[p,q])$ for p=5 and q=1 while *Figure 3* (d) shows the structure (graph) of $(Si_2C_3 - II[p,q])$ for p=5 and q=2.

Table 3 Frequency partition of $E(Si_2C_3 - II[p,q])$

(d_i, d_j)	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Frequency	2	1	$2(p+q)$	$2(4p+4q-7)$	$15pq-13(p+q)+11$

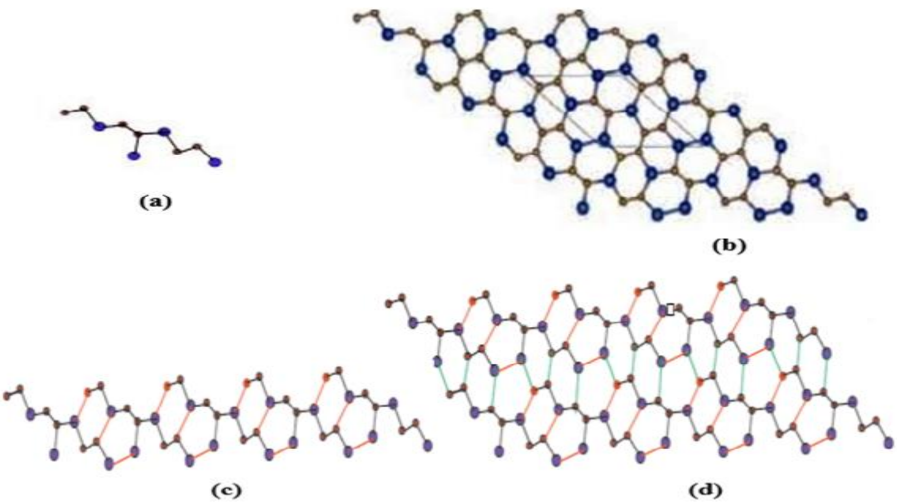

Figure 3. Two Dimensional structure of $(Si_2C_3 - II[p,q])$ with carbon (brown) and silicon (blue). a) One dimensional unit cell of $(Si_2C_3 - II[p,q]$. b) Structure of $(Si_2C_3 - II[3,3])$. c) Structure of $(Si_2C_3 - II[5,1])$. d) Structure of $(Si_2C_3 - II[5,2])$.

Theorem 4.1. Consider the Silicon carbide $(Si_2C_3 - II[p,q])$, then the ordinary Sombor index of the Silicon carbide $(Si_2C_3 - II[p,q]$) is

$$SO(Si_2C_3 - II[p,q]) = \left[2\sqrt{5} + \sqrt{10} + 4(p+q)\sqrt{2} + 2(4p+4q-7)\sqrt{13} + 3(15pq - 13(p+q) + 11)\sqrt{2}\right]$$

Proof: The ordinary Sombor index is defined as $SO(G) = \sum_{i\sim j} \sqrt{{d_i}^2 + {d_j}^2}$.

The total number of vertices and edges for silicon carbide $Si_2C_3 - II[p,q]$ are $8pq$ and $15pq - 3p - 3q$ respectively. For $Si_2C_3 - II[p,q]$, we have vertices of degrees 1, 2 and 3. The edge partition for the degree of vertices of $Si_2C_3 - II[p,q]$ is shown in Table 3, in which we have 2 edges of degree (1,2), 1 edge of degree (1,3), $(2(p+q))$ edges of degree (2,2), $(2(4p+4q-7))$ edges of degree (2,3) and $(15pq - 13(p+q) + 11)$ edges of degree (3,3). After putting values from Table 3 in the above equation *(3)*, we acquired the required results, i.e.

$$\begin{aligned} SO(G) &= (2)\sqrt{1^2+2^2} + (1)\sqrt{1^2+3^2} + (2(p+q))\sqrt{2^2+2^2} + (2(4p+4q-7))\sqrt{2^2+3^2} + (15pq \\ &\quad - 13(p+q) + 11)\sqrt{3^2+3^2}. \\ &= 2\sqrt{5} + \sqrt{10} + 2(p+q)2\sqrt{2} + \big(2(4p+4q-7)\big)\sqrt{13} + (15pq - 13(p+q) + 11)\sqrt{18} \\ &= 2\sqrt{5} + \sqrt{10} + 4(p+q)\sqrt{2} + 2(4p+4q-7)\sqrt{13} + 3(15pq - 13(p+q) + 11)\sqrt{2}. \end{aligned}$$

Theorem 4.2. Consider the Silicon carbide $(Si_2C_3 - II[p,q])$, then the reduced Sombor index of the Silicon carbide $(Si_2C_3 - II[p,q]$) is

$$SO_{red}(Si_2C_3 - II[p,q]) = \big(2(4p+4q-7)\big)\sqrt{5} + (2(15pq - 12(p+q) + 11))\sqrt{2} + 4.$$

Proof: The reduced Sombor index is defined as $SO_{red}(G) = \sum_{i\sim j} \sqrt{(d_i - 1)^2 + (d_j - 1)^2}$.

After putting values from the Table 3 and using above equation *(4)*, we acquired the required result, i.e.,

$$\begin{aligned} &SO_{red}(Si_2C_3 - II[p,q]) \\ &= (2)\sqrt{(1-1)^2+(2-1)^2} + (1)\sqrt{(1-1)^2+(3-1)^2} + 2(p+q)\sqrt{(2-1)^2+(2-1)^2} \\ &+ 2(4p+4q-7)\sqrt{(2-1)^2+(3-1)^2} + (15pq - 13(p+q) + 11)\sqrt{(3-1)^2+(3-1)^2} \\ &= 2 + 2 + 2(p+q)\sqrt{2} + \big(2(4p+4q-7)\big)\sqrt{5} + (15pq - 13(p+q) + 11)2\sqrt{2} \\ &= \big(2(4p+4q-7)\big)\sqrt{5} + (15pq - 13p - 13q + 11 + p + q)2\sqrt{2} + 4 \\ &= \big(2(4p+4q-7)\big)\sqrt{5} + (2(15pq - 12(p+q) + 11))\sqrt{2} + 4. \end{aligned}$$

Theorem 4.3. Consider the Silicon carbide $(Si_2C_3 - II[p,q])$, then the average Sombor index of the Silicon carbide $(Si_2C_3 - II[p,q]$) is

$SO_{avr}(Si_2C_3-II[p,q])=\sqrt{(1-\bar{d})^2+(2-\bar{d})^2}+\sqrt{(1-\bar{d})^2+(3-\bar{d})^2}+2(p+q)\sqrt{(2-\bar{d})^2+(2-\bar{d})^2}+\big(2(4p+4q-7)\big)\sqrt{(2-\bar{d})^2+(3-\bar{d})^2}(15pq-13(p+q)+11)\sqrt{(3-\bar{d})^2+(3-\bar{d})^2}$

Proof: The average Sombor index is defined as $SO_{avr}(G)=\sum_{i\sim j}\sqrt{(d_i-\bar{d})^2+(d_j-\bar{d})^2}$, where $\bar{d}=\frac{2|E(G)|}{|V(G)|}$. But For $(Si_2C_3-II[p,q])$, we have $|E(Si_2C_3-II[p,q])|=15pq-3p-3q$, $|V(Si_2C_3-II[p,q])|=8pq$. Then $\bar{d}=\frac{15pq-3p-3q}{4pq}$.
Now, putting values from the Table 3 in above equation (5), we acquired the desired result, i.e.,

$$\begin{aligned}SO_{avr}(Si_2C_3-II[p,q])\\ &=\sqrt{(1-\bar{d})^2+(2-\bar{d})^2}+\sqrt{(1-\bar{d})^2+(3-\bar{d})^2}+2(p+q)\sqrt{(2-\bar{d})^2+(2-\bar{d})^2}\\ &+\big(2(4p+4q-7)\big)\sqrt{(2-\bar{d})^2+(3-\bar{d})^2}\\ &+(15pq-13(p+q)+11)\sqrt{(3-\bar{d})^2+(3-\bar{d})^2}\end{aligned}$$

Where $\bar{d}=\frac{15pq-3p-3q}{4pq}$.

Comparison

Here, we present a numerical and graphical comparison of ordinary Sombor index, reduced Sombor index and average Sombor index for the Silicon carbide $Si_2C_3-II[p,q]$, where (p,q)=1, 2, 3,..., 8.

Table 4. Computation of Sombor Indices for Silicon Carbides $Si_2C_3-II[p,q]$.

(p,q)	(1,1)	(2,2)	(3,3)	(4,4)	(5,5)	(6,6)	(7,7)	(8,8)
$SO(Si_2C_3-II[p,q])$	26.159	175.77	452.66	856.83	1388.3	2047.0	2833.0	3746.2
$SO_{red}(Si_2C_3-II[p,q])$	14.129	109.30	289.33	554.20	903.93	1338.6	1857.9	2462.2
$SO_{avr}(Si_2C_3-II[p,q])$	4.9686	207.88	948.28	2300.3	4277.7	6885.6	10126	14000

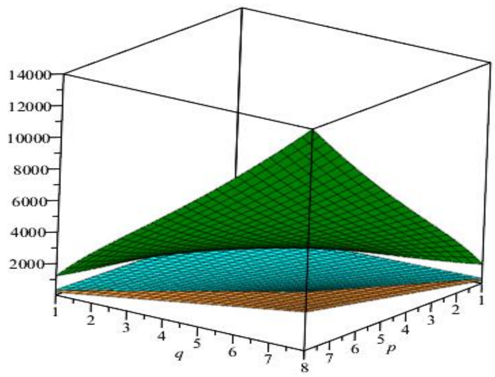

Figure 4. Graphical representation of Computation of Sombor Indices for Silicon Carbides $Si_2C_3 - II[p,q]$.

Computation of $(\boldsymbol{Si_2C_3 - III[p,q]})$

Consider the silicon carbide $(Si_2C_3 - III[p,q])$ as shown in the *Figure 5*. In order to understand the structure [20] of molecule of $(Si_2C_3 - III[p,q])$, we consider p represents the number of unit cells connected in a chain and q represents the number of rows in a connection and red lines shows linkage between two chains. *Figure 5* (a) shows the structure of one dimensional unit cell of $(Si_2C_3 - III[p,q])$ in which brown vertices shows carbon atoms and blue vertices shows silicon atoms, *Figure 5* (b) shows the structure of $(Si_2C_3 - III[p,q])$ for p=5 and q=4 and *Figure 5* (c) shows the structure of $(Si_2C_3 - III[p,q])$ for p=5 and q=1 while *Figure 5* (d) shows the structure of $(Si_2C_3 - III[p,q])$ for p=5 and q=2.

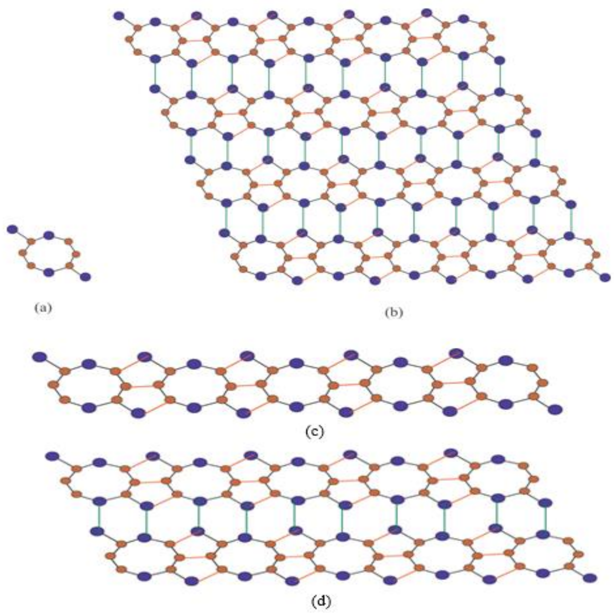

Figure 5. Two Dimensional structure of $(Si_2C_3 - III[p,q])$ *with carbon (brown) and silicon (blue). a) One dimensional unit cell of* $(Si_2C_3 - III[p,q])$. *b)* $Structure\ of\ (Si_2C_3 - III[5,4])$. *c) Structure of* $(Si_2C_3 - III[5,1])$. *d) Structure of* $(Si_2C_3 - III[5,2])$.

Table 5. Frequency partition of $E(Si_2C_3 - III[p,q])$

(d_i, d_j)	(1,3)	(2,2)	(2,3)	(3,3)
Frequency	2	$2p+2$	$4(2p+2q-3)$	$5p(3q-2)-13q+8$

Theorem 6.1. Consider the Silicon carbide $(Si_2C_3 - III[p,q])$, then the ordinary Sombor index of the Silicon carbide $(Si_2C_3 - III[p,q]\ )$ is

$$SO(Si_2C_3 - III[p,q]) = 2(2p+2)\sqrt{2} + \big(4(2p+2q-3)\big)\sqrt{13} + (15p(3q-2) - 39q + 24)\sqrt{2} + 2\sqrt{10}.$$

Proof: The ordinary Sombor index is defined as $SO(G) = \sum_{i\sim j}\sqrt{{d_i}^2 + {d_j}^2}$. The total number of vertices and edges for silicon carbide $Si_2C_3 - III[p,q]$ are $10pq$ and $15pq - 2p - 3q$ respectively. For $Si_2C_3 - III[p,q]$, we have vertices of degrees 1, 2 and 3. The edge partition for the degree of vertices of $Si_2C_3 - III[p,q]$ is shown in Table 5, in which we have 2 edges of degree (1,3), $(2p+2)$ edges of degree (2,2), $4(2p+2q-3)$ edges of degree (2,3) and $(5p(3q-2) - 13q + 8)$ edges of degree (3,3). After putting values from Table 5 in the above equation *(6)*, we acquired the required results, i.e.,

$$\begin{aligned} SO(Si_2C_3 - III[p,q]) &= (2)\sqrt{1^2+3^2} + (2p+2)\sqrt{2^2+2^2} + 4(2p+2q-3)\sqrt{2^2+3^2} \\ &+ (5p(3q-2) - 13q + 8)\sqrt{3^2+3^2} \\ &= 2\sqrt{10} + 2(2p+2)\sqrt{2} + \big(4(2p+2q-3)\big)\sqrt{13} + (5p(3q-2) - 13q + 8)\big(3\sqrt{2}\big) \\ &= 2(2p+2)\sqrt{2} + \big(4(2p+2q-3)\big)\sqrt{13} + (15p(3q-2) - 39q + 24)\sqrt{2} + 2\sqrt{10} \end{aligned}$$

Theorem 6.2. Consider the Silicon carbide $(Si_2C_3 - III[p,q])$, then the reduced Sombor index of the Silicon carbide $(Si_2C_3 - III[p,q]\ )$ is

$$SO_{red}(Si_2C_3 - III[p,q]) = [(2p+2)\sqrt{2} + (10p(3q-2) - 26q + 16)\sqrt{2} + \big(4(2p+2q-3)\big)\sqrt{5} + 4].$$

Proof: The reduced Sombor index is defined as $SO_{red}(G) = \sum_{i\sim j}\sqrt{(d_i-1)^2 + (d_j-1)^2}$.

After putting values from the Table 5 as in above equation *(7)*, we acquired the required result, i.e.,

$$\begin{aligned} SO_{red}(Si_2C_3 - III[p,q]) &= (2)\sqrt{(1-1)^2 + (3-1)^2} + (2p+2)\sqrt{(2-1)^2 + (2-1)^2} \\ &+ 4(2p+2q-3)\sqrt{(2-1)^2 + (3-1)^2} + (5p(3q-2) - 13q + 8)\sqrt{(3-1)^2 + (3-1)^2}. \\ &= 4 + (2p+2)\sqrt{2} + \big(4(2p+2q-3)\big)\sqrt{5} + (5p(3q-2) - 13q + 8)2\sqrt{2} \\ &= (2p+2)\sqrt{2} + (10p(3q-2) - 26q + 16)\sqrt{2} + \big(4(2p+2q-3)\big)\sqrt{5} + 4. \end{aligned}$$

Theorem 6.3. Consider the Silicon carbide $(Si_2C_3 - III[p,q])$, then the average Sombor index of the Silicon carbide $(Si_2C_3 - III[p,q]\ )$ is

$$SO_{avr}(Si_2C_3 - III[p,q]) = (2)\sqrt{(1-\bar{d})^2+(3-\bar{d})^2} + (2p+2)\sqrt{(2-\bar{d})^2+(2-\bar{d})^2} + \left(4(2p+2q-3)\right)\sqrt{(2-\bar{d})^2+(3-\bar{d})^2} + (5p(3q-2)-13q+8)\sqrt{(3-\bar{d})^2+(3-\bar{d})^2}$$

Proof: The average Sombor index is defined as $SO_{avr}(G) = \sum_{i\sim j}\sqrt{(d_i-\bar{d})^2+(d_j-\bar{d})^2}$,

where $\bar{d} = \frac{2|E(G)|}{|V(G)|}$.

But for silicon carbide $(Si_2C_3 - III[p,q])$, we have $|E(Si_2C_3 - III[p,q])| = 15pq - 2p - 3q$ and $|V(Si_2C_3 - III[p,q])| = 10pq$, where $\bar{d} = \frac{15pq-2p-3q}{5pq}$.

Now, putting values from the Table 5 in above equation (8), we get

$$SO_{avr}(Si_2C_3 - III[p,q]) = (2)\sqrt{(1-\bar{d})^2+(3-\bar{d})^2} + (2p+2)\sqrt{(2-\bar{d})^2+(2-\bar{d})^2} + \left(4(2p+2q-3)\right)\sqrt{(2-\bar{d})^2+(3-\bar{d})^2} + (5p(3q-2)-13q+8)\sqrt{(3-\bar{d})^2+(3-\bar{d})^2}.$$

$$\bar{d} = \frac{15pq-2p-3q}{5pq}.$$

Comparison

Here, we present a numerical and graphical comparison of ordinary Sombor index, reduced Sombor index and average Sombor index for the silicon carbide $Si_2C_3 - III[p,q]$, where (p,q)=1, 2, 3,..., 8.

Table 6. Computation of Sombor Indices for Silicon Carbides $Si_2C_3 - III[p,q]$.

(p,q)	(1,1)	(2,2)	(3,3)	(4,4)	(5,5)	(6,6)	(7,7)	(8,8)
$SO(Si_2C_3 - III[p,q])$	32.061	61.467	90.871	120.27	149.68	179.08	208.49	237.90
$SO_{red}(Si_2C_3 - III[p,q])$	18.601	34.580	50.559	66.540	82.512	98.493	114.47	130.46
$SO_{avr}(Si_2C_3 - III[p,q])$	6.8264	15.890	30.232	46.767	64.222	82.139	100.32	118.66

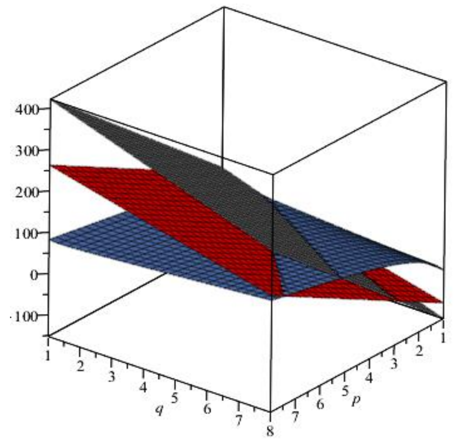

Figure 6. Graphical representation of Computation of Sombor Indices for Silicon Carbides$Si_2C_3 - III[p, q]$.

Computation of $(SiC_3 - III[p, q])$

Consider the silicon carbide $(\mathrm{SiC_3} - \mathrm{III}[\mathrm{p}, \mathrm{q}])$ as shown in the *Figure 7*. In order to understand the structure [20] of molecule of $(\mathrm{SiC_3} - \mathrm{III}[\mathrm{p}, \mathrm{q}])$, we consider p represents the number of unit cells connected in a chain and q represents the number of rows in a connection and red lines shows linkage between two chains. *Figure 7* (a) shows the structure of one dimensional unit cell of $(\mathrm{SiC_3} - \mathrm{III}[\mathrm{p}, \mathrm{q}])$ in which brown vertices shows carbon atoms and blue vertices shows silicon atoms, *Figure 7* (b) shows the structure of $(\mathrm{SiC_3} - \mathrm{III}[\mathrm{p}, \mathrm{q}])$ for p=5 and q=5 and *Figure 7* (c) shows the structure of $(\mathrm{Si_2C_3} - \mathrm{III}[\mathrm{p}, \mathrm{q}])$ for p=5 and q=1 while *Figure 7* (d) shows the structure of $(\mathrm{Si_2C_3} - \mathrm{II}[\mathrm{p}, \mathrm{q}])$ for p=5 and q=2.

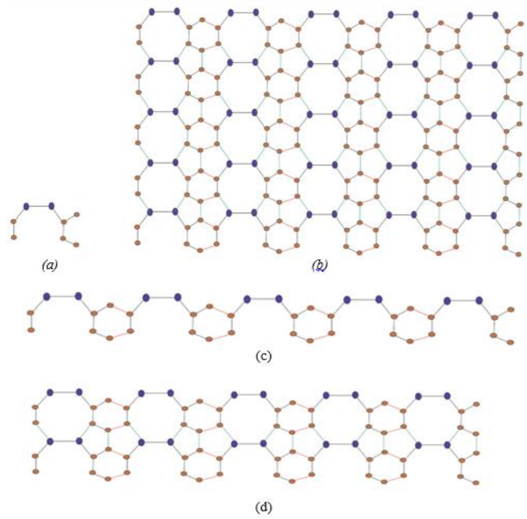

Figure 7. Two Dimensional structure of $(SiC_3 - III[p, q])$ with carbon (brown) and silicon (blue). a) One dimensional unit cell of $(SiC_3 - III[p, q])$. b) Structure of $(SiC_3 - III[5,5])$. c) Structure of $(SiC_3 - III[5,1])$. d) Structure of $(SiC_3 - III[5,2])$.

Table 7. Frequency partition of $E(SiC_3 - III[p,q])$

(d_i,d_j)	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Frequency	2	1	$3p+2q-3$	$2(3p+2q-4)$	$4(3pq-3p-2q+2)$

Theorem 8.1. Consider the Silicon carbide $(SiC_3 - III[p,q])$, then the ordinary Sombor index of the Silicon carbide $(SiC_3 - III[p,q])$ is

$$SO(SiC_3 - III[p,q]) = 2\sqrt{5} + \sqrt{10} + 2(3p+2q-3)\sqrt{2} + (2(3p+2q-4)\sqrt{13} +12(3pq-3p-2q+2)\sqrt{2}.$$

Proof: The ordinary Sombor index is defined as $SO(G) = \sum_{i\sim j}\sqrt{{d_i}^2 + {d_j}^2}$.

The total number of vertices and edges for silicon carbide $SiC_3 - III[p,q]$ are $8pq$ and $12pq - 3p - 2q$ respectively. For $SiC_3 - III[p,q]$, we have vertices of degrees 1, 2 and 3. The edge partition for the degree of vertices of $SiC_3 - III[p,q]$ is shown in Table 7, in which we have 2 edges of degree (1,2), 1 edge of degree (1,3), $(3p+2q-3)$ edges of degree (2,2), $2(3p+2q-4)$ edges of degree (2,3) and $4(3pq-3p-2q+2)$ edges of degree (3,3). After putting values from Table 7 in the above equation *(9)*, we acquired the required results, i.e.

$$\begin{aligned} SO(SiC_3 - III[p,q]) &= (2)\sqrt{1^2+2^2} + (1)\sqrt{1^2+3^2} + (3p+2q-3)\sqrt{2^2+2^2} \\ &+ (2(3p+2q-4))\sqrt{2^2+3^2} + \big(4(3pq-3p-2q+2)\big)\sqrt{3^2+3^2} \\ &= 2\sqrt{5} + \sqrt{10} + 2(3p+2q-3)\sqrt{2} + (2(3p+2q-4)\sqrt{13} \\ &+ 12(3pq-3p-2q+2)\sqrt{2}. \end{aligned}$$

Theorem 8.2. Consider the Silicon carbide $(SiC_3 - III[p,q])$, then the reduced Sombor index of the Silicon carbide $(SiC_3 - III[p,q])$ is

$$SO_{red}(SiC_3 - III[p,q]) = (3p+2q-3)\sqrt{2} + 8(3pq-3p-2q+2)\sqrt{2} + (2(3p+2q-4))\sqrt{5} + 4.$$

Proof: The reduced Sombor index is defined as $SO_{red}(G) = \sum_{i\sim j}\sqrt{(d_i-1)^2 + (d_j-1)^2}$.
After putting values from the Table 7 as in above equation *(10)*, we acquired the required result, i.e.,

$$\begin{aligned} SO_{red}(SiC_3 - III[p,q]) &= (2)\sqrt{(1-1)^2+(2-1)^2} + (1)\sqrt{(1-1)^2+(3-1)^2} \\ &+ (3p+2q-3)\sqrt{(2-1)^2+(2-1)^2} + \big(2(3p+2q-4)\big)\sqrt{(2-1)^2+(3-1)^2} \\ &+ \big(4(3pq-3p-2q+2)\big)\sqrt{(3-1)^2+(3-1)^2} \\ &= (3p+2q-3)\sqrt{2} + 8(3pq-3p-2q+2)\sqrt{2} + (2(3p+2q-4))\sqrt{5} + 4. \end{aligned}$$

Theorem 8.3. Consider the Silicon carbide ($SiC_3 - III[p,q]$), then the average Sombor index of the Silicon carbide ($SiC_3 - III[p,q]$) is

$$SO_{avr}(SiC_3 - III[p,q]) = (2)\sqrt{(1-\bar{d})^2 + (2-\bar{d})^2} + \sqrt{(1-\bar{d})^2 + (3-\bar{d})^2} + (3p+2q-3)\sqrt{(2-\bar{d})^2 + (2-\bar{d})^2} + \big(2(3p+2q-4)\big)\sqrt{(2-\bar{d})^2 + (3-\bar{d})^2} + \big(4(3pq-3p-2q+2)\big)\sqrt{(3-\bar{d})^2 + (3-\bar{d})^2}.$$

Proof: The average Sombor index is defined as $SO_{avr}(G) = \sum_{i\sim j}\sqrt{(d_i-\bar{d})^2 + (d_j-\bar{d})^2}$,where $\bar{d} = \frac{2|E(G)|}{|V(G)|}$. But for ($SiC_3 - III[p,q]$), we have $|E(SiC_3 - III[p,q])| = 12pq - 3p - 2q$ and $|V(SiC_3 - III[p,q])| = 8pq$, where $\bar{d} = \frac{12pq-3p-2q}{4pq}$.

Now, putting values from the Table 7 in above equation (11), we get

$$SO_{avr}(SiC_3 - III[p,q]) = (2)\sqrt{(1-\bar{d})^2 + (2-\bar{d})^2} + \sqrt{(1-\bar{d})^2 + (3-\bar{d})^2} + (3p+2q-3)\sqrt{(2-\bar{d})^2 + (2-\bar{d})^2} + \big(2(3p+2q-4)\big)\sqrt{(2-\bar{d})^2 + (3-\bar{d})^2} + \big(4(3pq-3p-2q+2)\big)\sqrt{(3-\bar{d})^2 + (3-\bar{d})^2}$$

where $\bar{d} = \frac{12pq-3p-2q}{4pq}$.

9. Comparison

Here, we present a numerical and graphical comparison of ordinary Sombor index, reduced Sombor index and average Sombor index for the Silicon carbide $SiC_3 - III[p,q]$, where (p,q)=1, 2, 3,..., 8.

Table 8. Computation of Sombor Indices for Silicon Carbides $SiC_3 - III[p,q]$

(p,q)	(1,1)	(2,2)	(3,3)	(4,4)	(5,5)	(6,6)	(7,7)	(8,8)
$SO(SiC_3 - III[p,q])$	20.502	138.58	358.48	680.20	1103.8	1629.1	2256.2	2985.3
$SO_{red}(SiC_3 - III[p,q])$	11.301	85.987	228.55	439.00	717.34	1063.6	1477.6	1959.6
$SO_{avr}(SiC_3 - III[p,q])$	6.2956	30.962	63.680	99.089	135.65	172.80	210.27	247.96

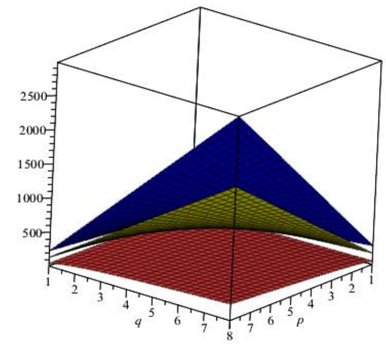

Figure 8. Graphical representation of Computation of Sombor Indices for Silicon Carbide $SiC_3 - III[p,q]$.

Conclusion

In this paper, we have computed the newly introduced ordinary Sombor index, reduced Sombor index and average Sombor index for the Silicon carbide graphs $Si_2C_3 - I[p,q]$, $Si_2C_3 - II[p,q]$, $Si_2C_3 - III[p,q]$ and $SiC_3 - III[p,q]$ in drugs. We have also determined formulas of respective Sombor indices for all given structures of Silicon carbides. These formulas would help in investigation of chemical and biological properties of silicon carbides in drugs.

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