

On Modified Topological Invariants of Various Networks

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Abstract

Chemical Structures are being studied to understand the insight of mathematical models of chemical molecules and this phenomenon is known as chemical graph theory. In this aspect, the role of topological indices (which tag to each chemical structure) is vital in making the difference between the base of molecules and its branching pattern. It is also a technique which use to explain the characteristics of compounds such as temperature and oscillation during their chemical reaction. These are million in counting which is based on a single edge but in this article, we try to enhance this idea for a path of length two between certain pair $(u, v) \in V(G)$ and calculate productive and compact informative results which are numerically and graphically representing better results than single edge formulas by using this notion by edge path we can drive smoothly millions of existing formulas of topological indices Bi-distance edge-based topological indices. In this article, we calculate different Bi-Distance degree-based topological indices namely; Randic index, Forgotten index, Arithmetic Geometric index, Geometric Arithmetic index, Zagreb indices, Sanskruti index, Second Arithmetic Geometric index, and Forth Atom-bond Connectivity index for Oxide Chain and Silicate Networks.

Keywords: Chain of Oxide Network, Silicate Network, Topological indices and Bi-distance degree based topological indices.

1. Introduction

A graph is the pictorial representation of different types of data or information. All the graphs presented in this article are two-dimensional, regular, simple and planer in nature with a set of points called vertices (nodes) connected with lines called edges (links).

Mathematical chemistry is an important approach of theoretical chemistry in which we study molecular structure by different mathematical techniques without discussing quantum mechanics. For the development and advancement of chemical sciences, this theory acts as the backbone. For the development of QSAR models, molecular descriptors play an efficient role. Molecular

connectivity indices (MCI) or topological indices (TI) are famous molecular descriptors also called graph invariants because these are formed by concepts of graph theory.

TIs are the translator of the topology of a chemical structure. It is a function in which we give numerical values as input and get information about the variations in the properties of chemical structure. TIs are significant and very easy to calculate by using simple mathematical techniques and tools. These indices have vast applications in theoretical chemistry, chemical graph theory, pharmacy, and nano-technology. Harold Wiener gave the idea of this by introducing the 1st topological index as the Wiener index in 1947 then he wrote a series papers to justify the relationship between the Wiener index and hydrocarbons. By inspiring his work hundreds of TIs are formed to understand the complex structure of different compounds easily.

In this paper, we discuss the degree-based TIs like RI, FI, AG index, GA index, Zagreb indices, Sanskruti index, AG2 index, and ABC4 index for oxide and silicate networks.

2. Parameter Assignment and Basic definitions

Let us have a group G with $E(G)$ and $V(G)$ are the collection of links (edges) and nodes (vertices) respectively. A vertex v is any point in the graph and the line connecting these two points uv said to be an edge. The degree of a node v is the count of edges incident on the node v denoted as $d(v)$. Some basic definitions related to topological indices are given below:-

The idea of the Randic index was given by Milan Randic [1] to investigate the physical and chemical properties of compounds. Randic index is denoted by R mathematically it is described as :-

$$RI(G) = \sum_{uv \in E} \frac{1}{\sqrt{d(u) + d(v)}}$$

M. Randic published a paper "on the history of randic index and emerging hospitality toward chemical graph theory" in 2008 [2]. The algebraic connection between RI and normalized Laplacian matrix is given by K.C. Das, S. Sun, I. Gutman [3-5].

Forgotten index in an advanced form of MI used to calculate the pi-electron energy. M.K. Siddiqui, M. Imran and M.K. Jamil study the forgotten index in drugs [6].Forgotton index is mathematically defined as:-

$$F(G) = \sum_{uv \in E} (d(u)^2 + d(v)^2)$$

AG index is an inverse TI of GA-index invented in 2015 [7] denoted by AG1 index and computed as:-

$$AG_1(G) = \sum_{uv \in E} \left(\frac{d(u) + d(v)}{2\sqrt{d(u) \times d(v)}} \right)$$

AG index of most attractive and conductive material for electromagnetic shielding which is grapheme, determined in [8]. The AG index for some tress of carbon compounds are computed and for spectrum and energy of AG index see [9-10]. The main purpose to study these papers, related to AG index to understand and compare its properties with graph of oxide and silicate structure.

In [11] D. Vukicevic, B. Furtula invented the GA index. GA-index is introduced by inspiring the connectivity index. It is mathematically computed as:

$$GA(G) = \sum_{uv \in E} \left(\frac{2\sqrt{d(u) \times d(v)}}{d(u) + d(v)} \right)$$

It gives us better and fast prediction for structural and chemical characteristics like enthalpy of vaporization, enthalpy of formation and acentric factor of molecular structure. A large number of articles are published on qualities of GA index [12-15].

The Zagreb indices M_1 and M_2 were proposed by Gutman [16] in 1972. Zagreb indices are denoted by M- indices. This index is the base of many indices. Due to its great importance lots of time, it is redefined and modified by different ways. The mathematical description of for four M-indices is:

$$\begin{aligned} M_1(G) &= \sum_{uv \in E} (d(u) + d(v)) \\ M_2(G) &= \sum_{uv \in E} (d(u) \times d(v)) \\ HM(G) &= \sum_{uv \in E} (d(u) \times d(v))^2 \\ AM(G) &= \sum_{uv \in E} \left(\frac{d(u) \times d(v)}{d(u) + d(v) - 2} \right)^3 \end{aligned}$$

For huge amount of information about Zagreb indices see [17]. ZIs are used to understand the branching skeleton structure of carbon atoms in hydrocarbons [18-20].

Sanskriti index is computed by using the concept of "total sum of degrees of end vertices" represented by SI and defined :

$$S(G) = \sum_{uv \in E} \left(\frac{S(u) \times S(v)}{S(u) + S(v) - 2} \right)^3$$

The Sanskriti index involve sum of end vertices and its values are comparatively larger than other indices. To estimate the properties and behavior of Sanskriti index see [21-22].

The fifth version of arithmetic-geometric index is denoted by AG_5 and mathematically described as:

$$AG_5(Q_1) = \sum_{uv \in E} \left(\frac{S(u) + S(v)}{2\sqrt{S(u) \times S(v)}} \right)$$

M. Ghorbani et al. proposed the latest TI; Fourth Atom-Bond Connectivity index ABC_4 in 2010 [23, 24]. ABC_4 index defined as:

$$ABC_4(Q_1) = \sum_{uv \in E} \sqrt{\frac{S(u) + S(v) - 2}{S(u) \times S(v)}}$$

The last three indices are the "sum of degree" based indices where $S(u) = \sum_{uv \in E} d(v)$ and $S(v) = \sum_{uv \in E} d(u)$. For more detail information see [26-28].

3. Bi-Distance Degree Based Topological Indices

In literature, distance-based TIs have been invented by H.Wiener [25]. In these all types of TIs we deal with the single distance ($d(u,v)=1$) edge but in this article, we proposed a new concept named "Bi-distance edges" ($d(u,v)=2$) is the shortest path of two vertices between u and v . We partitioned the edges set $E(G)$ according to Bi-distance concept.

For instant first, we discuss the single edge distance-based topological index like Forgotten Index for Friend- ship graph.

Forgotton index for friendship graph is computed as:-

$$F(G) = \sum_{uv \in E} (d(u)^2 + d(v)^2)$$

$$F(F_3^4) = 4(2^2 + 2^2) + 8(8^2 + 2^2)$$

$$F(F_3^4) = 576$$

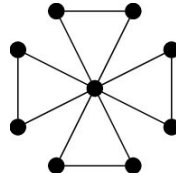


Figure 1: Friendship Graph F_3^4

d(u),d(v)	Total Number of Edges
(2,2)	4
(8,2)	8

Table 1: Single Distance Edge Partition For F_3^4

Now, we discuss about our new idea named as "Bi-Distance edges" for topological index such as Forgotten index. By using Bi-distance concept Forgotten index is determined as:-

d(u),d(v)	Total Number of Edges
(2,2)	24

Table 2: Bi-Distance Edge Partition For F_3^4

$$F(G) = \sum_{uv \in E} (d(u)^2 + d(v)^2)$$

$$F(F_3^4) = 24(2^2 + 2^2)$$

$$F(F_3^4) = 192$$

4. Main Result For Chain Oxide Network COX_n

In this segment, we talk about oxide networks and calculate different degree-based topological indices like Randic index, Forgotten index, AG index, GA index, Zagreb indices, Sanskruti index, AG5 index and ABC4 index. An oxide network is formed by deleting the silicon atom

from the silicide network. The triangular structure of the oxide network is consisting of three oxygen atoms. The linear oxide chain is composed when one oxygen of oxide network gets shared with another oxide network as shown in Figure 2.

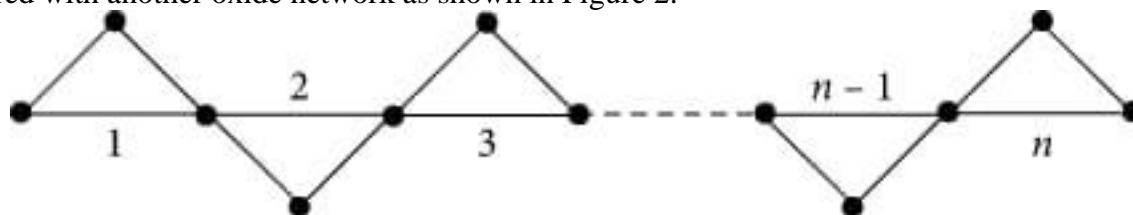


Figure 2: Chain Oxide Network COX_n of Order n

Remark: The total number of vertices and bi-distance edges are $2n + 1$ and $4n - 4$ respectively.

4.1 Edge partition

The oxide chain consists of three edge partitions. The integer n represents the order of the oxide chain and order is the number of unit cells in the chain. The bi-distance edge for $d(u)=d(v)=2$ has $n + 1$ numbers of edges. The second distance edge partitions has frequency $2n - 2$ where $d(u)=2$ and $d(v)=4$. The 3rd parcel of the edges $d(u)=d(v)=4$ has $n - 3$ edges. Total edges as shown in Table 3.

$d(u), d(v)$	Total number of edges
(2,2)	$n+1$
(4,2)	$2n-2$
(4,4)	$n-3$

Table 3: Edges Partition of Oxide Network for $n \geq 3$

Theorem 4.1. Suppose Q_1 is the oxide network of order n then its randic index is:

$$RI(Q_1) = \left(\frac{3}{4} + \frac{1}{\sqrt{2}}\right)n - \left(\frac{1}{4} + \frac{1}{\sqrt{2}}\right)$$

Proof. The oxide chain COX_n where $n \geq 3$ and n is integer so the formula of RI is

$$RI(Q_1) = \sum_{uv \in E(Q_1)} \frac{1}{\sqrt{d(u) + d(v)}}$$

By utilizing table 3 we get

$$\begin{aligned} R_{-\frac{1}{2}}(Q_1) &= \left(\frac{n+1}{\sqrt{2 \times 2}}\right) + \left(\frac{2n-2}{\sqrt{4 \times 2}}\right) + \left(\frac{n-3}{\sqrt{4 \times 4}}\right) \\ &= \left(\frac{3}{4} + \frac{1}{\sqrt{2}}\right)n - \left(\frac{1}{4} + \frac{1}{\sqrt{2}}\right) \\ R_{-\frac{1}{2}}(Q_1) &= 1.45n - 0.957 \end{aligned}$$

Theorem 4.2. Suppose Q_1 is the oxide network of order n then its forgotten index is;

$$F(Q_1) = 80n - 128$$

Proof. Let $Q_1 = COX_n$ where n is an integer and $n \geq 3$ than

$$F(Q_1) = \sum_{uv \in E(Q_1)} (d(u)^2 + d(v)^2)$$

By consuming the results given in Table 3 we have

$$F(Q_1) = (n + 1)(2^2 + 2^2) + (2n - 2)(4^2 + 2^2) + (n - 3)(4^2 + 4^2)$$

$$F(Q_1) = 80n - 128$$

Theorem 4.3. Consider Q_1 is oxide chain with n order then its AG_1 -index is;

$$AG_1(Q_1) = \left(\frac{3}{\sqrt{2}} + 2\right)n - \left(2 + \frac{3}{\sqrt{2}}\right)$$

Proof. We have oxide network with order n and n is an integer than the AG_1 index is

$$AG_1(Q_1) = \sum_{uv \in E(Q_1)} \frac{(d(u) + d(v))}{2\sqrt{d(u) \times d(v)}}$$

With the help of Table 3 we have

$$AG_1(Q_1) = (n + 1) \times \frac{(2 + 2)}{2\sqrt{2} \times 2} + (2n - 2) \times \frac{(4 + 2)}{2\sqrt{4} \times 2} + (n - 3) \times \frac{(4 + 4)}{2\sqrt{4} \times 4}$$

$$AG_1(Q_1) = \left(\frac{3}{\sqrt{2}} + 2\right)n - \left(2 + \frac{3}{\sqrt{2}}\right)$$

$$AG_1(Q_1) = 4.12n - 4.12$$

Theorem 4.4. Consider Q_1 is oxide network with n order then GA index is

$$GA(Q_1) = \left(\frac{4\sqrt{2}}{3} + 2\right)n - \left(2 + \frac{4\sqrt{2}}{3}\right)$$

Proof. Q_1 is an oxide network with n order than its GA index is

$$GA(Q_1) = \sum_{uv \in E(Q_1)} \frac{2\sqrt{d(u) \times d(v)}}{(d(u) + d(v))}$$

By the mean of Table 3 we get

$$GA(Q_1) = (n + 1) \times \frac{2\sqrt{2 \times 2}}{(2 + 2)} + (2n - 2) \times \frac{2\sqrt{4 \times 2}}{(4 + 2)} + (n - 3) \times \frac{2\sqrt{4 \times 4}}{(4 + 4)}$$

$$GA(Q_1) = \left(\frac{4\sqrt{2}}{3} + 2\right)n - \left(2 + \frac{4\sqrt{2}}{3}\right)$$

$$GA(Q_1) = 3.88n - 3.88$$

Theorem 4.5. Suppose Q_1 is oxide network with n order then its zegreb indices are

$$M_1(Q_1) = 24n - 32$$

$$M_2(Q_1) = 36n - 60$$

$$HM(Q_1) = 400n - 880$$

$$AM(Q_1) = \left(\frac{1160}{27}\right)n - \frac{584}{9}$$

Proof. In the oxide network n is an integer and $n \geq 3$ by defination of zegreb indices

$$M_1(Q_1) = \sum_{uv \in E(Q_1)} (d(u) + d(v))$$

$$M_2(Q_1) = \sum_{uv \in E(Q_1)} (d(u) \times d(v))$$

$$HM(Q_1) = \sum_{uv \in E(Q_1)} (d(u) \times d(v))^2$$

$$AM(Q_1) = \sum_{uv \in E(Q_1)} \left(\frac{d(u) \times d(v)}{d(u) + d(v) - 2} \right)^3$$

By utilizing Table 3 of edges division we have;

The values of first zagreb index for the chain of oxide are

$$M_1(Q_1) = (n + 1)(2 + 2) + (2n - 2)(4 + 2) + (n - 3)(4 + 4)$$

$$M_1(Q_1) = 24n - 32$$

The values for the TIs named as second zagreb index are

$$M_2(Q_1) = (n + 1)(2 \times 2) + (2n - 2)(4 \times 2) + (n - 3)(4 \times 4)$$

$$M_2(Q_1) = 36n - 60$$

Hyper zagreb index is an advanced form of the M-indices useful for many purposes and its values for the chain are

$$HM(Q_1) = (n + 1)(2 \times 2)^2 + (2n - 2)(4 \times 2)^2 + (n - 3)(4 \times 4)^2$$

$$HM(Q_1) = 400n - 880$$

Arithmetic geometric inverse is converse of GA-index and its values for the oxide chain are calculated as

$$AM(Q_1) = (n + 1) \left(\frac{2 \times 2}{2 + 2 - 2} \right)^3 + (2n - 2) \left(\frac{4 \times 2}{4 + 2 - 2} \right)^3 + (n - 3) \left(\frac{4 \times 4}{4 + 4 - 2} \right)^3$$

$$AM(Q_1) = \left(\frac{1160}{27} \right)n - \frac{584}{9}$$

$$AM(Q_1) = 42.96 - 64.88$$

Which are our required results

4.2 Comparison Of Degree Based Topological indices

In this portion, we describe a comparison between all above mentioned TI's graphically for n=1,2,3, 10 in Figure 3. The variation in the TIs is described by lines of different colors. We have only one parameter n so the graphs are just two dimensional. The variation trend of some indices are very fast and some run with slow speed as shown in Figure 3.

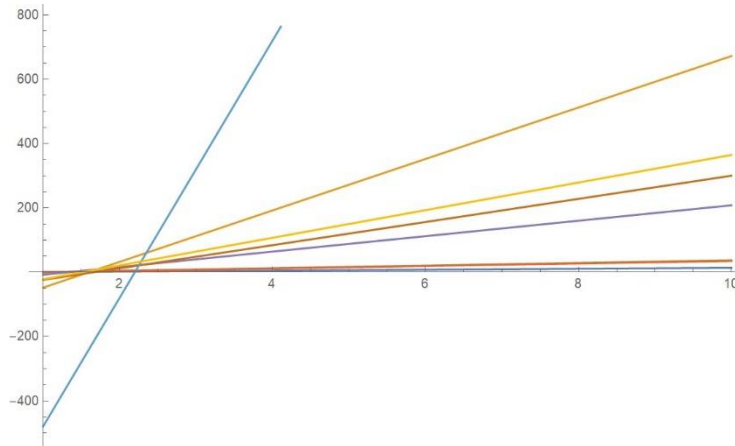


Figure 3: Comparison of Degree Based Topological Indices for the Oxide Chain

4.3 Total Sum of degrees of end vertices

As all the above TIs are dependent on the degree of edges but in the next indices, we concern with the sum of degrees of edges. The partition of edges according to this degree is given in Table 4.

$(d(u), d(v))$	$(S(v), S(u))$	Number of Edges
(2,2)	(8,6)	4
	(8,8)	$n-3$
(4,2)	(6,12)	4
	(8,10)	2
	(8,12)	$2n-8$
(4,4)	(10,12)	2
	(12,12)	$n-4$

Table 4: Edge Partition with respect to Degree Total of End Vertices of Oxide Network

Theorem 4.6. Let Q_1 is oxide network with n order then Sanskruti index is;

$$S(Q_1) = \left(\frac{8374151680}{12326391}\right)n - \left(\frac{3662359}{18522}\right)$$

Proof. Let we have oxide chain $Q_1 \sim COX_n$ for $n \geq 4$ than by definition $S(Q_1)$ is;

$$S(Q_1) = \sum_{uv \in E(Q_1)} \left(\frac{S(u) \times S(v)}{S(u) + S(v) - 2}\right)^3$$

By utilizing table 2 we get

$$S(Q_1) = 4 \times \left(\frac{8 \times 6}{8 + 6 - 2}\right)^3 + (n - 3) \times \left(\frac{8 \times 8}{8 + 8 - 2}\right)^3 + 4 \times \left(\frac{6 \times 12}{6 + 12 - 2}\right)^3 + 2 \times \left(\frac{8 \times 10}{8 + 10 - 2}\right)^3$$

$$+ (2n - 8) \times \left(\frac{8 \times 12}{8 + 12 - 2}\right)^3 + 2 \times \left(\frac{10 \times 12}{10 + 12 - 2}\right)^3 + (n - 4) \times \left(\frac{12 \times 12}{12 + 12 - 2}\right)^3$$

After some easy and simple calculation we get;

$$S(Q_1) = \left(\frac{8374151680}{12326391}\right)n - \left(\frac{3662359}{18522}\right)$$

$$S(Q_1) = 679.36n - 197.73$$

Which is required result.

Theorem 4.7. Let Q_1 is an n order oxide network then its AG_2 index is;

$$AG_2(Q_1) = \left(2 + \frac{5}{\sqrt{6}}\right)n + \left(\frac{14}{\sqrt{3}} + \frac{6}{\sqrt{2}} + \frac{9}{2\sqrt{5}} + \frac{20}{\sqrt{6}} + \frac{11}{\sqrt{30}} - 7\right)$$

Proof. A we have $Q_1 \sim COX_n$ for $n \geq 4$ and n is an integer by the definition of ;

$$AG_2(Q_1) = \sum_{uv \in E(Q_1)} \frac{S(u) + S(v)}{2\sqrt{S(u) \times S(v)}}$$

With the help of Table 4, putting values in formula and we get;

$$\begin{aligned} AG_2(Q_1) &= 4 \times \frac{(8+6)}{2\sqrt{8 \times 6}} + (n-3) \times \frac{(8+8)}{2\sqrt{8 \times 8}} + 4 \times \frac{(6+12)}{2\sqrt{6 \times 12}} + 2 \times \frac{(8+10)}{2\sqrt{8 \times 10}} \\ &+ (2n-8) \times \frac{(8+12)}{2\sqrt{8 \times 12}} + 2 \times \frac{(10+12)}{2\sqrt{10 \times 12}} + (n-4) \times \frac{(12+12)}{2\sqrt{12 \times 12}} \\ AG_2(Q_1) &= \left(2 + \frac{5}{\sqrt{6}}\right)n + \left(\frac{14}{\sqrt{3}} + \frac{6}{\sqrt{2}} + \frac{9}{2\sqrt{5}} + \frac{20}{\sqrt{6}} + \frac{11}{\sqrt{30}} - 7\right) \\ AG_2(Q_1) &= 4.04n + 1.18 \end{aligned}$$

Theorem 4.8. Suppose Q_1 is an oxide of n order than its ABC_4 index is

$$ABC_4(Q_1) = \left(\frac{\sqrt{14}}{8} + \frac{\sqrt{3}}{2} + \frac{\sqrt{22}}{12}\right)n + \left(2\sqrt{\frac{3}{5}} - \frac{3\sqrt{14}}{8} + \frac{4\sqrt{2}}{3} + \frac{2}{\sqrt{5}} - 2\sqrt{3} + \frac{2}{\sqrt{6}} - \frac{\sqrt{22}}{3}\right)$$

Proof. Let $Q_1 = COX_n$ where n is an integer and $n \geq 4$ than according to by definition

$$ABC_4(Q_1) = \sum_{uv \in E(Q_1)} \sqrt{\frac{S(u) + S(v) - 2}{S(u) \times S(v)}}$$

By putting the values in table two we get

$$\begin{aligned} ABC_4(Q_1) &= 4 \times \sqrt{\frac{8+6-2}{8 \times 6}} + (n-3) \times \sqrt{\frac{8+8-2}{8 \times 8}} + 4 \times \sqrt{\frac{6+12-2}{6 \times 12}} + 2 \times \left(\sqrt{\frac{8+10-2}{8 \times 10}}\right) \\ &+ (2n-8) \times \sqrt{\frac{8+12-2}{8 \times 12}} + 2 \times \sqrt{\frac{10+12-2}{10 \times 12}} + (n-4) \times \sqrt{\frac{12+12-2}{12 \times 12}} \end{aligned}$$

After some simple computation we get

$$\begin{aligned} ABC_4(Q_1) &= \left(\frac{\sqrt{14}}{8} + \frac{\sqrt{3}}{2} + \frac{\sqrt{22}}{12}\right)n + \left(2\sqrt{\frac{3}{5}} - \frac{3\sqrt{14}}{8} + \frac{4\sqrt{2}}{3} + \frac{2}{\sqrt{5}} - 2\sqrt{3} + \frac{2}{\sqrt{6}} - \frac{\sqrt{22}}{3}\right) \\ ABC_4(Q_1) &= 1.72n + 1.28 \end{aligned}$$

4.4 Comparison Of TIs For Oxide Network

In this section, we conferred the comparison of three topological indices that are computed above for the oxide network in Figure 4. We have only one parameter that is "n" so our graph is two-dimensional.

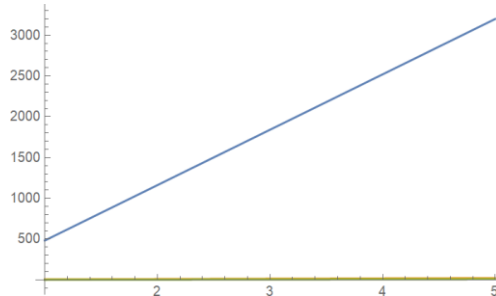


Figure 4: Comparison of Degree Based Topological Indices for Oxide network

5. Main Results Of Silicate Network CSn

In this segment, we study and calculate the degree-based TIs for the chain silicate network namely; RI, FI, AG, GA, Zagreb indices, AG2, ABC4 and GA5 indices. The structure of silicate is a tetrahedron having bond length 109.5° . These are large molecules that can make chains and rings. Silicate has unique properties used for different purposes. The shape of the tetrahedron is just like pyramids with a triangular base. It is formed by four oxygen atoms at corners and with one central silicon atom. The bond length of each silicon and oxygen bond is 162 pm. In Figure 5 we show that silicate network.

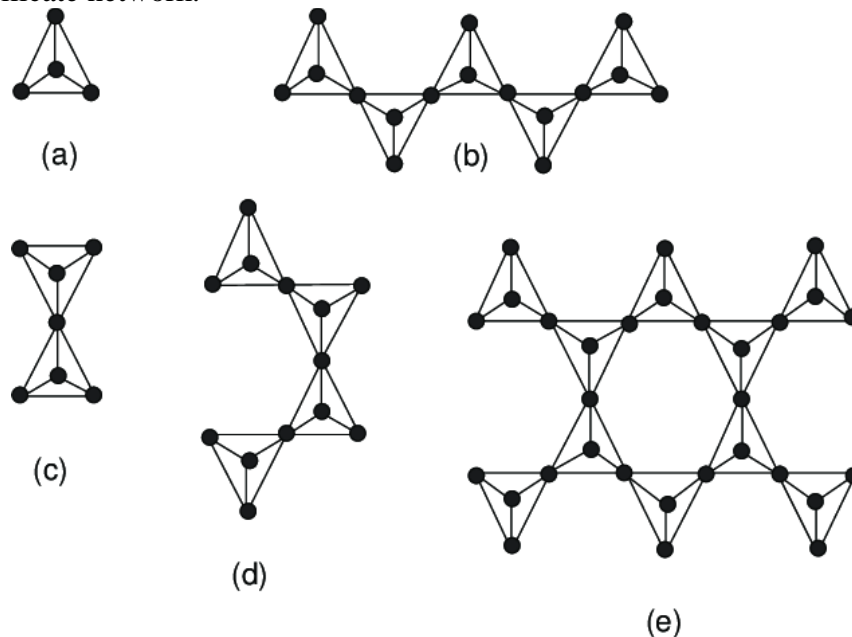


Figure 5: Silicate Network

Remark: The total number of vertices and bi-distance edges are $3n + 1$ and $9n - 9$ respectively.
 Edge partition

There are three type of edge parcels in chain of silicate network. There are two method used here standard edge partition and combinatorial counting. The first edge parcel consists of $4n$ edges where $d(u)=d(v)=3$. The second edge parcel consists of $4n - 6$ edges, where $d(u)=3$ and $d(v)=6$. The third edge parcel contains $n - 3$ edges uv , where $d(u) = d(v) = 2$, as shown in Table 5.

$(d(u),d(v))$	Frequency
$(3,3)$	2
$(3,6)$	$3m-2$
$(6,6)$	$m+2n-2$

Table 5: Edges partition of CS $_n$ where $n \geq 3$.

Theorem 5.1. Suppose Q_2 is the chain of silicate network with order n then its Randic index is;

$$RI(Q_2) = \left(\frac{3}{2} + \frac{4}{3\sqrt{2}}\right)n - \left(\frac{2}{\sqrt{2}} + \frac{1}{2}\right)$$

Proof. Let $Q_2 \sim COX_n$ where $n \geq 3$ and n is integer so by definition;

$$RI(Q_2) = \sum_{uv \in E(Q_2)} \frac{1}{\sqrt{d(u) + d(v)}}$$

By putting the values from Table 5 we get

$$\begin{aligned} R_{-\frac{1}{2}}(Q_2) &= \frac{4n}{\sqrt{3 \times 3}} + \frac{4n - 6}{\sqrt{3 \times 6}} + \frac{n - 3}{\sqrt{6 \times 6}} \\ &= \left(\frac{3}{2} + \frac{4}{3\sqrt{2}}\right)n - \left(\frac{2}{\sqrt{2}} + \frac{1}{2}\right) \\ R_{-\frac{1}{2}}(Q_2) &= 2.44n - 1.91 \end{aligned}$$

Theorem 5.2. Consider Q_2 is the chain of silicate network with order n then its forgotten index is;

$$F(Q_2) = 324n - 486$$

Proof. Suppose $Q_2 \sim COX_n$ where n is an integer and $n \geq 3$ than

$$F(Q_2) = \sum_{uv \in E(Q_2)} (d(u)^2 + d(v)^2)$$

Utilizing Table 5 we have

$$F(Q_1) = (4n) \times (3^2 + 3^2) + (4n - 6) \times (3^2 + 6^2) + (n - 3) \times (6^2 + 6^2)$$

$$F(Q_1) = 324n - 486$$

Theorem 5.3. Suppose Q_2 is chain of silicate network with n order then its AG1 is

$$AG_1(Q_2) = \left(\frac{6}{\sqrt{2}} + 5\right)n - \left(3 + \frac{9}{\sqrt{2}}\right)$$

Proof. Let Q_2 represents the silicate network and by definition AG1 index is

$$AG_1(Q_2) = \sum_{uv \in E(Q_2)} \frac{(d(u) + d(v))}{2\sqrt{d(u) \times d(v)}}$$

With the help of Table 5 we get

$$AG_1(Q_2) = (4n) \times \frac{(3+3)}{2\sqrt{3 \times 3}} + (4n-6) \times \frac{(6+3)}{2\sqrt{6 \times 3}} + (n-3) \times \frac{(6+6)}{2\sqrt{6 \times 6}}$$

$$AG_1(Q_2) = \left(\frac{6}{\sqrt{2}} + 5\right)n - \left(3 + \frac{9}{\sqrt{2}}\right)$$

$$AG_1(Q_1) = 9.242n - 9.36$$

Theorem 5.4. Let Q_2 is the silicate network given in Figure 5 with n order then GA index is;

$$GA(Q_2) = \left(\frac{8\sqrt{2}}{3} + 5\right)n - \left(3 + \frac{12\sqrt{2}}{3}\right)$$

Proof. As $Q_2 \cong COX_n$ where n is an integer $n \geq 3$ so;

$$GA(Q_2) = \sum_{uv \in E(Q_2)} \frac{2\sqrt{d(u) \times d(v)}}{d(u) + d(v)}$$

From the edge partition Table 5 we get

$$GA(Q_2) = (4n) \times \frac{2\sqrt{3 \times 3}}{3+3} + (4n-6) \times \frac{2\sqrt{6 \times 3}}{6+3} + (n-3) \times \frac{2\sqrt{6 \times 6}}{6+6}$$

$$GA(Q_2) = \left(\frac{8\sqrt{2}}{3} + 5\right)n - \left(3 + \frac{12\sqrt{2}}{3}\right)$$

$$GA(Q_1) = 8.77n - 8.65$$

Theorem 5.5. Consider Q_2 is graph of CS_n network with n is the number of tetrahedrons then its zagreb indices are;

$$M_1(Q_2) = 72n - 90$$

$$M_2(Q_2) = 144 - 214$$

$$HM(Q_2) = 2916n - 5832$$

$$AM(Q_2) = \left(\frac{439671564}{2744000}\right)n - \frac{10375128}{42875}$$

Proof. Let $Q_2 \cong COX_n$ where $n \geq 3$ and n is an integer we have four different categories of Zagreb indices like 1_{st} zagreb index , 2_{nd} zagreb index, HM index and Argumented zagreb index are;

$$M_1(Q_2) = \sum_{uv \in E} (d(u) + d(v))$$

$$M_2(Q_2) = \sum_{uv \in E} (d(u) \times d(v))$$

$$HM(Q_2) = \sum_{uv \in E} (d(u) \times d(v))^2$$

$$AM(Q_2) = \sum_{uv \in E} \left(\frac{d(u) \times d(v)}{d(u) + d(v) - 2} \right)^3$$

There are three types of different edges in the linear chain structure of silicate. With the help of Table 5 of edge partition we have

$$M_1(Q_2) = (4n)(3 + 3) + (4n - 6)(6 + 3) + (n - 3)(6 + 6)$$

$$M_1(Q_2) = 72n - 90$$

$$M_2(Q_2) = (4n)(3 \times 3) + (4n - 6)(6 \times 3) + (n - 3)(6 \times 6)$$

$$M_2(Q_2) = 144n - 216$$

$$HM(Q_2) = (4n)(3 \times 3)^2 + (4n - 6)(6 \times 3)^2 + (n - 3)(6 \times 6)^2$$

$$HM(Q_2) = 2916n - 5832$$

$$AM(Q_2) = (4n) \left(\frac{3 \times 3}{3 + 3 - 2} \right)^3 + (4n - 6) \left(\frac{6 \times 3}{6 + 3 - 2} \right)^3 + (n - 3) \left(\frac{6 \times 6}{6 + 6 - 2} \right)^3$$

$$AM(Q) = \left(\frac{439671564}{2744000} \right) n - \frac{10375128}{42875}$$

$$AM(Q_1) = 160.2n + 241.98$$

Which are our required results.

5.2 Comparison Of Degree Based Topological Indices For CS_n

In this section, we compare the above computed TIs Graphically. The graphs are 2-dimension because of one parameter n and n=1,2,3,...5. There are different colors in the 2D graphs that representing the variation of different TIs with changing the inputs.

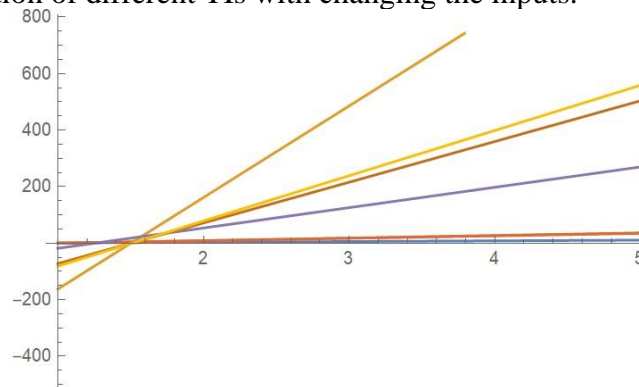


Figure 6: Comparison of Above Calculated Topological Indices for the Silicate Network

(d(u),d(v))	(S(v),S(u))	Number of Edges
(3,3)	(15,12)	12
	(15,15)	4n-12
(3,6)	(12,24)	6
	(15,21)	4
	(15,24)	4n-16
(6,6)	(21,24)	2
	(24,24)	n-5

Table 6: Edge partition for Silicate network CS_n for n ≥ 3

Theorem 5.6. Let Q₂ is an n order chain of silicate network then its AG₂ index is;

$$AG_2(Q_2) = \left(5 + \frac{13}{\sqrt{10}}\right)n + \left(\frac{27}{\sqrt{5}} + \frac{9}{\sqrt{2}} + \frac{24}{\sqrt{24}} - \frac{52}{\sqrt{10}} + \frac{55}{6\sqrt{14}} - 7\right)$$

Proof. Suppose Q₁ ≅ COX_n where n ≥ 4 and n is an integer so according to definition

$$AG_2(Q_2) = \sum_{uv \in E(Q_2)} \frac{S(u) + S(v)}{2\sqrt{S(u) \times S(v)}}$$

By using Table 6 we have

$$\begin{aligned} AG_2(Q_2) &= 12 \times \frac{(12 + 15)}{2\sqrt{12 \times 15}} + (4n - 12) \times \frac{(15 + 15)}{2\sqrt{15 \times 15}} + 6 \times \frac{(12 + 24)}{2\sqrt{12 \times 24}} + 4 \times \frac{(15 + 21)}{2\sqrt{15 \times 21}} \\ &\quad + (4n - 16) \times \frac{(15 + 24)}{2\sqrt{15 \times 24}} + 2 \times \frac{(21 + 24)}{2\sqrt{21 \times 24}} + (n - 5) \times \frac{(24 + 24)}{2\sqrt{24 \times 24}} \\ AG_2(Q_2) &= \left(5 + \frac{13}{\sqrt{10}}\right)n + \left(\frac{27}{\sqrt{5}} + \frac{9}{\sqrt{2}} + \frac{24}{\sqrt{24}} - \frac{52}{\sqrt{10}} + \frac{55}{6\sqrt{14}} - 7\right) \\ AG_2(Q_2) &= 9.11n - 8.49 \end{aligned}$$

Theorem 5.7. Consider Q₂ is silicate chain of n order which means there are total n tetrahedrons in this chain than its ABC₄ index is;

$$ABC_4(Q_2) = \left(\frac{8\sqrt{7}}{15} + \frac{2}{3}\sqrt{\frac{37}{10}} + \frac{\sqrt{46}}{24}\right)n + \left(2\sqrt{\frac{3}{5}} - \frac{3\sqrt{14}}{8} + \frac{4\sqrt{2}}{3} + \frac{2}{\sqrt{5}} - 2\sqrt{3} + \frac{2}{\sqrt{6}} - \frac{\sqrt{22}}{3}\right)$$

Proof. Let the chain of silicate is represented by Q₁ ≅ COX_n where n is an integer and n ≥ 4. For n = 3 the behaviour of TIs is different from all values of n by definition

$$ABC_4(Q_2) = \sum_{uv \in E(Q_1)} \sqrt{\frac{S(u) + S(v) - 2}{S(u) \times S(v)}}$$

By utilizing Table 6 we get

$$\begin{aligned} ABC_4(Q_2) &= 12 \times \sqrt{\frac{12 + 15 - 2}{12 \times 15}} + (4n - 12) \times \sqrt{\frac{15 + 15 - 2}{15 \times 15}} + 6 \times \sqrt{\frac{12 + 24 - 2}{12 \times 24}} + 4 \times \sqrt{\frac{15 + 21 - 2}{15 \times 21}} \\ &\quad + (4n - 16) \times \sqrt{\frac{15 + 24 - 2}{15 \times 24}} + 2 \times \sqrt{\frac{21 + 24 - 2}{21 \times 24}} + (n - 5) \times \sqrt{\frac{24 + 24 - 2}{24 \times 24}} \end{aligned}$$

After some simple computation we get

$$ABC_4(Q_2) = \left(\frac{8\sqrt{7}}{15} + \left(\frac{2}{3}\right)\sqrt{\frac{37}{10} + \frac{\sqrt{46}}{24}}\right)n + \left(2\sqrt{\frac{3}{5}} - \frac{3\sqrt{14}}{8} + \frac{4\sqrt{2}}{3} + \frac{2}{\sqrt{5}} - 2\sqrt{3} + \frac{2}{\sqrt{6}} - \frac{\sqrt{22}}{3}\right)$$

$$ABC_4(Q_2) = 2.97n + 2.34$$

Theorem 5.8. Suppose Q2 is the chain of silicate network with n order than its fifth version of Geometric Arithmetic index is

$$GA_5(Q_2) = \left(5 + \frac{6\sqrt{10}}{13}\right)n + \left(\frac{16\sqrt{5}}{3} + 4\sqrt{2} + \frac{\sqrt{35}}{2} + \frac{64\sqrt{10}}{13} + \frac{8\sqrt{14}}{15} - 17\right)$$

Proof. Let Q2 representing the chain Q2~ = COXn where n ≥ 4 so, by definition

$$GA_5(Q_2) = \sum_{uv \in E(Q_2)} \left(\frac{\sqrt{S(u) \times S(v)}}{S(u) + S(v)}\right)$$

By utilizing Table 4 we get

$$GA_5(Q_2) = 12\left(\frac{2\sqrt{12 \times 15}}{12 + 15}\right) + (4n - 12)\left(\frac{2\sqrt{15 \times 15}}{15 + 15}\right) + 6\left(\frac{\sqrt{12 \times 24}}{12 + 24}\right) + 4\left(\frac{2\sqrt{15 \times 21}}{15 + 21}\right)$$

$$+ (4n - 16)\left(\frac{2\sqrt{15 \times 24}}{15 + 24}\right) + 2\left(\frac{2\sqrt{21 \times 24}}{21 + 24}\right) + (n - 5)\left(\frac{\sqrt{24 \times 24}}{24 + 24}\right)$$

After some simple computation we get

$$GA_5(Q_2) = \left(5 + \frac{6\sqrt{10}}{13}\right)n + \left(\frac{16\sqrt{5}}{3} + 4\sqrt{2} + \frac{\sqrt{35}}{2} + \frac{64\sqrt{10}}{13} + \frac{8\sqrt{14}}{15} - 17\right)$$

$$GA_5(Q_2) = 8.89n + 10.03$$

5.3 Comparison Of Topological Indices For CSn

In this segment, we graphically compare the three TIs that we have computed for the chain of silicate network CSn. The comparison gives us information about the variation of TIs at different points. As all graphs are 2 dimensional because we on single parameter n.

Comparison of TIs for a chain of silicate network like ABC4 index, AG2 index and GA5 index. Different colors are used to represent the different TIs graph.

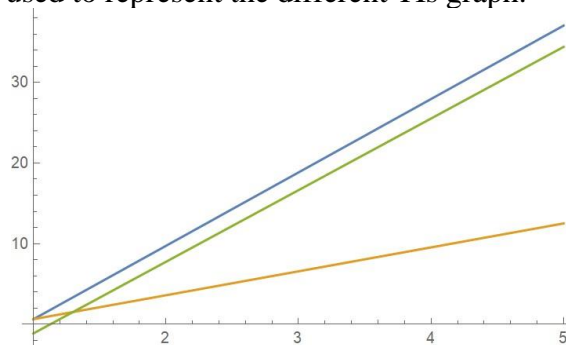


Figure 7: Comparison of above Calculated Topological Indices for the Silicate Network

6. Discussion Of Numerical and Graphical Comparison

In this segment, we have calculated all TIs for the oxide network and silicate network for different values of parameter n .

n	RI	FI	AG ₁	GA	M ₁	M ₂	HM	AM	S	AG ₂	ABC ₄
1	0.49	-48	0	0	-8	-24	-480	-21.92	446	5.22	0.44
2	1.94	32	4.12	3.88	10	12	-80	21.04	1160	9.26	2.16
3	3.39	112	8.24	7.76	40	48	320	64	1840	13.3	3.88
4	5.04	192	12.36	11.64	64	84	720	106.9	2519	17.34	5.6
5	6.29	272	16.48	15.52	88	120	1120	149	3198	21.38	7.32

Table 7: Numerical computation of all TIs for oxide network

n	RI	FI	AG ₁	GA	M ₁	M ₂	HM	AM	S	AG ₂	ABC ₄
1	0.53	-162	-0.12	-18	-72	-2916	-81	0.12	0.62	0.63	-1.41
2	2.97	162	9.12	54	72	0	79	8.89	9.73	3.6	7.75
3	5.41	486	18.36	126	216	2916	239	17.66	18.44	6.57	16.64
4	7.85	810	27.6	198	360	5832	399	26.43	27.95	9.54	25.33
5	10.29	1134	36.85	270	504	8748	559	35.2	37.06	12.51	34.42

Table 8: Comparison of all TIs for Silicate Network

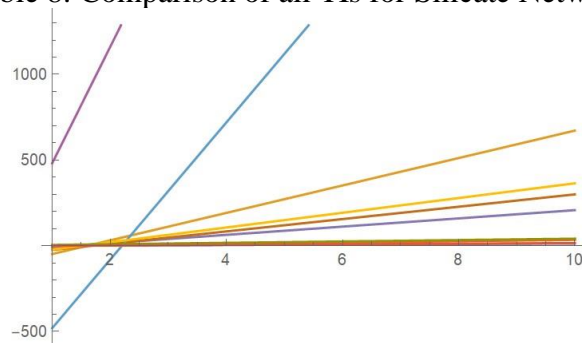


Figure 8: Comparison of Topological Indices for the Oxide Network

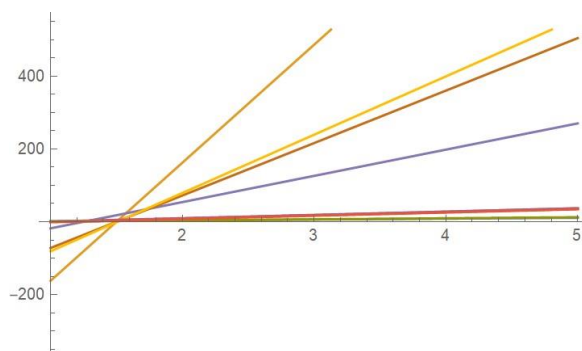


Figure 9: Comparison of Topological Indices for the Silicate Network

The graph is the pictorial representation of the data. It is a modified and simple way to check the variation in data. There are many types of graphs i.e 2D or 3D. The graphs used in our paper are 2 dimensional because our TIs have only one parameter. Table 7 represents all the values of TIs for the oxide network. All the TIs increase by increasing the value of parameter n. Topological indices like $R^{-1/2}$, ABC4 and AG2 increase at a 2 slow rate concerning the other TIs.

The numerical calculation also tells us about the variation in data but it is time-consuming method. The numerical values in Table 8 also increase by increasing the input values of n. The graphical representation for both chain network of oxide and network of silicate.

7. Conclusion

Topological Indices is a mathematical formula that may be applied to any network that represents a molecule structure. It is feasible to explore various physicochemical features of a molecule using this index. Topological indices are used for example in the establishment of quantitative structure-activity relationships (QSARs). QSARs are prediction models developed from statistical methods associating chemical activity (including desired therapeutic benefits and unpleasant side effects) with descriptors reflective of molecular structure and/or characteristics. We are modifying the concept of single edge degree-based topological indices in Bi- distance degree-based topological indices. We are discussing some topological indices in the Chain of Oxide Network and Silicate Network. In the future, we will work on molecular structures with the help of Bi-distance edge-based topological indices.

Data Availability

In this article, no data were utilized.

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Conflicts of Interest

Authors have no conflict of interest.

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