

COMPUTING TOPOLOGICAL INDICES OF SiO₂ LAYER STRUCTURE AND BENZENOID SERIES

M.H. MUHAMMAD^{†1,2}, J.L.G. GUIRAO[‡], N.A. REHMAN[§] and M.K. SIDDIQUI^{§§}

^{†1} College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou, 450001, China,

^{†2} School of Chemical Engineering and energy, Zhengzhou University, Zhengzhou 450001, China
mehwish@foxmail.com

[‡] Department of Mathematics, Matemática Aplicada y Estadística, Universidad Politécnica de Cartagena, 30203-Cartagena, Región de Murcia, Spain, juan.garcia@upct.es

[§] Department of Mathematics, Comsats University Islamabad, Sahiwal campus, 57000, Pakistan, najma_ar@hotmail.com

^{§§} Department of Mathematics, Comsats University Islamabad, Lahore campus, 54000, Pakistan, kamransiddiqui75@gmail.com

Abstract— A molecular graph can be transformed using map operations, one of these, named Capra, being defined by Diudea (2005). Topological indices are closely related to the toxicological, physicochemical, pharmacological properties of a chemical compound. These topological indices correlate certain physicochemical properties like boiling point, stability and strain energy of chemical compounds. In this paper, we focus on the Silicate SiO₂ layer structure and the structure of Capra-designed planar benzenoid series $Ca_k(C_6)$, ($k \geq 0$). We determined Zagreb type indices, Forgotten index, Augmented index and Balaban index for these structures.

Keywords— Zagreb types indices; Forgotten, Augmented and Balaban index; Silicate; benzenoid series.

I. INTRODUCTION

Molecules and molecular compounds are often modeled by molecular graphs. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds.

The Silicon oxide SiO₂ samples were prepared for different analysis by cleaning in organic solvents, and chemical etching in aqueous solution of hydrofluoric acid. There were examined samples exposed to air oxidation for a long period of time together with samples maintained for 2-3 hours in atmosphere after a chemical etching as well as chemical etched fresh samples.

A graph $G(V, E)$ with vertex set V and edge set E is connected, if there exists a connection between any pair of vertices in G . A *network* is simply a connected graph having no multiple edges and no loops. For a graph G , the degree of a vertex v is the number of edges incident with v and denoted by $\gamma(v)$. The total number of vertices in the graph is called order of the graph and the total number of edges in the graph is called the size of the graph.

A topological index is a numeric quantity associated with a graph which characterizes the topology of the graph and is invariant under graph automorphism. There

are some major classes of topological indices such as distance based topological indices, degree based topological indices and counting related polynomials and indices of graphs. The concept of topological index came from work done by Wiener (1947) while he was working on boiling point of paraffin. He named this index as *path number*. Later on, the path number was renamed as Wiener index. The *Wiener index* is the first and most studied topological index, both from theoretical point of view and applications, and defined as the sum of distances between all pairs of vertices in G , for more details see Gutman and Polansky (1986). Also, in the same paper of Wiener, another topological index Wiener polarity index was proposed. Wiener index and Wiener polarity index can characterize the chemical and physical properties of molecules (see Du *et al.*, 2009).

One of the oldest topological indices is the first Zagreb index introduced by Gutman and Trinajstić (1972) based on degree of vertices of G . The first and second Zagreb indices of a graph G are defined as:

$$M_1(G) = \sum_{u,v \in E(G)} [\gamma(u) + \gamma(v)], \quad (1)$$

$$M_2(G) = \sum_{u,v \in E(G)} [\gamma(u) \times \gamma(v)]. \quad (2)$$

Shirdel *et al.* (2013) introduced a new degree based Zagreb index named “hyper-Zagreb index” as:

$$HM(G) = \sum_{u,v \in E(G)} [\gamma(u) + \gamma(v)]^2. \quad (3)$$

Ghorbani and Azimi (2012) defined two new versions of Zagreb indices of a graph G . The first multiple Zagreb index $PM_1(G)$, second multiple Zagreb index $PM_2(G)$ and these indices are defined as:

$$PM_1(G) = \prod_{u,v \in E(G)} [\gamma(u) + \gamma(v)]. \quad (4)$$

$$PM_2(G) = \prod_{u,v \in E(G)} [\gamma(u) \times \gamma(v)]. \quad (5)$$

For further new result about multiple Zagreb indices see Gao *et al.* (2017) and Gharibi *et al.* (2016).

The first Zagreb polynomial $M_1(G, x)$ and second Zagreb polynomial $M_2(G, x)$ are defined as:

$$M_1(G, x) = \sum_{u,v \in E(G)} x^{[\gamma(u) + \gamma(v)]}, \quad (6)$$

$$M_2(G, x) = \sum_{u,v \in E(G)} x^{[\gamma(u) \times \gamma(v)]}. \quad (7)$$

Some recent result about Zagreb polynomials can be found from Idrees *et al.* (2017); Imran *et al.* (2018a) and Kang *et al.* (2018a,b).

Followed by the first and second Zagreb indices, Furtula and Gutman (2015) introduced forgotten topological index (also called F-index) which was defined as:

$$F(G) = \sum_{u,v \in E(G)} (\gamma(u)^2 + \gamma(v)^2). \quad (8)$$

Furtula *et al.* (2013) raised that the predictive ability of forgotten topological index is almost similar to that of first Zagreb index and for the acentric factor and entropy, and both of them obtain correlation coefficients larger than 0.95. This fact implies the reason why forgotten topological index is useful for testing the chemical and pharmacological properties of drug molecular structures. Sun *et al.* (2014) deduced some basic nature of forgotten topological index and reported that this index can reinforce the physico-chemical flexibility of Zagreb indices. Very recently, Gao *et al.* (2016a) manifested the forgotten topological index of some significant drug molecular structures (see also Basavanagoud *et al.* 2017).

Motivated by the success of the ABC index, Furtula *et al.* (2010) put forward its modified version, that they somewhat inadequately named augmented Zagreb index and is defined as:

$$AZI(G) = \sum_{u,v \in E(G)} \left(\frac{\gamma(u) \times \gamma(v)}{\gamma(u) + \gamma(v) - 2} \right)^3. \quad (9)$$

Another topological index based on the degree of the vertex is the Balaban index (Balaban, 1982). This index for a graph G of order N , size M is defined as:

$$J(G) = \frac{M}{M-N+2} \sum_{u,v \in E(G)} \frac{1}{\sqrt{\gamma(u) \times \gamma(v)}}. \quad (10)$$

For further study of Balaban index about various graph families see Gutman (2013), Ramane and Jumman- naver (2016) and Siddiqui *et al.* (2016a).

II. APPLICATIONS OF TOPOLOGICAL INDICES

The atom bond connectivity index (ABC) is a topological descriptor that has correlated with a lot of chemical characteristics of the molecules and has been found to be parallel to computing the boiling point and Kovats constants of the molecules (see Farahani *et al.*, 2016; Furtula *et al.*, 2013; Gao *et al.*, 2016b,c). Moreover, the atom bond connectivity (ABC) index provides a very good correlation for the stability of linear alkanes as well as the branched alkanes and for computing the strain energy of cyclo alkanes (Gao and Siddiqui, 2017; Gao *et al.*, 2018). To correlate with certain physico-chemical properties, GA index has much better predictive power than the predictive power of the Randic connectivity index (Siddiqui *et al.*, 2016b).

The first Zagreb index and second Zagreb index were found to occur for computation of the total π -electron energy of the molecules within specific approximate expressions (Gutman *et al.*, 1975; Imran *et al.*, 2018b). These are among the graph invariants, who were proposed for measurement of skeleton of branching of the carbon-atom Gutman and Trinajstić (1972) and Gutman and Das (2004).

III. RESULTS FOR SiO_2 LAYER STRUCTURE

The silicates (SiO_2) consist of one silicon ion and four oxygen ions, as shown in Fig. 1(a). Silicates from various

systems, in light of their polymerization yet the systems are normally persuaded by the first silicate arrange. Silicate SiO_2 , in its naturally occurring form, forms an octagon of sorts as shown in Fig. 1(b).

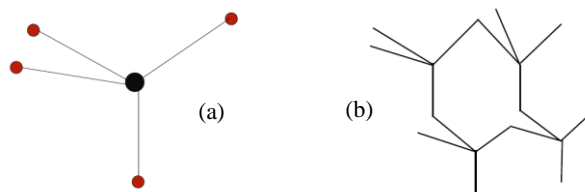


Figure 1. (a) SiO_2 ion (b) SiO_2 octagon.

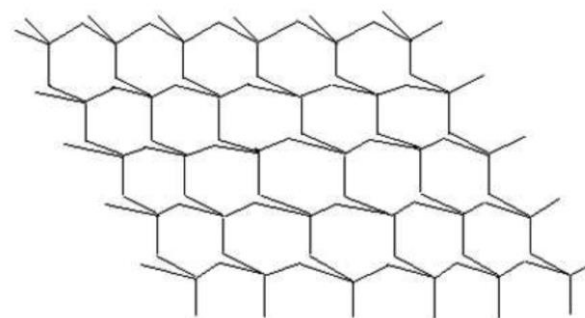


Figure 2. $SiO_2(4,5)$.

Table 1: (d_u, d_v) -type edge partition of SiO_2 .

$\gamma(u), \gamma(v)$	No. of edges
(1,4)	$2p+2q+4$
(2,4)	$2p+2q+4pq$

And finally, these octagons join together to form the SiO_2 layer structure. We define the rows as the number of lines of vertical octagons and columns as the number of lines of horizontal octagons. We denote the number of rows with p and the number of columns with q . Moreover, it is easy to see that the order of SiO_2 is $4pq+5q+1$ and size is $4pq+4(p+q)+4$. Figure 2 gives the SiO_2 layer structure with $p=4$ and $q=5$. The concept can be extended to any number of rows and columns.

Let G be a graph of Silicate SiO_2 layer structure. The edge set is partitioned into two sets, say, $E_1(SiO_2)$, $E_2(SiO_2)$, based on the degree of end vertices of each edge. First the set $E_1(SiO_2)$ contains $2p+2q+4$ edges of type uv such that $\gamma(u) = 1, \gamma(v) = 4$ and the set $E_2(SiO_2)$ contains $2p+2q+4pq$ edges of type uv such that $\gamma(u) = 2, \gamma(v) = 4$. More precisely the edge partition of the Silicate SiO_2 with respect to degrees of the end-vertices of edges is given by Table 1.

Now we compute first Zagreb index, second Zagreb, hyper-Zagreb index $HM(G)$, first multiple Zagreb index $PM_1(G)$, second multiple Zagreb index $PM_2(G)$ and Zagreb polynomials $M_1(G, x)$, $M_2(G, x)$ for Silicate SiO_2 as follows.

A. The first and second Zagreb indices of SiO_2

Now using Eqs. (1-2), we have:

$$M_1(G) = \sum_{u,v \in E(G)} [\gamma(u) + \gamma(v)],$$

$$\begin{aligned}
 M_1(SiO_2) &= \sum_{u,v \in E_1(SiO_2)} [\gamma(u) + \gamma(v)] \\
 &+ \sum_{u,v \in E_2(SiO_2)} [\gamma(u) + \gamma(v)] \\
 &= 5|E_1(SiO_2)| + 6|E_2(SiO_2)|, \\
 M_1(SiO_2) &= 5 \times (2p + 2q + 4) + 6 \times (2p + 2q + 4pq) \\
 &= 22p + 22q + 24pq + 20. \\
 M_2(G) &= \sum_{u,v \in E(G)} [\gamma(u) \times \gamma(v)], \\
 M_2(SiO_2) &= \sum_{u,v \in E_1(SiO_2)} [\gamma(u) \times \gamma(v)] \\
 &+ \sum_{u,v \in E_2(SiO_2)} [\gamma(u) \times \gamma(v)] \\
 &= 4|E_1(SiO_2)| + 8|E_2(SiO_2)|, \\
 M_2(SiO_2) &= 4 \times (2p + 2q + 4) + 8 \times (2p + 2q + 4pq) \\
 &= 24p + 24q + 32pq + 16.
 \end{aligned}$$

B. The Hyper Zagreb index of SiO_2

Now using Eq. (3), we have:

$$\begin{aligned}
 HM(G) &= \sum_{u,v \in E(G)} [\gamma(u) + \gamma(v)]^2, \\
 HM(SiO_2) &= \sum_{u,v \in E_1(SiO_2)} [\gamma(u) + \gamma(v)]^2 \\
 &+ \sum_{u,v \in E_2(SiO_2)} [\gamma(u) + \gamma(v)]^2 \\
 &= 25|E_1(SiO_2)| + 36|E_2(SiO_2)|, \\
 HM(SiO_2) &= 25 \times (2p + 2q + 4) + 36 \times (2p + 2q + 4pq) \\
 &= 122p + 122q + 144pq + 100.
 \end{aligned}$$

C. The first and second Multiple Zagreb indices of SiO_2

Now using Eqs. (4-5), we get our required result as follows:

$$\begin{aligned}
 PM_1(G) &= \prod_{u,v \in E(G)} [\gamma(u) + \gamma(v)] \\
 PM_1(SiO_2) &= \prod_{u,v \in E_1(SiO_2)} [\gamma(u) + \gamma(v)] \\
 &\times \prod_{u,v \in E_2(SiO_2)} [\gamma(u) + \gamma(v)] \\
 &= 5^{|E_1(SiO_2)|} \times 6^{|E_2(SiO_2)|} \\
 &= 5^{(2p+2q+4)} \times 6^{(2p+2q+4pq)} \\
 PM_2(G) &= \prod_{u,v \in E(G)} [\gamma(u) \times \gamma(v)] \\
 PM_2(SiO_2) &= \prod_{u,v \in E_1(SiO_2)} [\gamma(u) \times \gamma(v)] \\
 &\times \prod_{u,v \in E_2(SiO_2)} [\gamma(u) \times \gamma(v)] \\
 &= 4^{|E_1(SiO_2)|} \times 8^{|E_2(SiO_2)|} \\
 &= 4^{(2p+2q+4)} \times 8^{(2p+2q+4pq)} \\
 &= 2^{(10p+10q+12pq+8)}.
 \end{aligned}$$

D. The first and second Zagreb polynomials of SiO_2

Now using Eqs. (6-7), we get our required result as follows:

$$M_1(G, x) = \sum_{u,v \in E(G)} x^{[d_u + d_v]},$$

$$\begin{aligned}
 M_1(SiO_2, x) &= \sum_{u,v \in E_1(SiO_2)} x^{[\gamma(u) + \gamma(v)]} \\
 &+ \sum_{u,v \in E_2(SiO_2)} x^{[\gamma(u) + \gamma(v)]} \\
 &= |E_1(SiO_2)|x^5 + |E_2(SiO_2)|x^6 \\
 &= (2p + 2q + 4)x^5 \\
 &+ (2p + 2q + 4pq)x^6 \\
 M_2(G, x) &= \sum_{u,v \in E(G)} x^{[\gamma(u) \times \gamma(v)]} \\
 M_2(SiO_2, x) &= \sum_{u,v \in E_1(SiO_2)} x^{[\gamma(u) \times \gamma(v)]} \\
 &+ \sum_{u,v \in E_2(SiO_2)} x^{[\gamma(u) \times \gamma(v)]} = \\
 &= |E_1(SiO_2)|x^4 + |E_2(SiO_2)|x^8 \\
 &= (2p + 2q + 4)x^4 \\
 &+ (2p + 2q + 4pq)x^8.
 \end{aligned}$$

E. The Forgotten index, Augmented Zagreb index and Balaban index of SiO_2

From Table 1 and using Eqs. (8-10), we have

$$\begin{aligned}
 F(G) &= \sum_{u,v \in E(G)} (\gamma(u)^2 + \gamma(v)^2), \\
 F(SiO_2) &= 17|E_1(SiO_2)| + 20|E_2(SiO_2)| \\
 &= 17 \times (2p + 2q + 4) \\
 &+ 20 \times (2p + 2q + 4pq) \\
 &= 74p + 74q + 80pq + 68. \\
 AZI(G) &= \sum_{u,v \in E(G)} \left(\frac{\gamma(u) \times \gamma(v)}{\gamma(u) + \gamma(v) - 2} \right)^3 \\
 AZI(SiO_2) &= \sum_{u,v \in E_1(SiO_2)} \left(\frac{\gamma(u) \times \gamma(v)}{\gamma(u) + \gamma(v) - 2} \right)^3 \\
 &+ \sum_{u,v \in E_2(SiO_2)} \left(\frac{\gamma(u) \times \gamma(v)}{\gamma(u) + \gamma(v) - 2} \right)^3 = \\
 &= \frac{64}{27} |E_1(SiO_2)| + 8|E_2(SiO_2)| \\
 &= \frac{64}{27} (2p + 2q + 4) + 8(2p + 2q + 4pq) \\
 &= \frac{560}{27} p + \frac{560}{27} q + 32pq + \frac{256}{273} \\
 J(G) &= \frac{M}{M - N + 2} \sum_{u,v \in E(G)} \frac{1}{\sqrt{\gamma(u) \times \gamma(v)}} \\
 J(SiO_2) &= \frac{M}{M - N + 2} \left[\sum_{u,v \in E_1(SiO_2)} \frac{1}{\sqrt{\gamma(u) \times \gamma(v)}} \right. \\
 &\quad \left. + \sum_{u,v \in E_2(SiO_2)} \frac{1}{\sqrt{\gamma(u) \times \gamma(v)}} \right] = \\
 &\frac{4pq + 4p + 4q + 4}{4p - q + 5} \times \left[\frac{(2p + 2q + 4)}{2} + \frac{(2p + 2q + 4pq)}{2\sqrt{2}} \right] \\
 &= \frac{8p^2q + 8p^2 + 8pq^2 + 32pq + 24p}{8p - 2q + 10} \\
 &+ \frac{8q^2 + 24q + 16}{8p - 2q + 10} \\
 &+ \frac{16p^2q^2 + 24p^2q + 8p^2 + 24pq^2}{\sqrt{2}(8p - 2q + 10)} \\
 &+ \frac{32pq + 8p + 8q^2 + 8q}{\sqrt{2}(8p - 2q + 10)}.
 \end{aligned}$$

IV. RESULTS FOR CAPRA-DESIGNED PLANAR BENZENOID SERIES $Ca_k(C_6)$

Let G be a cyclic planar graph. Capra map operation is achieved as follows:

1. Insert two vertices on every edge of G
2. Add pendant vertices to the above inserted ones
3. Connect the pendant vertices in order $(-1, +3)$ around the boundary of a face of G .

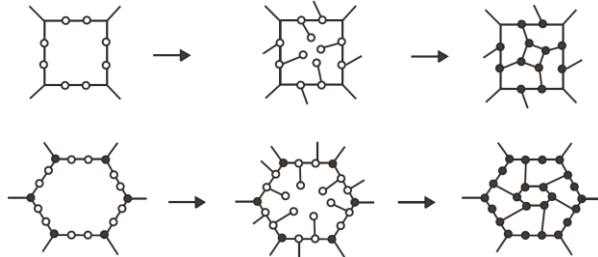


Figure 3. Capra map operation on the square and hexagonal face, respectively.

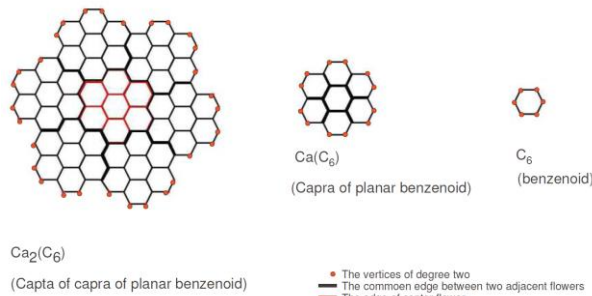


Figure 4. The first two graphs: $Ca(C_6)$ and $Ca_2(C_6)$ of the benzenoid family $Ca_k(C_6)$.

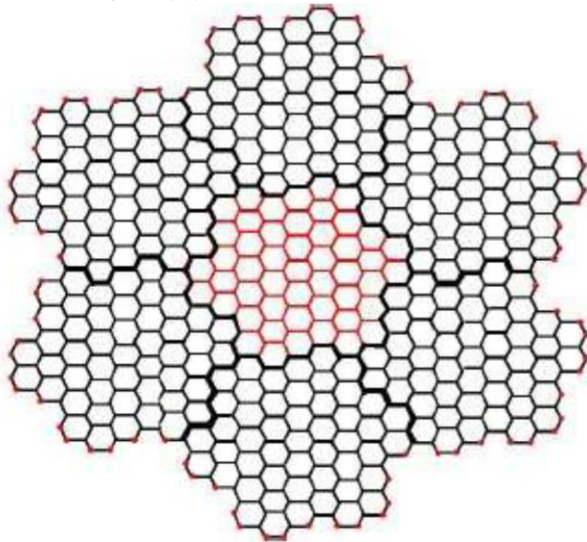


Figure 5. Graph $Ca_3(C_6)$ is the third member of Capra-designed planar benzenoid series.

Table 2. $(\gamma(u), \gamma(v))$ -type edge partition of $Ca_k(C_6)$.

$(\gamma(u), \gamma(v))$	No. of edges
(2,2)	$3^k + 3$
(2,3) and (3,2)	4×3^k
(3,3)	$3 \times (7^k - 2 \times 3^{k-1} - 1)$

By running these steps for every face/cycle of G , one obtains the Capra-transform of G $Ca(G)$, see Fig. 3. By

iterating the Capra-operation on the hexagon (i.e. benzene graph C_6) and its Ca-transforms, a benzenoid series, as shown in Figs. 4 and Fig. 5, can be designed.

Let G be the graph of Capra-Designed Planar Benzenoid series $Ca_k(C_6)$. The edge set is partitioned into three sets, say, according to the structure of $Ca_k(C_6)$, the number of vertices with degree two of graph $Ca_k(C_6)$ based on the degree of end vertices of each edge. The set $E_4(Ca_k(C_6))$ contains $3^k + 3$ edges of type uv with $\gamma(u) = 2, \gamma(v) = 2$, $E_5(Ca_k(C_6))$ contains 4×3^k edges of type uv with $\gamma(u) = 2, \gamma(v) = 3$ or $\gamma(u) = 3, \gamma(v) = 2$ and the set $E_6(Ca_k(C_6))$ contains $3 \times (7^k - 2 \times 3^{k-1} - 1)$ edges of type uv such that $\gamma(u) = 3, \gamma(v) = 3$. More preciously, the edge partition of C_6 with respect to the degrees of the end-vertices of edges given by Table 2.

Now, we compute first Zagreb index, second Zagreb index, hyper-Zagreb index $HM(G)$, first multiple Zagreb index $PM_1(G)$, second multiple Zagreb index $PM_2(G)$ and Zagreb polynomials $M_1(G, x)$, $M_2(G, x)$ for $Ca_k(C_6)$ as follows.

A. The first and second Zagreb indices of $Ca_k(C_6)$

Now using Eqs. (1-2), we have:

$$\begin{aligned}
 M_1(G) &= \sum_{u,v \in E(G)} [\gamma(u) + \gamma(v)], \\
 M_1(Ca_k(C_6)) &= \sum_{u,v \in E_4(Ca_k(C_6))} [\gamma(u) + \gamma(v)] \\
 &\quad + \sum_{u,v \in E_5(Ca_k(C_6))} [\gamma(u) + \gamma(v)] \\
 &\quad + \sum_{u,v \in E_6(Ca_k(C_6))} [\gamma(u) + \gamma(v)] \\
 &= 4|E_4(Ca_k(C_6))| + 5|E_5(Ca_k(C_6))| + 6|E_6(Ca_k(C_6))| \\
 &= 4(3^k + 3) + 5(4 \times 3^k) + 6(3 \times (7^k - 2 \times 3^{k-1} - 1)) \\
 &= 4 \times 3^{k+1} + 18 \times 7^k - 6. \\
 M_2(G) &= \sum_{u,v \in E(G)} [\gamma(u) \times \gamma(v)], \\
 M_2(Ca_k(C_6)) &= \sum_{u,v \in E_4(Ca_k(C_6))} [\gamma(u) \times \gamma(v)] \\
 &\quad + \sum_{u,v \in E_5(Ca_k(C_6))} [\gamma(u) \times \gamma(v)] \\
 &\quad + \sum_{u,v \in E_6(Ca_k(C_6))} [\gamma(u) \times \gamma(v)] \\
 &= 4|E_4(Ca_k(C_6))| + 6|E_5(Ca_k(C_6))| + 9|E_6(Ca_k(C_6))| \\
 &= 4(3^k + 3) + 6(4 \times 3^k) + 9(3 \times (7^k - 2 \times 3^{k-1} - 1)) \\
 &= 10 \times 3^k + 27 \times 7^k - 15.
 \end{aligned}$$

B. The Hyper Zagreb index of $Ca_k(C_6)$

Now using Eq. (3), we have:

$$\begin{aligned}
 HM(G) &= \sum_{u,v \in E(G)} [\gamma(u) + \gamma(v)]^2, \\
 HM(Ca_k(C_6)) &= \sum_{u,v \in E_4(Ca_k(C_6))} [\gamma(u) + \gamma(v)]^2 \\
 &\quad + \sum_{u,v \in E_5(Ca_k(C_6))} [\gamma(u) + \gamma(v)]^2 \\
 &\quad + \sum_{u,v \in E_6(Ca_k(C_6))} [\gamma(u) + \gamma(v)]^2 \\
 &= 16|E_4(Ca_k(C_6))| + 25|E_5(Ca_k(C_6))| + 36|E_6(Ca_k(C_6))|
 \end{aligned}$$

$$= 16(3^k + 3) + 25(4 \times 3^k) + 36(3 \times (7^k - 2 \times 3^{k-1} - 1)) \\ = 44 \times 3^k + 108 \times 7^k - 60.$$

C. The first and second Multiple Zagreb indices of $Ca_k(C_6)$

Now using Eqs. (4-5), we get our required result as follows:

$$PM_1(G) = \prod_{u,v \in E(G)} [\gamma(u) + \gamma(v)] \\ PM_1(Ca_k(C_6)) = \prod_{u,v \in E_4(Ca_k(C_6))} [\gamma(u) + \gamma(v)] \\ \times \prod_{u,v \in E_5(Ca_k(C_6))} [\gamma(u) + \gamma(v)] \\ \times \prod_{u,v \in E_6(Ca_k(C_6))} [\gamma(u) + \gamma(v)] \\ = 4^{|E_4(Ca_k(C_6))|} \times 5^{|E_5(Ca_k(C_6))|} \times 6^{|E_6(Ca_k(C_6))|} \\ = 4^{3^k+3} \times 5^{4 \times 3^k} + 6^{3 \times (7^k - 2 \times 3^{k-1} - 1)} \\ PM_2(G) = \prod_{u,v \in E(G)} [\gamma(u) \times \gamma(v)] \\ PM_2(Ca_k(C_6)) = \prod_{u,v \in E_4(Ca_k(C_6))} [\gamma(u) \times \gamma(v)] \\ \times \prod_{u,v \in E_5(Ca_k(C_6))} [\gamma(u) \times \gamma(v)] \\ \times \prod_{u,v \in E_6(Ca_k(C_6))} [\gamma(u) \times \gamma(v)] \\ = 4^{|E_4(Ca_k(C_6))|} \times 6^{|E_5(Ca_k(C_6))|} \times 6^{|E_6(Ca_k(C_6))|} \\ = 4^{3^k+3} \times 6^{4 \times 3^k} + 9^{3 \times (7^k - 2 \times 3^{k-1} - 1)}$$

D. The first and second Zagreb polynomials of $Ca_k(C_6)$

Now using Eqs. (6-7), we get our required result as follows:

$$M_1(G, x) = \sum_{u,v \in E(G)} x^{[\gamma(u)+\gamma(v)]}, \\ M_1(Ca_k(C_6), x) = \sum_{u,v \in E_4(Ca_k(C_6))} x^{[\gamma(u)+\gamma(v)]} \\ + \sum_{u,v \in E_5(Ca_k(C_6))} x^{[\gamma(u)+\gamma(v)]} \\ + \sum_{u,v \in E_6(Ca_k(C_6))} x^{[\gamma(u)+\gamma(v)]} \\ = |E_4(Ca_k(C_6))| x^4 + |E_5(Ca_k(C_6))| x^5 + |E_6(Ca_k(C_6))| x^6 \\ = (3^k + 3) x^4 + (4 \times 3^k) x^5 + 3(7^k - 2 \times 3^{k-1} - 1) x^6. \\ M_2(G, x) = \sum_{u,v \in E(G)} x^{[\gamma(u) \times \gamma(v)]} \\ M_2(Ca_k(C_6), x) = \sum_{u,v \in E_4(Ca_k(C_6))} x^{[\gamma(u) \times \gamma(v)]} \\ + \sum_{u,v \in E_5(Ca_k(C_6))} x^{[\gamma(u) \times \gamma(v)]} \\ + \sum_{u,v \in E_6(Ca_k(C_6))} x^{[\gamma(u) \times \gamma(v)]} \\ = |E_4(Ca_k(C_6))| x^4 + |E_5(Ca_k(C_6))| x^6 + |E_6(Ca_k(C_6))| x^9 \\ = (3^k + 3) x^4 + (4 \times 3^k) x^6 + 3(7^k - 2 \times 3^{k-1} - 1) x^9.$$

E. The Forgotten index, Augmented Zagreb index and Balaban index of $Ca_k(C_6)$

From Table 2 and using Eqs. (8-10), we have

$$F(G) = \sum_{u,v \in E(G)} (\gamma(u)^2 + \gamma(v)^2), \\ F(Ca_k(C_6)) = 8|E_4(Ca_k(C_6))| + 26|E_5(Ca_k(C_6))| \\ + 18|E_6(Ca_k(C_6))| \\ = 8(3^k + 3) + 26(4 \times 3^k) + 18(3(7^k - 2 \times 3^{k-1} - 1)) \\ = (76 \times 3^k) + (54 \times 3) - 30 \\ AZI(G) = \sum_{u,v \in E(G)} \left(\frac{\gamma(u) \times \gamma(v)}{\gamma(u) + \gamma(v) - 2} \right)^3 \\ AZI(Ca_k(C_6)) = \sum_{u,v \in E_4(Ca_k(C_6))} \left(\frac{\gamma(u) \times \gamma(v)}{\gamma(u) + \gamma(v) - 2} \right)^3 \\ + \sum_{u,v \in E_5(Ca_k(C_6))} \left(\frac{\gamma(u) \times \gamma(v)}{\gamma(u) + \gamma(v) - 2} \right)^3 \\ + \sum_{u,v \in E_6(Ca_k(C_6))} \left(\frac{\gamma(u) \times \gamma(v)}{\gamma(u) + \gamma(v) - 2} \right)^3 \\ = 8|E_4(Ca_k(C_6))| + 8|E_5(Ca_k(C_6))| + \frac{729}{64}|E_6(Ca_k(C_6))| \\ = 8(3^k + 3) + 8(4 \times 3^k) + \frac{729}{64}(3(7^k - 2 \times 3^{k-1} - 1)) \\ = \frac{551 \times 3^k}{32} + \frac{2187 \times 7^k}{64} - \frac{651}{64}. \\ J(G) = \frac{M}{M - N + 2} \sum_{u,v \in E(G)} \frac{1}{\sqrt{\gamma(u) \times \gamma(v)}} \\ J(Ca_k(C_6)) = \frac{M}{M - N + 2} \sum_{u,v \in E_4(Ca_k(C_6))} \frac{1}{\sqrt{\gamma(u) \times \gamma(v)}} \\ + \frac{M}{M - N + 2} \sum_{u,v \in E_5(Ca_k(C_6))} \frac{1}{\sqrt{\gamma(u) \times \gamma(v)}} \\ + \frac{M}{M - N + 2} \sum_{u,v \in E_6(Ca_k(C_6))} \frac{1}{\sqrt{\gamma(u) \times \gamma(v)}} \\ = \frac{3(7^k + 3^k)}{7^k + 1} \times \left[\frac{1}{2}(3^k + 3) + \frac{1}{\sqrt{6}}(4 \times 3^k) \right. \\ \left. + \frac{1}{3}(3(7^k - 2 \times 3^{k-1} - 1)) \right] \\ = \left(\frac{3 + 4\sqrt{6} - 4}{6} \right) 3^k + 7^k + \frac{1}{2}.$$

V. CONCLUSION

In this paper, we focus on the Silicate SiO_2 layer structure and the structure of Capra-designed planar benzenoid series $Ca_k(C_6)$ ($k \geq 0$). We determined Zagreb type indices, Forgotten index, Augmented index and Balaban index for these structures. Also we provide the importance of these indices for application point of view as well. However, computing the distance based and counting related topological indices for these structures still remain open for investigation and as a challenge for researchers.

ACKNOWLEDGMENTS

This research is Completed in Henan joint international research laboratory of green construction of functional Molecular and their bioanalytical application.

REFERENCES

Balaban, A.T. (1982) "Highly discriminating distance-based topological index," *Chem. Phys. Lett.*, **89**,

- 399-404.
- Basavanagoud, B., Gao W., Patil S., Desai V.R., Mirajkar V. and Pooja B. (2017) "Computing First Zagreb index and F-index of New C-products of Graphs," *Applied Mathematics and Nonlinear Sciences*, **21**, 285-298.
- Diudea, M.V. (2005) "Nanoporous carbon allotropes by septupling map operations," *J. Chem. Inf. Model*, **45**, 1002-1110.
- Du, W., Li X. and Shi Y. (2009) "Algorithms and extremal problem on Wiener polarity index," *MATCH Commun. Math. Comput. Chem.*, **62**, 235-244.
- Farahani, M.R., Siddiqui H.M.A., Baby S., Imran M. and Siddiqui M.K. (2016) "The second and second-sum-connectivity indices of $TUC_4C_8(s)$ nanotubes," *Journal of Optoelectronic and Biomedical Materials*, **8**, 107-111.
- Furtula, B., Graovac A. and Vukicevic D. (2010), "Augmented Zagreb index," *J. Math. Chem.*, **48**, 370-380.
- Furtula, B., Gutman I. and Dehmer M. (2013) "On structure-sensitivity of degree-based topological indices," *Appl. Math. Comput*, **219**, 8973-8978.
- Furtula, B. and Gutman I. (2015) "A forgotten topological index," *J. Math. Chem.*, **53**, 1184-1190.
- Gao, W., Siddiqui M.K., Imran M., Jamil M.K. and Farahani M.R. (2016a) "Forgotten Topological Index of Chemical Structure in Drugs," *Saudi Pharmaceutical Journal*, **24**, 258-267.
- Gao, W., Farahani M.R., Siddiqui M.K. and Jamil M.K. (2016b) "On the First and Second Zagreb and First and Second Hyper-Zagreb Indices of Carbon Nanocones $CNCK[n]$," *J. Comput. Theor. Nanosci.*, **13**, 7475-7482.
- Gao, W., Farahani M.R., Jamil M.K. and Siddiqui M.K. (2016c) "The Redefined First, Second and Third Zagreb Indices of Titania Nanotubes $TiO_2[m; n]$," *The Open Biotechnology Journal*, **10**, 272-277.
- Gao, W., Siddiqui M.K., Naeem M. and Rehman N.A. (2017) "Topological Characterization of Carbon Graphite and Crystal Cubic Carbon Structures," *Molecules*, **22**, 1496-1507.
- Gao, W. and Siddiqui M.K. (2017) "Molecular Descriptors of Nanotube, Oxide, Silicate, and Triangulene networks," *Journal of Chemistry*, **2017**, 1-10.
- Gao, W., Siddiqui M.K., Naeem M. and Imran M. (2018) "Computing multiple ABC index and multiple GA index of some grid graphs," *Open Physic*, **16**, 588-598.
- Ghorbani, M. and Azimi N. (2012) "Note on multiple Zagreb indices," *Iran. J. Math. Chem.*, **3**, 137-143.
- Gharibi, W., Ahmad A. and Siddiqui M.K. (2016) "On Zagreb Indices, Zagreb Polynomials of Nanocone and Nanotubes," *J. Comput. Theor. Nanosci.*, **13**, 5086-5092.
- Gutman, I. and Trinajstić N. (1972) "Graph theory and molecular orbitals total π -electron energy of alternant hydrocarbons," *Chem. Phys. Lett.*, **17**, 535-538.
- Gutman, I., Ruscic B., Trinajstić N. and Wilcox C.F. (1975) "Graph theory and molecular orbitals, XII. Acyclic polyenes," *J. Chem. Phys.*, **62**, 3399-3405.
- Gutman, I. and Polansky O.E. (1986) *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, New York.
- Gutman, I. and Das K.C. (2004) "Some Properties of the Second Zagreb Index," *MATCH Commun. Math. Comput. Chem.*, **50**, 103-112.
- Gutman, I. (2013) "Degree-based topological indices," *Croat. Chem. Acta*, **86**, 351-361.
- Idrees, N., Naeem M.N., Hussain F., Sadiq A. and Siddiqui M.K. (2017) "Molecular Descriptors of Benzenoid System," *Quimica Nova*, **40**, 143-145.
- Imran, S., Siddiqui M.K., Imran M. and Nadeem M.F. (2018a) "Computing Topological Indices and Polynomials for Line Graphs," *Mathematics*, **6**, 1-10.
- Imran, M., Siddiqui M.K., Naeem M. and Iqbal M.A. (2018b) "On Topological Properties of Symmetric Chemical Structures," *Symmetry*, **10**, 1-21.
- Kang, S.M., Siddiqui M.K., Rehman N.A., Naeem M. and Muhammad M.H. (2018) "Topological Properties of 2-Dimensional Silicon-Carbons," *IEEE Access*, **6**, 59362-59373.
- Ramane, H.S. and Jummannaver R.B. (2016) "Note on forgotten topological index of chemical structure in drugs," *Applied Mathematics and Nonlinear Sciences*, **12**, 369-374.
- Shirdel, G.H., Pour H.R. and Sayadi A.M. (2013) "The Hyper-Zagreb Index of Graph Operations," *Iran. J. Math. Chem.*, **4**, 213-220.
- Siddiqui, M.K., Imran M. and Ahmad A. (2016a) "On Zagreb indices, Zagreb polynomials of some nanostar dendrimers," *Appl. Math. Comput.*, **280**, 132-139.
- Siddiqui, M.K., Naeem M., Rahman N.A. and Imran M. (2016b) "Computing topological indices of certain networks," *J. Optoelectronics and Advanced Materials*, **18**, 884-892.
- Sun, Y.C., Lin Z., Peng W.X., Yuan T.Q., Xu F., Wu Y.Q., Yang J., Wang Y.S. and Sun R.C. (2014) "Chemical changes of raw materials and manufactured binderless boards during hot pressing: lignin isolation and characterization," *Bioresources*, **9**, 1055-1071.
- Wiener, H. (1947) "Structural determination of paraffin boiling points," *J. Am. Chem. Soc.*, **69**, 17-20.

Received October 31, 2018.

Sent to Guest Editor November 4, 2018.

Accepted July 25, 2019.

Recommended by Editor In Chief Alberto Bandoni