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Harmonic Polynomial and Harmonic Index of Silicon Carbide Graphs $SiC_3 - I$ and $SiC_3 - II$

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Abstract. In mathematical chemistry topological index is a type of molecular descriptor that is computed based on chemical graph of chemical compound. In chemical graph atoms and bond corresponds to vertices and edges. In this paper we compute harmonic index and harmonic polynomial for silicon carbide graphs for the list of silicon carbide graphs.

Keywords: Mathematical chemistry, harmonic index, harmonic polynomial, silicon carbon.

AMS Mathematics Subject Classification (2010): 05C12, 05C90

1. Introduction

Chemical graph theory is a branch of mathematical chemistry which deals with the non-trivial applications of graph theory to solve molecular problems. In general, a graph is used to represent a molecule by considering the atoms as the vertices of the graph and the molecular bonds as the edges. Let $G(V,E)$ be a simple connected graph, with vertex set $V(G)$ and edge set $E(G)$. The number of vertices in vertex set is called the order and number of edges in edge set is called the size of graph $G(V,E)$. Degree of a vertex v is the number of vertices adjacent with that vertex v, is denoted as d_v.

Topological descriptors are derived from hydrogen-suppressed molecular graphs, in which the atoms are represented by vertices and the bonds by edges. The connections between the atoms can be described by various types of topological matrices (e.g., distance or adjacency matrices), which can be mathematically manipulated so as to derive a single number, usually known as graph invariant, graph-theoretical index or topological index. As a result, the topological index can be defined as two-dimensional descriptors that can be easily calculated from the molecular graphs, and do not depend on the way the graph is depicted or labeled and no need of energy minimization of the chemical structure. These topological indices are numeric numbers that are used to co-relate physco-chemical properties of graph, readers can see [8, 12, 13]. They are playing significant role in QSAR/QSPR studies [4], [11]. In 1975 [15], first degree based topological index was proposed by Randi c', which is defined as

$$R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-\frac{1}{2}}$$

Later on, Amic [2] and Bollobas [3] introduced general Randic' index seperately, he substituted any real number α in the place of exponent $-\frac{1}{2}$, which is defined as

$$R(G) = \sum_{uv \in E(G)} (d_u d_v)^{\alpha}$$

Harmonic index is one of the important degree based topological indices in the field of mathematical chemistry. It was introduced by Fajtlowicz in 1980 [5]. Consider a graph G with vertex set $V(G)$ and edge set $E(G)$, the harmonic index $H(G)$ for a graph G is defined as:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$$

Harmonic index is a variant of well-known Randi´c index. As compared to Randi´c index, harmonic index gives somewhat better correlations with chemical and physical properties of graphs. Recently, Hosmani et al. [6] explored the chemical applications of the harmonic index. They discovered that harmonic index is also a useful tool in predicting the heats of vaporization and critical temperatures of alkanes. They also represented explicit formulas of harmonic polynomial for different families of graphs and gave lower and upper bounds of harmonic polynomials for Caterpillar graph of diameter four. For the first time the harmonic polynomial was introduced by Iranmanesh et al. [7] as follows:

$$H(G, x) = 2 \sum_{uv \in E(G)} x^{d_u + d_v - 1}$$

The relation between harmonic index and harmonic polynomial is established as

$$H(G) = \int_0^1 H(G, x) dx.$$

2. Results and discussions

Silicon is a low cost, non-toxic, easily producible inpure form, device manufacturing semi-conductor material which is being utilized in almost all the latest electronic based devices. The 2D silicon carbon $Si - C$ single layers can be seen as tunable materials between the pure 2D carbon single layer-graphene and the pure 2D silicon single layer-silicene.

In this paper we compute exact formulas for harmonic polynomial and harmonic index for the silicon carbide graphs $SiC_3 - I[n, m]$ and $SiC_3 - II[n, m]$, where m and n are any natural numbers, for more details readers can see [1, 8]. First of all we compute harmonic polynomial and index of the silicon carbide graph $SiC_3 - I[n, m]$. The 2D structure of silicon carbide graph $SiC_3 - I[n, m], n, m \geq 1$ is shown in following figure.The left picture is of one unit cell and right picture is the sheet of $SiC_3 - I[n, m]$ for $n = 4, m = 3$. Carbon atoms C are colored red and silicon atoms Si are colored blue, red lines show how two cells are connected in a row and green lines show how two rows are connected. This structure consists of n cells (in a row) and m

connected rows. The order of the graph is $8mn$ where its size is $12mn - 2n - 3m$. For further studies and results see [1, 9, 10, 14, 16].

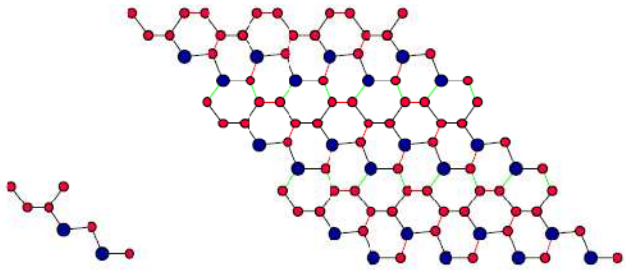

Figure 1:

Theorem 2.1. Let $G \cong SiC_3 - I[n,m]$ be the silicon carbide graph, where $m,n \in \mathbb{N}$. Then harmonic polynomial and harmonic index are equal to

1. For $n = 1, m \geq 1$

$$H(G,x) = 4x^2 + 6mx^3 + 2(6m - 4)x^4 + 2(12mn - 2n - 12m + 2)x^5.$$
$$H(G) = 4mn - \frac{2}{3}n - \frac{1}{10}m + \frac{2}{5}.$$

2. For $n > 1, m \geq 1$

$$H(G,x) = 4x^2 + 2(2n + 2m - 2)x^3 + 2(4n + 8m - 8)x^4 + 2(12mn - 8n - 13m + 8)x^5.$$
$$H(G) = 4mn - \frac{1}{15}n - \frac{2}{15}m - \frac{1}{5}.$$

Proof: From the graph of $SiC_3 - I[n,m]$ we can see that edge set of $SiC_3 - I[n,m]$ has following five partitions with $m,n \geq 1$, based on the degrees of their end vertices namely:

$$\begin{aligned}
E_{\{1,2\}} &= \{uv \in E(SiC_3 - I[n,m]) | d_u = 1, d_v = 2\},\\
E_{\{1,3\}} &= \{uv \in E(SiC_3 - I[n,m]) | d_u = 1, d_v = 3\},\\
E_{\{2,2\}} &= \{uv \in E(SiC_3 - I[n,m]) | d_u = 2, d_v = 2\},\\
E_{\{2,3\}} &= \{uv \in E(SiC_3 - I[n,m]) | d_u = 2, d_v = 3\},\\
E_{\{3,3\}} &= \{uv \in E(SiC_3 - I[n,m]) | d_u = 3, d_v = 3\},
\end{aligned}$$

The cardinalities of edge sets are

$$| E_{\{1,2\}}(SiC_3 - I[n,m]) | = 2$$
$$| E_{\{1,3\}}(SiC_3 - I[n,m]) | = 1$$

$$| E_{\{2,2\}}(SiC_3 - I[n,m]) | = \begin{cases} 3m - 1 & \text{for } n = 1, m \geq 1 \\ 2n + 2m - 3 & \text{for } n > 1, m \geq 1 \end{cases}$$

$$| E_{\{2,3\}}(SiC_3 - I[n,m]) | = \begin{cases} 6m - 4 & \text{for } n = 1, m \geq 1 \\ 4n + 8m - 8 & \text{for } n > 1, m \geq 1 \end{cases}$$

$$| E_{\{3,3\}}(SiC_3 - I[n,m]) | = \begin{cases} 12mn - 2n - 12m + 2 & \text{for } n = 1, m \geq 1 \\ 12mn - 8n - 13n + 8 & \text{for } n > 1, m \geq 1 \end{cases}$$

Now we are able to compute harmonic polynomial

1. For $n = 1, m \geq 1$

$$H(G,x) = 2\sum_{uv\in E(G)} x^{d_u+d_v-1}$$
$$= 2\sum_{uv\in E_{\{1,2\}}} x^{d_u+d_v-1} + 2\sum_{uv\in E_{\{1,3\}}} x^{d_u+d_v-1} + 2\sum_{uv\in E_{\{2,2\}}} x^{d_u+d_v-1}$$
$$+2\sum_{uv\in E_{\{2,3\}}} x^{d_u+d_v-1} + 2\sum_{uv\in E_{\{3,3\}}} x^{d_u+d_v-1}$$
$$= 2(2)x^{1+2-1} + 2(1)x^{1+3-1} + 2(3m-1)x^{2+2-1} + 2(6m-4)x^{2+3-1}$$
$$+2(12mn - 2n - 12m + 2)x^{3+3-1}$$
$$= 4x^2 + 6mx^3 + 2(6m - 4)x^4 + 2(12mn - 2n - 12m + 2)x^5$$

As a particular result harmonic index is

$$H(G) = \int_0^1 H(G,x)dx$$
$$= \int_0^1 [4x^2 + 6mx^3 + 2(6m - 4)x^4 + 2(12mn - 2n - 12m + 2)x^5]dx$$
$$= \left|(4) \times \frac{x^3}{3} + 2(3m) \times \frac{x^4}{4} + 2(6m-4) \times \frac{x^5}{5} + 2(12mn - 2n - 12m + 2) \times \frac{x^6}{6}\right|_0^1$$
$$= 4mn - \frac{2}{3}n - \frac{1}{10}m + \frac{2}{5}$$

2. For $n > 1, m \geq 1$

$$H(G,x) = 2\sum_{uv\in E(G)} x^{d_u+d_v-1}$$
$$= 2\sum_{uv\in E_{\{1,2\}}} x^{d_u+d_v-1} + 2\sum_{uv\in E_{\{1,3\}}} x^{d_u+d_v-1} + 2\sum_{uv\in E_{\{2,2\}}} x^{d_u+d_v-1}$$
$$+2\sum_{uv\in E_{\{2,3\}}} x^{d_u+d_v-1} + 2\sum_{uv\in E_{\{3,3\}}} x^{d_u+d_v-1}$$
$$= 2(2)x^{1+2-1} + 2(1)x^{1+3-1} + 2(2n + 2m - 3)x^{2+2-1}$$
$$+2(4n + 8m - 8)x^{2+3-1} + 2(12mn - 8n - 13m + 8)x^{3+3-1}$$
$$= 4x^2 + 2(2n + 2m - 3)x^3 + 2(4n + 8m - 8)x^4 + 2(12mn - 8n - 13m + 8)x^5.$$

As a particular result harmonic index is

$$H(G) = \int_0^1 H(G,x)dx$$
$$= \int_0^1 [4x^2 + 2(2n + 2m - 3)x^3 + 2(4n + 8m - 8)x^4 + 2(12mn - 8n - 13m + 8)x^5]dx$$

$$= \left|(4) \times \frac{x^3}{3} + 2(2n + 2m - 3) \times \frac{x^4}{4} + 2(4n + 8m - 8) \times \frac{x^5}{5} + 2(12mn - 8n - 13m + 8) \times \frac{x^6}{6}\right|_0^1 = 4mn - \frac{1}{15}n - \frac{1}{15}m - \frac{1}{5}.$$

Next we compute harmonic polynomial and index of silicon carbide graph ($SiC_3 - II[n, m]$), for $m, n \geq 1$. The graphical structure of ($SiC_3 - II[n, m]$) is shown in the following figure.The left picture is of one unit cell and right picture is the sheet of $SiC_3 - II[n, m]$ for $n = 4, m$ =3. Carbon atoms C are colored red and silicon atoms Si are colored blue, red lines show how two cells are connected in a row and green lines show how two rows are connected. This structure consists of n cells (in a row) and m connected rows. The order of the graph is $8mn$ where its size is $12mn - 2n - 2m$.

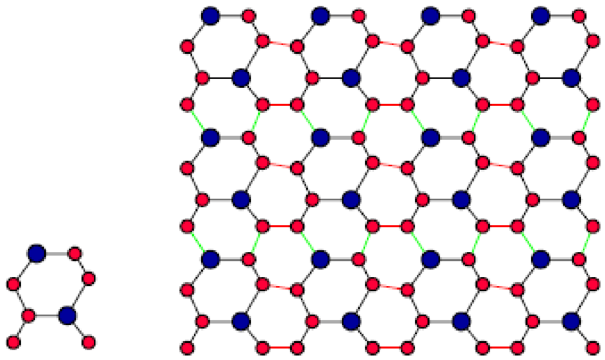

Figure 2:

Theorem 2.1. Let $G \cong SiC_3 - II[n, m]$ be the silicon carbide graph, where $m, n \in \mathbb{N}$. Then harmonic polynomial and harmonic index are equal to

$H(G, x) = 2(2n + 3)x^3 + 2(4n + 8m - 10)x^4 + 2(12mn - 8n - 10m + 7)x^5$

$H(G) = 4mn - \frac{1}{15}n - \frac{2}{15}m - \frac{1}{6}$.

Proof: From the graph of $SiC_3 - II[n, m]$ we can see that edge set of $SiC_3 - II[n, m]$ has following four partitions with $m, n \geq 1$, based on the degrees of their end vertices namely:

$$E_{\{1,3\}} = \{uv \in E(SiC_3 - II[n, m]) | d_u = 1, d_v = 3\},$$
$$E_{\{2,2\}} = \{uv \in E(SiC_3 - II[n, m]) | d_u = 2, d_v = 2\},$$
$$E_{\{2,3\}} = \{uv \in E(SiC_3 - II[n, m]) | d_u = 2, d_v = 3\},$$
$$E_{\{3,3\}} = \{uv \in E(SiC_3 - II[n, m]) | d_u = 3, d_v = 3\},$$

The cardinalities of edge sets are

$$| E_{\{1,3\}}(SiC_3 - II[n, m])| = 2$$
$$\left|E_{\{2,2\}}(SiC_3 - II[n, m])\right| = 2n + 1$$

$$| E_{\{2,3\}}(SiC_3 - II[n, m]) | = 4n + 8m - 10$$

$$|\, E_{\{3,3\}}(SiC_3 - II[n,m])\, | = 12mn - 8n - 10m + 7$$

Now we are able to compute harmonic polynomial

$$H(G,x) = 2\sum_{uv\in E(G)} x^{d_u+d_v-1}$$

$$= 2\sum_{uv\in E_{\{1,3\}}} x^{d_u+d_v-1} + 2\sum_{uv\in E_{\{2,2\}}} x^{d_u+d_v-1} + 2\sum_{uv\in E_{\{2,3\}}} x^{d_u+d_v-1}$$

$$+2\sum_{uv\in E_{\{3,3\}}} x^{d_u+d_v-1}$$

$$= 2(2)x^{1+3-1} + 2(2n+1)x^{2+2-1} + 2(4n+8m-10)x^{2+3-1}$$

$$+2(12mn-8n-10m+7)x^{3+3-1}$$

$$= 2(2n+3)x^3 + 2(4n+8m-10)x^4 + 2(12mn-8n-10m+7)x^5$$

As a particular result harmonic index is

$$H(G) = \int_0^1 H(G,x)dx$$

$$= \int_0^1 [2(2n+3)x^3 + 2(4n+8m-10)x^4$$

$$+ 2(12mn-8n-10m+7)x^5]dx$$

$$= \Big| 2(2n+3)x^3 \times \frac{x^4}{4} + 2(4n+8m-10)x^4 \times \frac{x^5}{5} + 2(12mn-8n-$$

$$10m+7) \times \frac{x^6}{6}\Big|_0^1 = 4mn - \frac{1}{15}n - \frac{2}{15}m - \frac{1}{6}.$$

3. Conclusion

In this paper, we computed harmonic polynomial and harmonic index for the silicon carbide graphs $SiC_3 - I[n,m]$ and $SiC_3 - II[n,m]$ where $m,n \geq 1$. These computations would help to investigate physical, chemical and bio-logical properties of silicon carbide graphs.

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