Research Article

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Topological Descriptor of 2-Dimensional Silicon Carbons and Their Applications

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Abstract: The Chemical graph theory is extensively used in finding the atomic supplementary properties of different chemical structures. Many results of graph theory are commonly used in molecular structures and in general in Chemistry. In a molecular graph vertices are atoms while chemical bonds are given by edges. This article is about computing the exact values for some degree based topological descriptors of two molecular structures. Namely we work on the silicon-carbon Si$_2$C$_3$-III and SiC$_3$-III for dimension two. We also discuss some applications of these results towards Chemistry.

Keywords: 2D silicon-carbon Si$_2$C$_3$-III and SiC$_3$-III; Zagreb indices.

1 Introduction

A combination of graph theory and Chemistry is an interesting branch of Mathematics called chemical graph theory. The molecules from Chemistry model in Mathematical ways in the form of molecular graph. A graph is a union of two sets namely vertices and edges. In a molecular graph vertices are atoms while chemical bonds are given by edges. Different techniques from graph theory use to apply on these molecular structures to get their different topological and structure properties. For example, the boiling point of chemical compound, which is a physical entity, can be estimated using degree and distance between the vertices of the chemical compound. Thus, we can say while modelling a chemical problem in terms of mathematical form, topology of its molecular structure plays an important role to give useful properties of corresponding chemical compound [1]. In 1988, it was accounted for that few hundred specialists worked in delivering around 500 research articles every year exploring various properties of chemical structures including two-volume of meticulous contents by Gutman in [2]. More applications of this interested branch of science particularly discussing topological indices are available in [3, 4, 5, 6, 7, 8, 9].

One of the promptly research directions among the researchers is the study of chemical compounds in term of mathematical modelling [4, 5]. A broad proportion of chemical compounds exists which have interesting mathematical structures and have wide range of applications in industrial, pharmaceutical, research and commercial chemistry. Arrangements of atoms among a chemical compound have definite structural rules which have useful hidden properties. Thus, to explore these properties by use of mathematical tools, in terms of combinatorics and topology, play a significant rule in applied research. It is worth mentioning here that the mathematical chemistry obtains considerable contributions from the field of chemical graph theory [6, 7]. There are many invariants of chemical graph theory namely, indices or descriptors, which are used in other sciences notably in pharmaceutical and chemical way [8, 9]. More precisely the study of distance based and degree-based indices takes active part in the development of related fields [10]. It helps to gather huge data in the form of numerical values associated to chemical structures and get their comparisons using modern computer systems [11]. During the last decade of nineteenth century many topological descriptors have been introduced to fulfil the requirements of the chemists [12,13].

A graph $G=(V,E)$ can be represented as combination of two sets namely edge set $E$ and vertex set $V$. Edges are denoted by lines in a graph $G$. Number of edges shared by
a vertex \( p \) called its degree \( \mu(p) \) while distance between two vertices \( p \) and \( q \) is the minimum of the cardinality of the sets of all edges between them and is denote by \( d(p,q) \). One can represent a graph by many ways including a value namely by different topological descriptors which could be distance based or degree based.

The Zagreb indices are defined as follows by Gutman and Trinajstić [14, 15]:

\[
M_1(G) = \sum_{pq \in E(G)} (\mu(p) + \mu(q))
\]

\[
M_2(G) = \sum_{pq \in E(G)} (\mu(p) \times \mu(q))
\]

The Zagreb coindices are defined as follows by Došlic’ [16]:

\[
\overline{M}_1(G) = \sum_{pq \in E(G)} [\mu(p) + \mu(q)]
\]

\[
\overline{M}_2(G) = \sum_{pq \in E(G)} \mu(p)\mu(q)
\]

Following theorem is proved by Gutman et al. [17]:

"**Theorem 1**: Let \( G \) be a graph with \( |V(G)| \) vertices, \( |E(G)| \) edges and \( \overline{M}_1(G) \) represents the first Zagreb coindex, then

\[
\overline{M}_1(G) = 2|E(G)|(|V(G)| - 1) - \overline{M}_2(G)
\]

**Theorem 2**: Let \( G \) be graph with \( |V(G)| \) vertices, \( |E(G)| \) edges and \( \overline{M}_2(G) \) represents the second Zagreb coindex, then

\[
\overline{M}_2(G) = 2|E(G)|^2 - \frac{1}{2} \overline{M}_1(G) - \overline{M}_2(G)
\]

The multiple Zagreb indices are defined as follows by Ghorbani and Azimi [18]:

\[
P.M_1(G) = \prod_{pq \in E(G)} [\mu(p) + \mu(q)]
\]

\[
P.M_2(G) = \prod_{pq \in E(G)} [\mu(p) \times \mu(q)]
\]

We recommend the reader to study [19-22] for more details.

Firstly this article deals with the computation of above mentioned indices for the molecular structures \( \text{Si}_2\text{C}_3\text{-III}[n,m] \) and \( \text{SiC}_3\text{-III}[n,m] \). Secondly we present comparisons of the results in the form of tables and functional graphs.

### 2 Methods

To process our outcomes, we utilize the strategy for combinatorial registering, vertex segment technique, edge segment strategy, graph hypothetical instruments, investigative strategies, degree tallying strategy and whole of degrees of neighbor’s technique. Likewise, we used computer algebra systems like Matlab and Maple for estimation and numerical sketching, respectively.

### 3 Two dimenstional Silicon Carbide \( \text{Si}_2\text{C}_3\text{-III}[n,m] \)

The silicones are semiconductor in nature that utilizes in assembling of some different materials. It is organism used nearly in all the most recent electronic based gadgets. A be notable among these discovered structures are the 2 dimensional silicon carbon having single layer blends having particular stoichiometric which were wrapped [23]. It’s based particle the molecule swarm streamlining given to be (PSO) system combined with deep practical postulate enhancement.

Some sheets of the graphene were effectively disconnected in 2004 [24]. This two-dimensional structure come out to be used in the additional conventional particularly in their mechanical and optical possessions. Moreover, these gadgets possess distinguish electric properties of graphene draw which attracts the researcher to work on this two dimensional structure.

Till this date study of these silicon sheets is quite open although a lot of work has already been done. There is another form of these structures namely two dimensional (Si-C) single layers which can be seen as distinctive objects among the pure 2 dimensional single-layer carbon-graphene and the pure 2 dimensional solitary layer-silicone. Many attempts are accompanied for forestalling the silicon carbon (Si-C) sheet [25]. Figure 1 give the structure for the above-mentioned sheets.

To have idea about the corresponding molecular graph, we characterize associated values of the one dimensional cells in succession (chain). It is easily seen in Figure 2 that in what way the cells associate in bolt (chain) and how one line interfaces with another line. As a first part we work on the molecular structure given by \( \text{Si}_2\text{C}_3\text{-III}[n,m] \).

#### 3.1 Results

For this structure the cardinality of vertex set is 10 mn. Also, the cardinality of the edge set is 15mn-2n-3. We make partitions of vertex set and edge set to compute the topological descriptors for this chemical structure. Let \( n, m \geq 1 \). The vertex is partitioned into three sets depending upon degrees of the vertices. Namely we denote by \( V_i \) the
Figure 1: Two dimensional constitution of $\text{Si}_2\text{C}_3\text{III}[n,m]$
(a) One dimensional cell of $\text{Si}_2\text{C}_3\text{III}[n,m]$, 
(b) $\text{Si}_2\text{C}_3\text{III}[5,4]$. Brown vertices as Carbon atom C and blue vertices as Silicon atom Si.

Figure 2: 2 dimensional $\text{Si}_2\text{C}_3\text{III}[n,m]$, (a) $\text{Si}_2\text{C}_3\text{I}[5,1]$ (b) $\text{Si}_2\text{C}_3\text{III}[5,2]$. 
set containing vertices of degree \(i\). For \(S_{i,j,3-III}[n,m]\), we have \(|V_1|=2\), \(|V_2|=4n+3m-1\) and \(|V_3|=10mn-4n-3m-1\). The partitions of edges are shown in the following Table.

### 3.1.1 Zagreb indices

By [35], we have:

\[
\mathcal{M}_1(S_{i,j,3-III}[n,m]) = 4 - 20n + 30m(3n - 1).
\]

\[
\mathcal{M}_2(S_{i,j,3-III}[n,m]) = 14 - 42n + 135mn - 61m.
\]

### 3.1.2 The first and second Zagreb coindices

Equations (3), (4) and Theorem 1,2 we get our results as:

\[
\overline{\mathcal{M}}_1(G) = \sum_{pq \in E(G)} (\nu(p) + \nu(q))
\]

\[
\overline{\mathcal{M}}_2(G) = 2|E(G)|(|V(G)| - 1) - \mathcal{M}_1(G)
\]

\[
= 2(-3m - 2n + 15mn)(10mn - 1)
\]

\[
= 300m^2n^2 + 36m + 24n - 120mn - 4 - 60m^2n - 40mn^2.
\]

\[
\overline{\mathcal{M}}_1(G) = \sum_{pq \in E(G)} (\nu(p)\nu(q))
\]

\[
\overline{\mathcal{M}}_2(G) = 2|E(G)|^2 - \frac{1}{2} \mathcal{M}_1(G) - \mathcal{M}_2(G)
\]

\[
= 2(-20n - 30m + 4 + 90mn)
\]

\[
= 450m^2n^2 + 8n^2 - 156mn + 76m + 18m^2 - 180m^2n - 120mn^2 + 52n - 16.
\]

### 3.1.3 Multiple Zagreb indices

Now equations (7), (8) are used to compute following indices as:

\[
P.M_1(G) = \prod_{p \in E(G)} [\nu(p) + \nu(q)]
\]

\[
= (2 + 2)^{(2+2m)} \times (3 + 1)^{(2)} \times (3 + 3)^{(15mn-13m-10n+8)}
\]

\[
= (4)^{(2m+2)} \times (4)^{(2)} \times (6)^{(15mn-13m-10n+8)}
\]

\[
P.M_2(G) = \prod_{p \in E(G)} [\nu(p) \times \nu(q)]
\]

\[
= (2 \times 2)^{(2+2m)} \times (1 \times 3)^{(2)} \times (3 \times 3)^{(15mn-13m-10n+8)}
\]

\[
= (4)^{(2+2m)} \times (6)^{(15mn-13m-10n+8)} \times (9)^{(15mn-13m-10n+8)}
\]
The two dimensional Silicon Carbide SiC$_3$-III, the molecular graph, is shown in Figure 6. The one dimensional cells are shown in the straight line in the form of chain. The rows are given by $n$ and columns are given by $m$. Figure 7 describes the structure exhibited in the way the cells interface straight (chain) and how one line associates with another column.

4.1 Results

For this structure the cardinality of vertex set is $8mn$. Also, the cardinality of the edge set is $12mn-3n-2m$. We make partitions of vertex set and edge set to compute the topological descriptors for this chemical structure. Let $n, m \geq 1$. The vertex is partitioned into three sets depending upon degrees of the vertices. Namely we denote by $V_i$ the set containing vertices of degree $i$. For Si$_2$C$_3$-III[$n,m$], we have $|V_1|=3$, $|V_2|=6n+4m-6$ and $|V_3|=8mn-6n-4m-1$. The partition of edges is shown in the following Table.

4.1.1 Zagreb indices

By [35], we have:

$$M_1(G) = 6 + 4m(18n - 5) - 30n.$$  
$$M_2(G) = 19 + 4m(27n - 10) - 60n.$$
Figure 6: 2 dimensional structure of SiC$_3$-III[$n,m$], (a) One dimensional cell, (b) SiC$_3$-III[5,5]. Carbon atoms(brown), Silicon atoms(blue).

Figure 7: 2 dimensional structure of SiC$_3$-III[$n,m$], (a) SiC$_3$-III[5,1], (b) SiC$_3$-III[5,2].
4.1.2 Zagreb Coincides

Equations (3), (4) and Theorem 1, 2 leads us to compute the following results as below:

\[ M_1(G) = \sum_{pq \in E(G)} (\mu(p) + \mu(q)) \]
\[ M_1(G) = 2|E(G)||V(G)| - 1 - M_1(G) \]
\[ = 2(12mn - 2m - 3n)(8mn - 1) \]
\[ = (2 + 2)(2m+3n-3) \times (1 + 2)^2 \times (1 + 3)^1 \]
\[ \times (2 + 3)^{4m+6n-8} \times (+2)^{6+12m-8m-12n} \]
\[ = (5)^6 \times (4)^{2m+3n-3} \times (6)^{12m-8m-12n+8} \]
\[ \times (6)^{12m-8m-12n+8} \times (4)^{2m+3n-3} \times (6)^{4m+6n-8} \times (9)^{12m-8m-12n+8} \times 12. \]

4.1.3 Multiple Zagreb indices

By (7) and (8), we have:

\[ PM_1(G) = \prod_{pq \in E(G)} [\mu(p) + \mu(q)] \]
\[ = (2 + 2)(2m+3n-3) \times (1 + 2)^2 \times (1 + 3)^1 \]
\[ \times (2 + 3)^{4m+6n-8} \times (+2)^{6+12m-8m-12n} \]
\[ = (5)^6 \times (4)^{2m+3n-3} \times (6)^{12m-8m-12n+8} \]
\[ \times (6)^{12m-8m-12n+8} \times (4)^{2m+3n-3} \times (6)^{4m+6n-8} \times (9)^{12m-8m-12n+8} \times 12. \]

5 Results Comparisons and Discussion

A brief comparison of the indices has shown growth in the values of the calculated topological descriptors. This is clear from the Table 3 and Table 4 that values of these descriptors for \( SiC_{-III}\) are in increasing order as values of \( n \) and \( m \) are increasing. The corresponding behaviour of the graphs of these indices are shown in Figures 3-5 for some estimated values of \( n \) and \( m \).

Now we give a comparison of different Zagreb indices computed for \( SiC_{-III}\). It is clear from the Table 5 and Table 6 that the numerical values of these indices are in increasing order as values of \( n \) and \( m \) are increasing. The corresponding behaviour of the graphs of these indices are shown in Figures 8-10 for some estimated values of \( n \) and \( m \).

The topological descriptors computed in this article are used to compute the energy of electron particles \( \pi \) [15]. Thus, above mentioned comparison shown that the energy of electron particles increases as we increase the value of \( m \) and \( n \) for both types of Silicon sheets.
6 Conclusions

6.1 Applications of Zagreb Indices

The Zagreb coindex demonstrates a virtuous correlation of the materialization in heat of heptane’s and octane. Thus, our calculation done for the Zagreb coindices has shown an imperative statute for the materialization heat absorbed by heptanes and octane as their standards are in growing behaviour [26, 27].

The multiple Zagreb indices are valuable for investigations of the ingredient and pharmacological
possessions of medication in nuclear configurations. Therefore, on account of SiC₃-III[n,m], and SiC₃-III[n,m], its expanding esteems are valuable in the fast activity during synthetic reaction for drugs [28].

In [29], the authors utilized these topological descriptors to demonstrate the mitigating movement of different acids particularly in N-arylanthranilic. In [30], the authors established the fact that these descriptors are important in demonstrating the division guaranteed and leeway of cephalosporin’s inhumaness [31].

**6.2 Applications of Silicone carbides**

In Physical perspective, unadulterated silicon carbide is gotten as dry gems, along with thickness of around 3 g/mL and a peak dissolving purpose of 2730°C. Moreover, generally this is found as a somewhat blue dark, radiant crystalline strong, because of modest quantities of iron or different polluting influences from the modern generation. In synthetic perspective, silicon carbide is an entirely steady furthermore, synthetically inactive multifaceted. This is indeed incredibly tough material, usually having 9 hardness rating, which is near to the precious stone.

This is additionally portrayed by there extraordinary warm conductivity, peak temperature equality, below warm extension, protection from substance response, and capacity to work as a semiconductor. For more details, see books [32,33].

In addition, silicon carbide is broadly utilized as a rough. It is utilized to make different materials, for example, polishes, granulating wheels, spitful apparatuses, hard earthenware production, vehicle parts, recalcitrant linings, high temperature blocks, warming components, wear-safe parts for siphons and even gems. It is additionally a significant material in the hardware business and utilized for making light LEDs and semiconductor electronic devices. Moreover, Silicon carbides residue and filaments delivered during the handling found to be primary dangers of this quantifiable. The silicon carbides residue may also bother eyes, coating, and superior respiratory framework and lead to lung cancer and fibrosis. For more details, see book [34].

**6.3 Concluding Remarks**

This article is about the computation of different topological descriptors of the chemical structures SiC₃-III[n,m], and SiC₃-III[n,m]. We have computed the exact values of Zagreb type indices. The results are very useful and helpful for both chemical and pharmaceutical point of view. It gives interesting comparisons in terms of tables and three dimensional graphs.

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