COMPUTING TOPOLOGICAL INDICES OF SiO₂ LAYER STRUCTURE AND BENZENOID SERIES

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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 physico-chemical 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 Cₖ₋₁(C₉), (k ≥ 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 oxidized for 2-3 hours in atmosphere after a chemical etch.

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 Trinajstic (1972) based on degree of vertices of \( G \). The first and second Zagreb indices of a graph \( G \) are defined as:

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

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

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

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

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:

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

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

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

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

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

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

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:

\[ F(G) = \sum_{u,v \in E(G)} \gamma(u)^2 + \gamma(v)^2. \] (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:

\[ AZI(G) = \sum_{u,v \in E(G)} \left( \frac{\gamma(u)\gamma(v)}{\gamma(u)+\gamma(v)} \right)^3. \] (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:

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

For further study of Balaban index about various graph families see Gutman (2013), Ramane and Jummannaver (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 the 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 \( \pi \)-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 Trinajstic (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.](image1)

![Figure 2. SiO\(_2\) (4,5).](image2)

<table>
<thead>
<tr>
<th>( d_u, d_v )-type edge partition of SiO(_2).</th>
<th>( \gamma(u), \gamma(v) )</th>
<th>No. of edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1,4)</td>
<td>2p+2q+4</td>
<td></td>
</tr>
<tr>
<td>(2,4)</td>
<td>2p+2q+4</td>
<td></td>
</tr>
</tbody>
</table>

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\(_2\)(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:

\[ M_1(G) = \sum_{u,v \in E(G)} [\gamma(u) + \gamma(v)]. \]
\[ M_1(\text{SiO}_2) = \sum_{u,v \in E(SiO_2)} [\gamma(u) + \gamma(v)] \]
\[ + \sum_{u \in E(SiO_2)} [\gamma(u) + \gamma(v)] \]
\[ = 5|E_1(\text{SiO}_2)| + 6|E_2(\text{SiO}_2)|, \]
\[ M_1(\text{SiO}_2) = 5 \times (2p + 2q + 4) + 6 \times (2p + 2q + 4pq) \]
\[ = 22p + 22q + 24pq + 20. \]
\[ M_2(G) = \sum_{u \in E(G)} [\gamma(u) \times \gamma(v)], \]
\[ M_2(\text{SiO}_2) = \sum_{u \in E(SiO_2)} [\gamma(u) \times \gamma(v)] \]
\[ + \sum_{u \in E(SiO_2)} [\gamma(u) \times \gamma(v)] \]
\[ = 4|E_1(\text{SiO}_2)| + 8|E_2(\text{SiO}_2)|, \]
\[ M_2(\text{SiO}_2) = 4 \times (2p + 2q + 4) + 8 \times (2p + 2q + 4pq) \]
\[ = 24p + 24q + 32pq + 16. \]

**B. The Hyper Zagreb index of SiO\(_2\)**

Now using Eq. (3), we have:
\[ HM(G) = \sum_{u \in E(G)} [\gamma(u) + \gamma(v)]^2, \]
\[ HM(\text{SiO}_2) = \sum_{u \in E(SiO_2)} [\gamma(u) + \gamma(v)]^2 \]
\[ + \sum_{u \in E(SiO_2)} [\gamma(u) + \gamma(v)]^2 \]
\[ = 25|E_1(\text{SiO}_2)| + 36|E_2(\text{SiO}_2)|, \]
\[ HM(\text{SiO}_2) = 25 \times (2p + 2q + 4) + 36 \times (2p + 2q + 4pq) \]
\[ = 122p + 122q + 144pq + 100. \]

**C. The first and second Multiple Zagreb indices of SiO\(_2\)**

Now using Eqs. (4-5), we get our required result as follows:
\[ PM_1(G) = \prod_{u \in E(G)} [\gamma(u) + \gamma(v)] \]
\[ PM_1(\text{SiO}_2) = \prod_{u \in E(SiO_2)} [\gamma(u) + \gamma(v)] \]
\[ \times \prod_{u \in E(SiO_2)} [\gamma(u) + \gamma(v)] \]
\[ = 5|E_1(\text{SiO}_2)| \times 6|E_2(\text{SiO}_2)| \]
\[ = 5(2p + 2q + 4) \times 6(2p + 2q + 4pq) \]
\[ PM_2(G) = \prod_{u \in E(G)} [\gamma(u) \times \gamma(v)] \]
\[ PM_2(\text{SiO}_2) = \prod_{u \in E(SiO_2)} [\gamma(u) \times \gamma(v)] \]
\[ \times \prod_{u \in E(SiO_2)} [\gamma(u) \times \gamma(v)] \]
\[ = 4|E_1(\text{SiO}_2)| \times 8|E_2(\text{SiO}_2)| \]
\[ = 4(2p + 2q + 4) \times 8(2p + 2q + 4pq) \]
\[ = 2(10p + 10q + 12pq + 8). \]

**D. The first and second Zagreb polynomials of SiO\(_2\)**

Now using Eqs. (6-7), we get our required result as follows:
\[ M_1(G,x) = \sum_{u \in E(G)} x^{[\gamma(u) + \gamma(v)]} \]
\[ + \sum_{u \in E(SiO_2)} x^{[\gamma(u) + \gamma(v)]} \]
\[ = |E_1(\text{SiO}_2)|x^5 + |E_2(\text{SiO}_2)|x^6 \]
\[ = (2p + 2q + 4)x^5 + (2p + 2q + 4pq)x^6 \]
\[ M_2(G,x) = \sum_{u \in E(G)} x^{[\gamma(u) \times \gamma(v)]} \]
\[ + \sum_{u \in E(SiO_2)} x^{[\gamma(u) \times \gamma(v)]} \]
\[ = |E_1(\text{SiO}_2)|x^4 + |E_2(\text{SiO}_2)|x^8 \]
\[ = (2p + 2q + 4)x^4 + (2p + 2q + 4pq)x^8. \]

**E. The Forgotten index, Augmented Zagreb index and Balaban index of SiO\(_2\)**

From Table 1 and using Eqs. (8-10), we have
\[ F(G) = \sum (\gamma(u) + \gamma(v))^2, \]
\[ F(\text{SiO}_2) = 17|E_1(\text{SiO}_2)| + 20|E_2(\text{SiO}_2)| \]
\[ = 17 \times (2p + 2q + 4) + 20 \times (2p + 2q + 4pq) \]
\[ = 74p + 74q + 80pq + 68. \]
\[ AZI(G) = \sum_{u \in E(G)} (\gamma(u) \times \gamma(v))^3 \]
\[ AZI(\text{SiO}_2) = \sum_{u \in E(SiO_2)} (\gamma(u) \times \gamma(v))^3 \]
\[ \times \sum_{u \in E(SiO_2)} (\gamma(u) \times \gamma(v) - 2) \]
\[ = 64 \times (2p + 2q + 4) + 8(2p + 2q + 4pq) \]
\[ = 64p + 64q + 128pq + 256 \]
\[ = \frac{560}{M} + \frac{560}{M_2} + \frac{256}{273}. \]
\[ J(G) = \frac{1}{M - N + 2} \sum_{u \in E(G)} \sqrt[4]{\gamma(u) \times \gamma(v)} \]
\[ J(SiO_2) = \frac{1}{M - N + 2} \sum_{u \in E(SiO_2)} \sqrt[4]{\gamma(u) \times \gamma(v)} \]
\[ = \frac{1}{4p + 4q + 4 + \frac{2(2p + 2q + 4pq)}{2p + 2q + 4pq}} \]
\[ = \frac{8pq + 8p^2 + 8p^2 + 32pq + 24p}{8p + 2q + 10} \]
\[ + \frac{8q^2 + 24q + 16}{8p + 2q + 10} + \frac{16p^2 q^2 + 24p^2 q + 8p^2 + 24pq^2}{\sqrt{2} (8p - 2q + 10)} \]
\[ + \frac{32pq + 8q^2 + 8q}{\sqrt{2} (8p - 2q + 10)}. \]
IV. RESULTS FOR CAPRA-DESIGNED PLANAR BENZENOID SERIES $Ca_k(G_6)$

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.](image)

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

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

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

$$M_2(Ca_k(G_6)) = \sum_{u,v \in E(Ca_k(G_6))} [\gamma(u) + \gamma(v)]$$

$$+ \sum_{u,v \in E(Ca_k(G_6))} [\gamma(u) \times \gamma(v)]$$

$$+ \sum_{u,v \in E(Ca_k(G_6))} [\gamma(u) \times \gamma(v)],$$

$$= 4|E_4(Ca_k(G_6))| + 6|E_6(Ca_k(G_6))| + 9|E_8(Ca_k(G_6))|$$

$$= 4(3^k + 3) + 6(4 \times 3^k) + 9(3 \times (7^k - 2 \times 3^{k-1} - 1))$$

$$= 10 \times 3^k + 27 \times 7^k - 15.$$  

B. The Hyper Zagreb index of $Ca_k(G_6)$

Now using Eq. (3), we have:

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

$$HM(Ca_k(G_6)) = \sum_{u,v \in E(Ca_k(G_6))} [\gamma(u) + \gamma(v)]^2$$

$$+ \sum_{u,v \in E(Ca_k(G_6))} [\gamma(u) \times \gamma(v)]^2$$

$$+ \sum_{u,v \in E(Ca_k(G_6))} [\gamma(u) \times \gamma(v)]^2,$$

$$= 16|E_4(Ca_k(G_6))| + 25|E_6(Ca_k(G_6))| + 36|E_8(Ca_k(G_6))|.$$
\[
= 16(3^k + 3) + 25(4 \times 3^k) + 36(3 \times (7^k - 2 \times 3^{k-1} - 1)) \\
= 44 \times 3^k + 108 \times 7^k - 60.
\]

C. The first and second Multiple Zagreb indices of \( C_a(G) \)

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

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

\[
PM_1(Ca(G)) = \prod_{u,v \in E(Ca(G))} [\gamma(u) + \gamma(v)]
\]

\[
PM_2(Ca(G)) = \prod_{u,v \in E(Ca(G))} [\gamma(u) + \gamma(v)]
\]

= \[ |E_4(Ca(G))| \times |E_4(Ca(G))| \times |E_4(Ca(G))| \times |E_4(Ca(G))| \times |E_4(Ca(G))| \times |E_4(Ca(G))| \]

= \[ |E_4(Ca(G))| \times |E_4(Ca(G))| \times |E_4(Ca(G))| \times |E_4(Ca(G))| \times |E_4(Ca(G))| \times |E_4(Ca(G))| \]

D. The first and second Zagreb polynomials of \( C_a(G) \)

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

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

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

\[
M_2(Ca(G),x) = \sum_{u,v \in E(Ca(G))} x^{[\gamma(u) + \gamma(v)]}
\]

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

\[
F(G) = \sum_{u,v \in E(G)} (\gamma(u)^2 + \gamma(v)^2),
\]

\[
F(Ca(G)) = 8|E_4(Ca(G))| + 26|E_6(Ca(G))| + 18|E_8(Ca(G))| \]

= \[ 8(3^k + 3) + 26(4 \times 3^k) + 18(3(7^k - 2 \times 3^{k-1} - 1)) \]

= \[ 76(3^k) + (54 \times 7^k) - 30 \]

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

\[
AZI(Ca(G)) = \sum_{u,v \in E(Ca(G))} \left( \frac{\gamma(u) \times \gamma(v)}{\gamma(u) + \gamma(v) - 2} \right)^3
\]

= \[ 8|E_4(Ca(G))| + 8|E_6(Ca(G))| + 729 \times 64 \]

\[ = 8(3^k + 3) + 8(4 \times 3^k) + 729 \times 64(3(7^k - 2 \times 3^{k-1} - 1)) \]

= \[ 551 \times 3^k + 2187 \times 7^k - 651 \]

\[
J(G) = \frac{32 M}{M - N + 2} \sum_{u,v \in E(G)} \frac{1}{\gamma(u) \times \gamma(v)}
\]

\[
J(Ca(G)) = \frac{M}{M - N + 2} \sum_{u,v \in E(Ca(G))} \frac{1}{\gamma(u) \times \gamma(v)}
\]

= \[ \frac{M}{M - N + 2} \sum_{u,v \in E(Ca(G))} \frac{1}{\gamma(u) \times \gamma(v)}
\]

= \[ \frac{3(7^k + 3^k)}{7^k + 1} \times \left( \frac{1}{2} (3^k + 3) + \frac{1}{6} (4 \times 3^k) \right)
\]

= \[ \left(3 + 4 \sqrt{6} - 4\right) 3^k + 7^k + 1 \]

V. CONCLUSION

In this paper, we focus on the Silicate SiO₄ layer structure and the structure of Capra-designed planar benzene series \( Ca(G) \) \( (k \geq 0) \). 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.

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REFERENCES


