# On Some Ve-Degree and Harmonic Molecular Topological Properties of Carborundum

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Abstract—Carborundum, also known as silicon carbide which containing carbon and silicon, is a semiconductor. Molecular topological properties of physical substances are important tools to investigate the underlying topology of these substances. Ev-degree and ve-degree based on the molecular topological indices have been defined as parallel to their corresponding classical degree based topological indices in chemical graph theory. Classical degree based topological properties of carborundum have been investigated recently. As a continuation of these studies, in this study, we compute novel ve-degree harmonic, ve-degree sum-connectivity, ve-degree geometric-arithmetic, and ve-degree atom-bond connectivity, the first and the fifth harmonic molecular topological indices of two carborundum structures.

*Index Terms*—Carborundum, Harmonic indices, Ve-degree topological indices.

## I. Introduction

This chemical graph theory study of molecules through topological indices enables to understand and to give information about underlying topology of these molecules. These studies are important part of quantitative structure±property relationship/quantitative structure—activity relationship studies in chemistry. Topological indices are grouped into five categories: Classical degree based topological indices such as Zagreb indices, distance based topological indices such as Wiener index, eccentric connectivity indices, classical degree, and distance based topological indices such as Gutman index, and eigenvalue based topological indices such as Estrada index and matching based topological indices such as Hosoya index. In recent

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5 years period, studies of calculating topological indices of molecules have been rising.

Carborundum (silicon carbide), an inorganic compound has a crystal structure like that of diamond and is almost as hard. It is used as an abrasive for cutting, grinding, and polishing, as an antislip additive, and as a refractory. Carborundum is not a natural mineral, but rather is produced in a number of industrial processes. Carborundum has a wide range of industrial uses; in electronic applications including high voltage/high temperature semiconductor and grains bonded together to form extremely hard ceramics, which are used in car brakes and clutches, and plates in bulletproof vests. Stored energy release in neutron irradiated silicon carbide was investigated in (Snead, et al., 2019). 3-D Wire bondless switching cell using flip-chip-bonded silicon carbide power devices were investigated by Seal, Glover and Mantooth (2018). Reddy, Kesavan and Ramnath (2018), mechanical properties of aluminum 6061-silicon carbide, boron carbide metal matrix composite, were investigated. Real-time junction temperature sensing for silicon carbide MOSFET with different gate drive topologies and different operating conditions was studied in (Van der Broeck, et al., 2018). Effect of carbon nanoparticle reinforcement on mechanical and thermal properties of silicon carbide ceramics was studied in (Kaźmierczak-Bałata and Mazur, 2018). Topologically protected interface phonons in two-dimensional nanomaterials: Hexagonal boron nitride and silicon carbide were investigated by Jiang, Wang and Park (2018). Relaxation of residual microstress in reaction bonded silicon carbide was studied in (Wing and Halloran, 2018). Manufacturing isotropic carbon fiber preforms for multilayered silicon carbide composites with a pyrolytic carbon interphase was investigated in (Mei, et al., 2018). Ion irradiation-induced novel microstructural change in silicon carbide nanotubes was studied by Taguchi, Yamamoto and Ohba (2018).

Topological indices of nanostructures have been conducting by many researches recently in chemical graph theory such as (Ediz, 2010), (Ediz, 2011), (Ediz, 2013), (Munir, et al., 2016), (Gao, Asif and Nazeer, 2018), (Anjum and Safdar, 2019), and (Shao, et al., 2019).

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Molecular classical degree based topological properties of silicon carbon structures have been investigated recently in (Imran, et al., 2018). The authors calculated general Randic, Zagreb types indices, geometric arithmetic index, atom-bond connectivity (ABC) index, fourth ABC and fifth geometric arithmetic index of Si<sub>2</sub>C<sub>3</sub>-I[p,q] and Si<sub>2</sub>C<sub>3</sub>-II[p,q]. As a continuation of this study, generalized first and multiplicative Zagreb indices, the multiplicative version of the ABC index and the generalized multiplicative geometric arithmetic index of Si<sub>2</sub>C<sub>3</sub>-I[p,q] and Si<sub>2</sub>C<sub>3</sub>-II[p,q] have been investigated in (Kwun, et al., 2018). Reverse Zagreb and reverse hyper-Zagreb Indices for silicon carbide have been computed by Virk, Jhangeer and Rehman (2018).

Harmonic index was defined in (Zhong, 2012). Novel harmonic indices have been defined by Ediz, Farahani and Imran (2017). Novel ev-degree and ve-degree concepts were defined in (Chellali, et al., 2017). Moreover, novel ev-degree and ve-degree topological indices have been defined in (Ediz, 2017; Sahin and Ediz, 2018; Ediz, 2018).

The aim of this study to investigate the first, fifth, sixth harmonic, and ve-degree atom-bond connectivity (ve-ABC), geometric-arithmetic (GA), sum-connectivity, harmonic topological properties of Si<sub>2</sub>C<sub>3</sub>-I[p,q] and Si<sub>2</sub>C<sub>3</sub>-II[p,q].

## II. Preliminaries

In this section, we give some basic and preliminary concepts which we shall use later. A graph G=(V,E) consists of two nonempty sets V and 2-element subsets of V, namely E. The elements of V are called vertices and the elements of E are called edges. For a vertex V, deg(V) show the number of edges that incident to V. The set of all vertices which adjacent to V is called the open neighborhood of V and denoted by V if we add the vertex V to V is then we get the closed neighborhood of V, V is a constant.

And now we give the definitions of ev-degree and vedegree concepts which were given in Chellali, et al. (2017).

Definition 1 (ve-degree) Let G be a connected simple graph and  $v \in V(G)$ . The ve-degree of the vertex v,  $deg_{ve}(v)$ , equals the number of different edges that incident to any vertex from the closed neighborhood of v.

We also can restate the definition 1 as follows: Let G be a connected simple graph and  $v \in V(G)$ . The ve-degree of the vertex v is the number of different edges between the other vertices with a maximum distance of two from the vertex v.

Definition 2 (ev-degree), let G be a connected graph and  $e=uv \in E(G)$ . The ev-degree of the edge e,  $deg_{ev}(e)$ , equals the number of vertices of the union of the closed neighborhoods of u and v.

The authors in (Chellali, et al. 2017) also can give the definition 2 as follows: Let G be a connected graph and  $e=uv \in E(G)$ . The ev-degree of the edge e,  $deg_{uv}(e)=degu+degv-n_e$ , where  $n_e$  means the number of triangles in which the edge e lies in.

Definition 3 (ve-ABC index), let G be a connected graph and  $e=uv \in E(G)$ . The ve-ABC index of the graph G defined as;

$$ABC^{ve}(G) = \sum\nolimits_{uv \in E(G)} \sqrt{\frac{deg_{ve}u + deg_{ve}v - 2}{deg_{ve}udeg_{ve}v}} \tag{1}$$

Definition 4 (ve-degree GA [ve-GA] index), let G be a connected graph and  $v \in V(G)$ . Ve-GA index of the graph G defined as;

$$GA^{ve}(G) = \sum_{uv \in E(G)} \frac{2\sqrt{deg_{ve}udeg_{ve}v}}{deg_{ve}u + deg_{ve}v}$$
(2)

Definition 5 (ve-degree harmonic (ve-H) index), let G be a connected graph and  $uv \in E(G)$ . ve-H index of the graph G defined as;

$$H^{ve}(G) = \sum_{uv \in E(G)} \frac{2}{\deg_{ve} u + \deg_{ve} v}$$
(3)

Definition 6 (ve-degree sum-connectivity [ve- $\chi$ ] index), let G be a connected graph and  $uv \in E(G)$ . Ve- $\chi$  index of the graph G defined as;

$$\chi^{ve}(G) = \sum_{uv \in E(G)} (deg_{ve}u + deg_{ve}v)^{-1/2}$$
 (4)

Let G be a simple connected graph G=(V,E). Harmonic indices may be defined as;

$$H_{general}(G) = \sum_{uv \in E(G)} \frac{2}{Q_u + Q_v} \tag{5}$$

where  $Q_u$  is a unique parameter which is acquired from the vertex  $u \in V(G)$ .

Definition 9 (First Harmonic Index), the first kind of this Harmonic indices by considering  $Q_u$  to be the degree of the vertex u:

$$H_1(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v} \tag{6}$$

Definition 10 (Second Harmonic Index), the second kind of this class can be defined by considering  $Q_u$  to be the number  $n_u$  of vertices of G lying closer to the vertex u than to the vertex v for the edge uv of the graph G:

$$H_2(G) = \sum_{uv \in E(G)} \frac{2}{n_u + n_v} \tag{7}$$

Definition 11 (Third Harmonic Index), the third type of this class can be defined by considering  $Q_u$  to be the number  $m_u$  of edges of G lying closer to the vertex u than to the vertex v for the edge uv of the graph G:

$$H_3(G) = \sum_{uv \in E(G)} \frac{2}{m_u + m_v} \tag{8}$$

Definition 12 (Fourth Harmonic Index), the fourth type of this class can be defined by considering  $Q_u$  to be the eccentricity of the vertex u:

$$H_4(G) = \sum_{uv \in E(G)} \frac{2}{e_u + e_v} \tag{9}$$

Definition 13 (Fifth Harmonic Index), the fifth type of this class can be defined by considering  $Q_u$  to be the

$$H_5(G) = \sum_{uv \in E(G)} \frac{2}{S_u + S_v} \tag{10}$$

Definition 14 (Sixth Harmonic Index), and the sixth type of this class can be defined by considering  $Q_u$  to be the  $M_u = \prod_{v \in N(u)} d_v$ 

$$H_6(G) = \sum_{uv \in E(G)} \frac{2}{M_u + M_v}$$
 (11).

#### III. METHODS

We use combinatorial computing method such as vertex partitioning method, edge partitioning strategy, degree counting strategy, discrete partitioning, and discrete counting strategy to compute our results.

## IV. RESULTS

In Imran, et al. (2018), two-dimensional lattices of Si<sub>2</sub>C<sub>3</sub>-I[p,q] and Si<sub>2</sub>C<sub>3</sub>-II[p,q] are given in the following Figs. 1 and 2, respectively.

Note that, two rows are being connecting, carbon atom C is brown and silicon atom Si is blue and red lines (edges) connects the upper and lower rows in Fig. 1.  $Si_2C_3$ -I[p,q] has 10 pg vertices and 15pg-2p-3q edges.

Note that, two rows are connecting and green lines (edges) connect the upper and lower rows in Fig. 2. Furthermore, red lines show the connection between the unit cells in Fig. 2. Si<sub>2</sub>C<sub>2</sub>-II[p,q] has 10pg vertices and 15pg-2p-3q edges.

From Fig. 1, we give the edge partition of Si<sub>2</sub>C<sub>3</sub>-I[p,q] with respect to ve-degrees in the following Table I.

From Fig. 2, we give the edge partition of Si<sub>2</sub>C<sub>3</sub> –II[p,q] with respect to ve-degrees in the following Table II.

And we begin to compute topological indices for  $Si_2C_3$ -I[p,q]. Theorem 1

The ve-degree, the first harmonic and the fifth harmonic topological indices of the Si<sub>2</sub>C<sub>3</sub>-I[p,q] are

$$ABC^{ve}\left(Si_{2}C_{3}-I\right) == \left(15pq-14p-21q+20\right)x\sqrt{\frac{11}{42}}+q-1$$

$$+\left(p+2q-4\right)x\sqrt{\frac{7}{32}}+\left(2q+2\right)x\sqrt{\frac{2}{7}}+\left(4p+2q-7\right)x\sqrt{\frac{11}{42}}$$

$$+\left(2p+2q-5\right)x\sqrt{\frac{5}{24}}+\left(2p+2q-3\right)x\sqrt{\frac{2}{7}}+\left(2p+4q-7\right)$$

$$x\sqrt{\frac{5}{24}}+\sqrt{\frac{1}{2}}+\sqrt{\frac{2}{5}}+\sqrt{\frac{8}{25}}+\sqrt{\frac{9}{28}}+\sqrt{\frac{9}{30}}+\sqrt{\frac{13}{56}}$$

$$GA^{ve}\left(Si_{2}C_{3}-I\right) = 15pq-12p-17q+17$$

$$+\left(2q+2\right)x\frac{\sqrt{35}}{6}+\left(4p+2q-7\right)x\frac{2\sqrt{42}}{13}+\left(2q-2\right)$$

$$x\frac{4\sqrt{3}}{7}+\left(2p+2q-5\right)x\frac{4\sqrt{10}}{13}+\left(2p+2q-3\right)$$

$$\cdot x\frac{3\sqrt{7}}{8}+\left(2p+4q-7\right)x\frac{12\sqrt{2}}{17}+\frac{2\sqrt{2}}{3}$$

$$+\frac{2\sqrt{15}}{8}+\frac{4\sqrt{7}}{11}+\frac{2\sqrt{30}}{11}+\frac{4\sqrt{14}}{15}$$

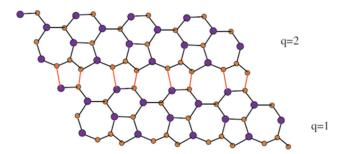


Fig. 1. Two-dimensional structure of Si, C3-I[4,2].

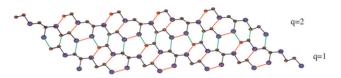


Fig. 2. Two-dimensional structure of Si<sub>2</sub>C<sub>2</sub>-II[5,2].

TABLE I VE-DEGREES OF THE END VERTICES OF  $Si_2C_3$ - $I[p_2Q]$ 

Edge	Ve-degrees of end vertices of edge	Number of edges
(2,1)	(4,2)	1
(3,1)	(5,3)	1
(2,2)	(5,5)	p+2q
(3,2)	(5,5)	1
(3,2)	(7,4)	1
(3,2)	(7,5)	2q+2
(3,2)	(5,6)	1
(3,2)	(7,6)	4p+2q-7
(3,2)	(8,6)	2q-2
(3,2)	(8,5)	2p+2q-5
(3,3)	(8,7)	1
(3,3)	(8,8)	p+2q-4
(3,3)	(9,7)	2p+2q-3
(3,3)	(9,8)	2p+4q-7
(3,3)	(9,9)	15pq-14p-21q+20

TABLE II  $\label{eq:Vedegrees} Ve\text{-degrees of the End Vertices of Si}_2C_3\text{-II}[p,\!q]$ 

Edge	Ve-degrees of end vertices of edge	Number of edges
(2,1)	(3,2)	2
(3,1)	(7,3)	1
(2,2)	(4,3)	2
(2,2)	(5,4)	2
(2,2)	(5,5)	2p+2q-4
(3,2)	(7,5)	2p+2q
(3,2)	(7,6)	2p+2q-2
(3,2)	(8,6)	2p+2q-6
(3,2)	(8,5)	2p+2q-6
(3,3)	(8,7)	2
(3,3)	(8,8)	2p+2q-8
(3,3)	(7,7)	2
(3,3)	(9,7)	2p+2q-3
(3,3)	(9,8)	2p+2q-5
(3,3)	(9,9)	15pq-19p-19q+23

$$x\frac{1}{9} + (2p + 4q - 7)x\frac{2}{17} + (p + 2q - 4)x\frac{1}{8}$$

$$+ (2p + 2q - 3)x\frac{1}{8} + (4p + 2q - 7)x\frac{2}{13} + (2q - 2)$$
•  $x\frac{1}{7} + (2p + 2q - 5)x\frac{2}{13} + (q + 1)x\frac{1}{3} + (p + 2q + 1)$ 

$$x\frac{1}{5} + \frac{2}{11} + \frac{1}{3} + \frac{1}{4} + \frac{2}{15}$$

$$x^{ve}(Si_2C_3 - I) = (15pq - 14p - 21q + 20)$$

$$x\frac{1}{3\sqrt{2}} + (2p + 4q - 7)x\frac{1}{\sqrt{17}} + (3p + 4q - 7)$$

$$x\frac{1}{4} + (2p + 2q - 5)x\frac{1}{\sqrt{13}} + (2q - 2)x\frac{1}{\sqrt{14}}$$
•  $+(4p + 2q - 7)x\frac{1}{\sqrt{13}} + (q + 1)x\frac{1}{\sqrt{3}} + (p + 2q + 1)$ 

$$x\frac{1}{\sqrt{10}} + \frac{1}{\sqrt{6}} + \frac{1}{2\sqrt{2}} + \frac{2}{\sqrt{11}} + \frac{1}{\sqrt{15}}$$

$$H_1(Si_2C_3 - I) = (15pq - 9p - 13q + 9)x\frac{1}{3} + (6p + 8q - 5)$$
•  $x\frac{2}{5} + +(p + 2q + 1)x\frac{1}{2}$ 

$$H_5(Si_2C_3 - I) = (15pq - 14p - 21q + 20)$$

$$x\frac{1}{9} + (2p + 4q - 7)x\frac{2}{17} + (p + 2q - 4)x\frac{1}{8}$$

$$+(2p + 2q - 3)x\frac{1}{8} + (4p + 2q - 7)x\frac{2}{13}$$
•  $+(2q - 2)x\frac{1}{7} + (2p + 2q - 5)x\frac{2}{13} + (q + 1)x\frac{1}{3}$ 

$$+(p + 2q + 1)x\frac{1}{5} + \frac{2}{11} + \frac{1}{3} + \frac{1}{4} + \frac{2}{11} + \frac{2}{15}$$

 $H^{ve}(Si_2C_3-I)=(15pq-14p-21q+20)$ 

Proof of Theorem 1. From Fig. 1, Table I and the definition of ve-ABC index, we can write directly;

$$ABC^{ve}(Si_{2}C_{3}-I) = \sum_{uv \in E(Si_{2}C_{3}-I)} \sqrt{\frac{deg_{ve}u + deg_{ve}v - 2}{deg_{ve}udeg_{ve}v}} =$$

$$= 1x\sqrt{\frac{4}{8}} + 1x\sqrt{\frac{6}{15}} + (p+2q)x\sqrt{\frac{6}{15}} + 1x\sqrt{\frac{8}{25}} + 1x\sqrt{\frac{9}{28}}$$

$$+ (2q+2)x\sqrt{\frac{10}{35}} + 1x\sqrt{\frac{9}{30}} + (4p+2q-7)x\sqrt{\frac{11}{42}}$$

$$+ (2q-2)x\sqrt{\frac{12}{48}} + (2p+2q-5)x\sqrt{\frac{15}{72}} + 1x\sqrt{\frac{13}{56}}$$

$$+ (p+2q-4)x\sqrt{\frac{14}{64}} + (2p+2q-3)x\sqrt{\frac{14}{63}} + (2p+4q-7)$$

$$x\sqrt{\frac{15}{72}} + (15pq-14p-21q+20)x\sqrt{\frac{11}{42}}$$

After simplification we get;

$$= (15pq - 14p - 21q + 20)x\sqrt{\frac{11}{42}}$$

$$+q - 1 + (p + 2q - 4)x\sqrt{\frac{7}{32}} + (2q + 2)x\sqrt{\frac{2}{7}}$$

$$+ (4p + 2q - 7)x\sqrt{\frac{11}{42}} + (2p + 2q - 5)x\sqrt{\frac{5}{24}}$$

$$+ (2p + 2q - 3)x\sqrt{\frac{2}{7}} + (2p + 4q - 7)x$$

$$\sqrt{\frac{5}{24}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{2}{5}} + \sqrt{\frac{8}{25}} + \sqrt{\frac{9}{28}} + \sqrt{\frac{9}{30}} + \sqrt{\frac{13}{56}}$$

Again from Fig. 1, Table I and the definition of ve-GA index, we can write directly;

$$GA^{ve}(Si_{2}C_{3}-I) = \sum_{uv \in E(Si_{2}C_{3}-I)} \frac{2\sqrt{deg_{ve}udeg_{ve}v}}{deg_{ve}u + deg_{ve}v}$$

$$= 1x \frac{2\sqrt{8}}{6} + 1x \frac{2\sqrt{15}}{8} + (p+2q)x \frac{2\sqrt{25}}{10} + 1x \frac{2\sqrt{25}}{10}$$

$$+1x \frac{2\sqrt{28}}{11} + (2q+2)x \frac{2\sqrt{35}}{12} + 1x \frac{2\sqrt{30}}{11} + (4p+2q-7)$$

$$x \frac{2\sqrt{42}}{13} + (2q-2)x \frac{2\sqrt{48}}{14} + (2p+2q-5)x \frac{2\sqrt{40}}{13}$$

$$+1x \frac{2\sqrt{56}}{15} + (p+2q-4)x \frac{2\sqrt{64}}{16} + (2p+2q-3)x \frac{2\sqrt{63}}{16}$$

$$+(2p+4q-7)x \frac{2\sqrt{72}}{17} + (15pq-14p-21q+20)x \frac{2\sqrt{81}}{18}$$

$$= 15pq-14p-21q+20+p+2q-4+p+2q$$

$$+(2q+2)x \frac{\sqrt{35}}{6} + (4p+2q-7)x \frac{2\sqrt{42}}{13} + (2q-2)$$

$$x \frac{4\sqrt{3}}{7} + (2p+2q-5)x \frac{4\sqrt{10}}{13} + (2p+2q-3)x \frac{3\sqrt{7}}{8}$$

$$+(2p+4q-7)x \frac{12\sqrt{2}}{17} + \frac{2\sqrt{2}}{3} + \frac{2\sqrt{15}}{8}$$

$$+1 + \frac{4\sqrt{7}}{11} + \frac{2\sqrt{30}}{11} + \frac{4\sqrt{14}}{15}$$

After simplification, we get it;

$$=15pq-12p-17q+17+\left(2q+2\right)x\frac{\sqrt{35}}{6}+\left(4p+2q-7\right)x\frac{2\sqrt{42}}{13}+\left(2q-2\right)x\frac{4\sqrt{3}}{7}+\left(2p+2q-5\right)x\frac{4\sqrt{10}}{13}\\+\left(2p+2q-3\right)x\frac{3\sqrt{7}}{8}+\left(2p+4q-7\right)x\frac{12\sqrt{2}}{17}\\+\frac{2\sqrt{2}}{3}+\frac{2\sqrt{15}}{8}+\frac{4\sqrt{7}}{11}+\frac{2\sqrt{30}}{11}+\frac{4\sqrt{14}}{15}$$

Now, we prove the ve-H index of Si<sub>2</sub> C<sub>3</sub>-I. From Fig. 1, Table I and the definition of ve-H index, we can write directly;

$$H^{ve}\left(Si_{2}C_{3}-I\right) = \sum_{uv \in E\left(Si_{2}C_{3}-I\right)} \frac{2}{deg_{ve}u + deg_{ve}v}$$

$$= 1x\frac{2}{6} + 1x\frac{2}{8} + (p+2q)x\frac{2}{10} + 1x\frac{2}{10} + 1x\frac{2}{11} + (2q+2)x\frac{2}{12}$$

$$+1x\frac{2}{11} + (4p+2q-7)x\frac{2}{13} + (2q-2)x\frac{2}{14} + (2p+2q-5)$$

$$x\frac{2}{13} + 1x\frac{2}{15} + (p+2q-4)x\frac{2}{16} + (2p+2q-3)x\frac{2}{16} + \binom{2p+4q-7}{4q-7}$$

$$x\frac{2}{17} + (15pq-14p-21q+20)x\frac{2}{18}$$

$$= \frac{1}{3} + \frac{1}{4} + (p+2q+1)x\frac{1}{5} + \frac{2}{11} + (q+1)x\frac{1}{3} + \frac{2}{11}$$

$$+ (4p+2q-7)x\frac{2}{13} + (2q-2)x\frac{1}{7} + (2p+2q-5)$$

$$x\frac{2}{13} + \frac{2}{15} + (p+2q-4)x\frac{1}{8} + (2p+2q-3)x\frac{1}{8}$$

$$+ (2p+4q-7)x\frac{2}{17} + (15pq-14p-21q+20)x\frac{1}{9}$$

After some simplifications, we get;

$$= (15pq - 14p - 21q + 20)x\frac{1}{9} + (2p + 4q - 7)x\frac{2}{17}$$

$$+ (p + 2q - 4)x\frac{1}{8} + (2p + 2q - 3)x\frac{1}{8} + (4p + 2q - 7)$$

$$x\frac{2}{13} + (2q - 2)x\frac{1}{7} + (2p + 2q - 5)x\frac{2}{13} + (q + 1)x\frac{1}{3}$$

$$+ (p + 2q + 1)x\frac{1}{5} + \frac{2}{11} + \frac{1}{3} + \frac{1}{4} + \frac{2}{11} + \frac{2}{15}$$

Now, we prove the ve- $\chi$  index of Si<sub>2</sub> C<sub>3</sub>-I. From Fig. 1, Table I and the definition of ve- $\chi$  index, we can write directly;

$$\chi^{ve}(Si_{2}C_{3}-I) = \sum_{uv \in E(Si_{2}C_{3}-I)} (deg_{ve}u + deg_{ve}v)^{-1/2}$$

$$= 1x \frac{1}{\sqrt{6}} + 1x \frac{1}{\sqrt{8}} + (p+2q)x \frac{1}{\sqrt{10}} + 1x \frac{1}{\sqrt{10}} + 1x \frac{1}{\sqrt{11}}$$

$$+ (2q+2)x \frac{1}{\sqrt{12}} + 1x \frac{1}{\sqrt{11}} + (4p+2q-7)x \frac{1}{\sqrt{13}}$$

$$+ (2q-2)x \frac{1}{\sqrt{14}} + (2p+2q-5)x \frac{1}{\sqrt{13}} + 1x \frac{1}{\sqrt{15}}$$

$$+ (p+2q-4)x \frac{1}{\sqrt{16}} + (2p+2q-3)x \frac{1}{\sqrt{16}} + (2p+4q-7)$$

$$x \frac{1}{\sqrt{17}} + (15pq-14p-21q+20)x \frac{1}{\sqrt{18}}$$

$$= \frac{1}{\sqrt{6}} + \frac{1}{2\sqrt{2}} + (p+2q+1)x \frac{1}{\sqrt{10}} + \frac{2}{\sqrt{11}} + (q+1)$$

$$x \frac{1}{\sqrt{3}} + (4p+2q-7)x \frac{1}{\sqrt{13}} + (2q-2)x \frac{1}{\sqrt{14}}$$

$$+ (2p+2q-5)x \frac{1}{\sqrt{13}} + \frac{1}{\sqrt{15}} + (3p+4q-7)x \frac{1}{4}$$

$$+ (2p+4q-7)x \frac{1}{\sqrt{17}} + (15pq-14p-21q+20)x \frac{1}{3\sqrt{2}}$$

After necessary simplifications, we get;

$$= (15pq - 14p - 21q + 20)x \frac{1}{3\sqrt{2}} + (2p + 4q - 7)$$

$$x \frac{1}{\sqrt{17}} + (3p + 4q - 7)x \frac{1}{4} + (2p + 2q - 5)x \frac{1}{\sqrt{13}}$$

$$+ (2q - 2)x \frac{1}{\sqrt{14}} + (4p + 2q - 7)x \frac{1}{\sqrt{13}} + (q + 1)$$

$$x \frac{1}{\sqrt{3}} + (p + 2q + 1)x \frac{1}{\sqrt{10}} + \frac{1}{\sqrt{6}} + \frac{1}{2\sqrt{2}} + \frac{2}{\sqrt{11}} + \frac{1}{\sqrt{15}}$$

Now, we prove the first harmonic index of Si<sub>2</sub> C<sub>3</sub>-I. From Fig. 1, Table I and the definition of the first harmonic index, we can write directly;

$$H_1\left(Si_2C_3 - I\right) = \sum_{uv \in E(GSi_2C_3 - I)} \frac{2}{d_u + d_v}$$

$$= 1x\frac{2}{3} + 1x\frac{2}{4} + (p + 2q)x\frac{2}{4} + 1x\frac{2}{5} + 1x\frac{2}{5} + (2q + 2)$$

$$x\frac{2}{5} + 1x\frac{2}{5} + (4p + 2q - 7)x\frac{2}{5} + (2q - 2)x\frac{2}{5} + {2p + 2q - 5}x\frac{2}{5}$$

$$+1x\frac{2}{6} + (p + 2q - 4)x\frac{2}{6} + (2p + 2q - 3)x\frac{2}{6}$$

$$+(2p + 4q - 7)x\frac{2}{6} + (15pq - 14p - 21q + 20)x\frac{2}{6}$$

After necessary simplifications, we can write that;

$$= \frac{2}{3} + \frac{1}{2} + (p+2q)x\frac{1}{2} + \frac{2}{5} + \frac{2}{5} + (2q+2)x\frac{2}{5} + \frac{2}{5}$$

$$+ (4p+2q-7)x\frac{2}{5} + (2q-2)x\frac{2}{5} + (2p+2q-5)x\frac{2}{5}$$

$$+ \frac{1}{3} + (p+2q-4)x\frac{1}{3} + (2p+2q-3)x\frac{1}{3} + \binom{2p+4q}{-7}$$

$$x\frac{1}{3} + (15pq-14p-21q+20)x\frac{1}{3}$$

$$= (15pq-9p-13q+9)x\frac{1}{3} + (6p+8q-5)x\frac{2}{5} + (p+2q+1)x\frac{1}{2}$$

And now, we prove the fifth harmonic index of Si<sub>2</sub> C<sub>3</sub>-I. From Fig. 1, Table I and the definition of the fifth harmonic index, we can write directly;

$$H_5(Si_2C_3 - I) = \sum_{uv \in E(Si_2C_3 - I)} \frac{2}{S_u + S_v}$$

$$= 1x\frac{2}{6} + 1x\frac{2}{8} + (p + 2q)x\frac{2}{10} + 1x\frac{2}{10} + 1x\frac{2}{11} + (2q + 2)$$

$$x\frac{2}{12} + 1x\frac{2}{11} + (4p + 2q - 7)x\frac{2}{13} + (2q - 2)x\frac{2}{14} + \binom{2p}{+2q - 5}$$

$$x\frac{2}{13} + 1x\frac{2}{15} + (p + 2q - 4)x\frac{2}{16} + (2p + 2q - 3)x\frac{2}{16}$$

$$+ (2p + 4q - 7)x\frac{2}{17} + (15pq - 14p - 21q + 20)x\frac{2}{18}$$

$$= \frac{1}{3} + \frac{1}{4} + (p+2q+1)x\frac{1}{5} + \frac{2}{11} + (q+1)x\frac{1}{3}$$

$$+ \frac{2}{11} + (4p+2q-7)x\frac{2}{13} + (2q-2)x\frac{1}{7}$$

$$+ (2p+2q-5)x\frac{2}{13} + \frac{2}{15} + (p+2q-4)x\frac{1}{8}$$

$$+ (2p+2q-3)x\frac{1}{8} + (2p+4q-7)$$

$$x\frac{2}{17} + (15pq-14p-21q+20)x\frac{1}{9}$$

After necessary simplifications, we can write that;

$$= (15pq - 14p - 21q + 20)x\frac{1}{9}$$

$$+ (2p + 4q - 7)x\frac{2}{17} + (p + 2q - 4)$$

$$x\frac{1}{8} + (2p + 2q - 3)x\frac{1}{8} + (4p + 2q - 7)x\frac{2}{13}$$

$$+ (2q - 2)x\frac{1}{7} + (2p + 2q - 5)x\frac{2}{13} + (q + 1)x\frac{1}{3}$$

$$+ (p + 2q + 1)x\frac{1}{5} + \frac{2}{11} + \frac{1}{3} + \frac{1}{4} + \frac{2}{11} + \frac{2}{15}$$

And now, we begin to compute topological indices for  $Si_2C_3$ -II[p,q].

Theorem 2

The ve-degree, the first and the fifth harmonic topological indices of the  $Si_2C_3$ -II[p,q] are

$$ABC^{ve}\left(Si_{2}C_{3}-II\right) = (15pq-19p-19q+23)$$

$$x\frac{4}{9}+p+q-3+(2p+2q-5)x\sqrt{\frac{5}{24}}$$

$$+(2p+2q-3)x\sqrt{\frac{14}{63}}+(2p+2q-8)x\sqrt{\frac{7}{32}}$$

$$+(2p+2q-6)x\sqrt{\frac{11}{40}}+(2p+2q-2)x\sqrt{\frac{11}{42}}+$$

$$+(2p+2q)x\sqrt{\frac{10}{35}}+(2p+2q-4)x\sqrt{\frac{8}{25}}+\sqrt{2}+\sqrt{\frac{8}{21}}$$

$$+2x\sqrt{\frac{5}{12}}+\sqrt{\frac{7}{5}}+\sqrt{\frac{13}{14}}+4x\sqrt{\frac{3}{49}}$$

$$GA^{ve}\left(Si_{2}C_{3}-II\right) = 15pq-15p-15q+(2p+2q)$$

$$x\frac{2\sqrt{35}}{12}+(2p+2q-2)x\frac{2\sqrt{42}}{13}+(2p+2q-6)$$

$$x\frac{4\sqrt{3}}{7}+(2p+2q-6)x\frac{8\sqrt{10}}{13}+(2p+2q-3)$$

$$x\frac{6\sqrt{7}}{16}+(2p+2q-5)x\frac{12\sqrt{2}}{17}+13+\frac{4\sqrt{6}}{5}$$

$$+\frac{\sqrt{21}}{5}+\frac{8\sqrt{2}}{7}+\frac{8\sqrt{5}}{9}+\frac{16\sqrt{7}}{15}$$

$$H^{ve}(Si_{2}C_{3}-II) = \frac{4}{5} + \frac{1}{5} + \frac{6}{7} + \frac{4}{9} + (2p+2q-4)x\frac{1}{5}$$

$$+(p+q)x\frac{1}{3} + (2p+2q-2)x\frac{2}{13} + \binom{2p}{+2q-6}x\frac{1}{7} + \binom{2p}{+2q-6}$$

$$\cdot x\frac{2}{13} + \frac{4}{15} + \binom{2p}{+2q-8}x\frac{1}{8} + \binom{2p}{+2q-3}x\frac{1}{8} + \binom{2p}{+2q-5}x\frac{2}{17}$$

$$+(15pq-19p-19q+23)x\frac{1}{9}$$

$$\chi^{ve}(Si_{2}C_{3}-II) = \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{10}} + \frac{2}{\sqrt{7}} + \frac{2}{3} + \frac{2}{\sqrt{15}} + \frac{2}{\sqrt{14}}$$

$$+\binom{2p+2q}{-4}x\frac{1}{\sqrt{16}} + (p+q)x\frac{1}{\sqrt{3}} + \binom{2p+2q}{-2}x\frac{1}{\sqrt{13}}$$

$$\cdot +\binom{2p+}{2q-6}x\frac{1}{\sqrt{16}} + (2p+2q-6)x\frac{1}{\sqrt{17}} + \binom{15pq-19p}{-19q+23}x\frac{1}{3\sqrt{2}}$$

$$+\binom{2p+}{2q-3}x\frac{1}{\sqrt{16}} + \binom{2p+}{2q-5}x\frac{2}{\sqrt{17}} + \binom{15pq-19p}{-19q+23}x\frac{1}{3\sqrt{2}}$$

$$+I_{1}(Si_{2}C_{3}-II) = 5+p+q+(8p+8q-14)x\frac{2}{5}$$

$$+(15pq-13p-13q+9)x\frac{1}{3}$$

$$+I_{2}(GSi_{2}C_{3}-II) = \frac{4}{5} + \frac{1}{5} + \frac{6}{7} + \frac{4}{9} + \binom{2p}{+2q-4}x\frac{1}{5}$$

$$+(p+q)x\frac{1}{3} + \binom{2p}{+2q-2}x\frac{2}{13} + \binom{2p}{+2q-6}x\frac{1}{7} + \binom{2p}{+2q-6}$$

$$\cdot x\frac{2}{13} + \frac{4}{15} + \binom{2p}{+2q-8}x\frac{1}{8} + \binom{2p}{+2q-3}x\frac{1}{8} + \binom{2p}{+2q-5}x\frac{2}{17}$$

$$+(15pq-19p-19q+23)x\frac{1}{9}$$

Proof of Theorem 2

From Fig. 2, Table II and the definition of ve-ABC index, we can write directly;

$$ABC^{ve}\left(Si_{2}C_{3}-II\right) = \sum_{uv \in E\left(Si_{2}C_{3}-I\right)} \sqrt{\frac{deg_{ve}u + deg_{ve}v - 2}{deg_{ve}udeg_{ve}v}}$$

$$= 2x\sqrt{\frac{3}{6}} + 1x\sqrt{\frac{8}{21}} + 2x\sqrt{\frac{5}{12}} + 2x\sqrt{\frac{7}{20}} + (2p + 2q - 4)$$

$$x\sqrt{\frac{8}{25}} + (2p + 2q)x\sqrt{\frac{10}{35}} + (2p + 2q - 2)x\sqrt{\frac{11}{42}}$$

$$+ (2p + 2q - 6)x\sqrt{\frac{12}{48}} + (2p + 2q - 6)x\sqrt{\frac{11}{40}} + 2x\sqrt{\frac{13}{56}}$$

$$+ (2p + 2q - 8)x\sqrt{\frac{14}{64}} + 2x\sqrt{\frac{12}{49}} + \binom{2p}{+2q - 3}x\sqrt{\frac{14}{63}}$$

$$+ (2p + 2q - 5)x\sqrt{\frac{15}{72}} + \binom{15pq - 19p}{-19q + 23}x\sqrt{\frac{16}{81}}$$

After necessary simplifications we get;

$$= (15pq - 19p - 19q + 23)x\frac{4}{9} + p + q - 3 + (2p + 2q - 5)$$

$$x\sqrt{\frac{5}{24}} + (2p + 2q - 3)x\sqrt{\frac{14}{63}} + (2p + 2q - 8)x\sqrt{\frac{7}{32}}$$

$$+ (2p + 2q - 6)x\sqrt{\frac{11}{40}} + (2p + 2q - 2)x\sqrt{\frac{11}{42}}$$

$$+ (2p + 2q)x\sqrt{\frac{10}{35}} + (2p + 2q - 4)x\sqrt{\frac{8}{25}} + \sqrt{2}$$

$$+\sqrt{\frac{8}{21}} + 2x\sqrt{\frac{5}{12}} + \sqrt{\frac{7}{5}} + \sqrt{\frac{13}{14}} + 4x\sqrt{\frac{3}{49}}$$

And now, we prove the ve-GA index of Si<sub>2</sub> C<sub>3</sub>-II. From Fig. 2, Table II and the definition of ve-GA index, we can write directly;

$$GA^{ve}(Si_{2}C_{3}-II) = \sum_{uv \in E(Si_{2}C_{3}-II)} \frac{2\sqrt{deg_{ve}udeg_{ve}v}}{deg_{ve}u + deg_{ve}v}$$

$$= 15pq - 19p - 19q + 23 + 2 + 2p + 2q - 8 + 2p + 2q - 4$$

$$+ \frac{4\sqrt{6}}{5} + \frac{\sqrt{21}}{5} + \frac{8\sqrt{2}}{7} + \frac{8\sqrt{5}}{9} + (2p + 2q)x\frac{2\sqrt{35}}{12} + \binom{2p}{+2q - 2}$$

$$x\frac{2\sqrt{42}}{13} + (2p + 2q - 6)x\frac{4\sqrt{3}}{7} + (2p + 2q - 6)x\frac{8\sqrt{10}}{13}$$

$$+ \frac{16\sqrt{7}}{15} + (2p + 2q - 3)x\frac{6\sqrt{7}}{16} + (2p + 2q - 5)x\frac{12\sqrt{2}}{17}$$

After necessary simplifications, we can write that;

$$=15pq-15p-15q+(2p+2q)x\frac{2\sqrt{35}}{12}+(2p+2q-2)$$

$$x\frac{2\sqrt{42}}{13}+(2p+2q-6)x\frac{4\sqrt{3}}{7}+(2p+2q-6)x\frac{8\sqrt{10}}{13}$$

$$+(2p+2q-3)x\frac{6\sqrt{7}}{16}+(2p+2q-5)x\frac{12\sqrt{2}}{17}$$

$$+13+\frac{4\sqrt{6}}{5}+\frac{\sqrt{21}}{5}+\frac{8\sqrt{2}}{7}+\frac{8\sqrt{5}}{9}+\frac{16\sqrt{7}}{15}$$

And now, we prove the ve-H index of Si<sub>2</sub> C<sub>3</sub>-II. From Fig. 2, Table II and the definition of ve-H index, we can write directly;

$$H^{ve}(Si_{2}C_{3}-II) = \sum_{uv \in E(Si_{2}C_{3}-II)} \frac{2}{deg_{ve}u + deg_{ve}v}$$

$$= 2x\frac{2}{5} + 1x\frac{2}{10} + 2x\frac{2}{7} + 2x\frac{2}{9} + (2p + 2q - 4)x\frac{2}{10}$$

$$+ (2p + 2q)x\frac{2}{12} + (2p + 2q - 2)x\frac{2}{13} + (2p + 2q - 6)x\frac{2}{14}$$

$$+ (2p + 2q - 6)x\frac{2}{13} + 2x\frac{2}{15} + (2p + 2q - 8)x\frac{2}{16}$$

$$+ 2x\frac{2}{14} + (2p + 2q - 3)x\frac{2}{16} + (2p + 2q - 5)x\frac{2}{17}$$

$$+ (15pq - 19p - 19q + 23)x\frac{2}{18}$$

After necessary simplifications, we can write that,

$$= \frac{4}{5} + \frac{1}{5} + \frac{6}{7} + \frac{4}{9} + (2p + 2q - 4)x\frac{1}{5} + (p + q)x\frac{1}{3}$$

$$+ (2p + 2q - 2)x\frac{2}{13} + (2p + 2q - 6)x\frac{1}{7} + (2p + 2q - 6)$$

$$x\frac{2}{13} + \frac{4}{15} + (2p + 2q - 8)x\frac{1}{8} + (2p + 2q - 3)x\frac{1}{8} + {2p \choose +2q - 5}$$

$$x\frac{2}{17} + (15pq - 19p - 19q + 23)x\frac{1}{9}$$

And now, we prove the ve- $\chi$  index of Si<sub>2</sub> C<sub>3</sub>-II. From Fig. 2, Table II and the definition of ve- $\chi$  index, we can write directly:

$$\chi^{ve}\left(Si_{2}C_{3}-II\right) = \sum_{uv \in E(GSi_{2}C_{3}-II)} (deg_{ve}u + deg_{ve}v)^{-1/2}$$

$$= 2x\frac{1}{5} + 1x\frac{1}{10} + 2x\frac{1}{7} + 2x\frac{1}{9} + (2p + 2q - 4)x\frac{1}{10}$$

$$+ (2p + 2q)x\frac{1}{12} + (2p + 2q - 2)x\frac{1}{13} + (2p + 2q - 6)$$

$$x\frac{1}{14} + (2p + 2q - 6)x\frac{1}{13} + 2x\frac{1}{15} + (2p + 2q - 8)$$

$$x\frac{1}{16} + 2x\frac{1}{14} + (2p + 2q - 3)x\frac{1}{16} + (2p + 2q - 5)$$

$$x\frac{1}{17} + (15pq - 19p - 19q + 23)x\frac{1}{18}$$

After some necessary simplifications, we can directly write that;

$$= \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{10}} + \frac{2}{\sqrt{7}} + \frac{2}{3} + \frac{2}{\sqrt{15}} + \frac{2}{\sqrt{14}} + (2p + 2q - 4)$$

$$x \frac{1}{\sqrt{10}} + (p+q)x \frac{1}{\sqrt{3}} + (2p + 2q - 2)x \frac{1}{\sqrt{13}}$$

$$+ (2p + 2q - 6)x \frac{1}{\sqrt{14}} + (2p + 2q - 6)x \frac{1}{\sqrt{13}}$$

$$+ (p+q-4)x \frac{1}{2} + (2p + 2q - 3)x \frac{1}{\sqrt{16}} + (2p + 2q - 5)$$

$$x \frac{2}{\sqrt{17}} + (15pq - 19p - 19q + 23)x \frac{1}{3\sqrt{2}}$$

And now, we prove the first harmonic index of Si<sub>2</sub> C<sub>3</sub>-II. From Fig. 2, Table II and the definition of the first harmonic index, we can write directly;

$$\begin{split} H_1 \Big( Si_2 C_3 - II \Big) &= \sum_{uv \in E(Si_2 C_3 - II)} \frac{2}{d_u + d_v} \\ &= 2x \frac{2}{3} + 1x \frac{2}{4} + 2x \frac{2}{4} + 2x \frac{2}{4} + \binom{2p}{+2q - 4} x \frac{2}{4} \\ &+ (2p + 2q)x \frac{2}{5} + (2p + 2q - 2)x \frac{2}{5} + \binom{2p}{+2q - 6} \\ &x \frac{2}{5} + \binom{2p}{+2q - 6} x \frac{2}{5} + 2x \frac{2}{6} + \binom{2p}{+2q - 8} x \frac{2}{6} + 2x \frac{2}{6} \\ &+ \binom{2p +}{2q - 3} x \frac{2}{6} + \binom{2p}{+2q - 5} x \frac{2}{6} + \binom{15pq - 19p}{-19q + 23} x \frac{2}{6} \end{split}$$

After necessary simplifications, we get;

$$= 5 + p + q + (8p + 8q - 14)x + \frac{2}{5} + (15pq - 13p - 13q + 9)x + \frac{1}{3}$$

And now, we prove the fifth harmonic index of Si<sub>2</sub> C<sub>3</sub>-II. From Fig. 2, Table II and the definition of the fifth harmonic index, we can write directly;

$$\begin{split} H_5 \left( GSi_2 C_3 - II \right) &= \sum_{uv \in E(GSi_2 C_3 - II)} \frac{2}{S_u + S_v} \\ &= 2x \frac{2}{5} + 1x \frac{2}{10} + 2x \frac{2}{7} + 2x \frac{2}{9} + \left( 2p + 2q - 4 \right) x \frac{2}{10} \\ &+ \left( 2p + 2q \right) x \frac{2}{12} + \left( 2p + 2q - 2 \right) x \frac{2}{13} + \left( 2p + 2q - 6 \right) \\ &x \frac{2}{14} + \left( 2p + 2q - 6 \right) x \frac{2}{13} + 2x \frac{2}{15} + \left( 2p + 2q - 8 \right) x \frac{2}{16} + \\ &2x \frac{2}{14} + \left( 2p + 2q - 3 \right) x \frac{2}{16} + \left( 2p + 2q - 5 \right) x \frac{2}{17} \\ &+ \left( 15pq - 19p - 19q + 23 \right) x \frac{2}{18} \end{split}$$

After necessary simplifications, we get;

$$= \frac{4}{5} + \frac{1}{5} + \frac{6}{7} + \frac{4}{9} + (2p + 2q - 4)x\frac{1}{5} + (p + q)x\frac{1}{3}$$

$$+ (2p + 2q - 2)x\frac{2}{13} + (2p + 2q - 6)x\frac{1}{7}$$

$$+ (2p + 2q - 6)x\frac{2}{13} + \frac{4}{15} + (2p + 2q - 8)x\frac{1}{8}$$

$$+ (2p + 2q - 3)x\frac{1}{8} + (2p + 2q - 5)x\frac{2}{17}$$

$$+ (15pq - 19p - 19q + 23)x\frac{1}{9}$$

# V. Conclusions

In this study, we calculated the ve-ABC, ve-GA, ve-H, and ve- $\chi$ , the first harmonic and the fifth harmonic molecular topological properties of the two silicon carbide structures: Si<sub>2</sub> C<sub>3</sub>-I and Si<sub>2</sub> C<sub>3</sub>-II. These calculations enable to understand and to give information about the underlying topology of Si<sub>2</sub> C<sub>3</sub>-I and Si<sub>2</sub> C<sub>3</sub>-II.

Mathematical properties of ev-degree, ve-degree, and novel harmonic topological indices are interesting studies for further studies. It is also interesting to compute ve-degree based topological indices and novel harmonic indices of naostructures and molecules for further studies.

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