On Modified Topological Invariants of Various Networks

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Abstract

A phenomenon known as chemical graph theory is being investigated in the field of chemical structures in order to comprehend the mathematical representations of chemical molecules and the insights they provide. In this respect, topolog-ical indices play an essential role in distinguishing between the bases of molecules and their branching patterns; these indices are attached to each chemical structure. Chemical reaction kinetics, including the effects of temperature and oscillation, may be better understood using this method. In this article, we aim to improve upon the idea of counting millions of edges based on a single edge by applying it to paths of length two between specific pairs (u, v) ε V(G). The goal is to compute efficient and concise informative results that outperform single edge formulas both numerically and graphically. This idea of an edge route allows us to effortlessly drive millions of formulae for topological indices. A topological index based on bi-distance edges! Different topological indices based on Bi-Distance degrees are computed in this article for oxide chain and silicate networks. These indices are Randic, Forgotten, Arithmetic Geometric, Geometric Arithmetic, Zagreb, Sanskruti, Second Arithmetic Geometric, and Fourth Atom-bond Connectivity.

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

1. Introduction

A graph is a graphical way to show many kinds of information or data. Each of the two-dimensional, regular, simple, and planar graphs discussed in this piece has a collection of points called vertices (nodes) linked together by lines called edges (links). Molecular structure is studied in mathematical chemistry using many mathematical approaches, apart from quantum mechanics, which is a significant part of theoretical chemistry. This theory provides a solid foundation for the growth and improvement of chemical sciences. In the process of creating QSAR models, molecular descriptors are quite useful. Molecular Commonly referred to as graph invariants, well-known molecular descriptors that derive from graph theory principles include connectivity indices (MCI) or topological indices (TI). Translators of chemical structural topology are TIs. Here, we may enter numerical numbers and get information on the variances in chemical structural attributes; it's a function. TIs are substantial and can be easily calculated using basic mathematical tools and methodologies. Numerous fields, including nanotechnology, theoretical chemistry, chemical graph theory, and pharmacology, make extensive use of these indexes. The concept was proposed by Harold

Wiener, who introduced the first topological index in 1947 and titled it the Wiener index.

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

Wiener went on to publish a number of studies that provided justification for the connection between the Wiener index and hydrocarbons. Hundreds of TIs have been inspired by his work to simplify the process of understanding the intricate structures of many compounds. This article delves into the topic of degree-based TIs such as RI, FI, AG index, GA index, Sanskruti index, AG2 index, and ABC4 index as they pertain to 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) respec- tively. 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

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

Milan Randic [1] to investigate the physical and chemical prop- erties of compounds. Randic index is denoted by R mathematically it is describedas :-

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:-

AG index is an inverse TI of GA-index invented in 2015 [7] denoted by AG1 index andcomputed 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, deter-
mined 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:

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

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 M1 and M2 were proposed by Gutman [16] in 1972. Zegrab indices are denoted by M- indices. This index is the base of many indices. Due to its great importance lots oftime , it is redefined and modified by different ways. The mathematical description of for four M-indices is:

$$M_1(G) = \sum_{uv\varepsilon E} (d(u) + d(v))$$

$$M_2(G) = \sum_{uv\varepsilon E} (d(u) \times d(v))$$

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

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

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]. Sanskruti index is computed by using the concept of ”total sum of degrees of end vertices” represented by SI and defined :

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

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

The fifth version of arithmetic-geometric index is denoted by AG5 and mathematically describedas:

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

M. Ghorbani et al. proposed the latest TI; Fourth Atom-Bond Connectivity index ABC4 in 2010[23, 24].ABC4index defined as:

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

The last three indices are the ”sum of degree” based indices where $S(u) = \sum_{uv\varepsilon E} d(v)$ and $S(v) = \sum_{uv\varepsilon E} d(u)$. 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:-

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

$$F(F_3^4) = 4(2^2 + 2^2) + 8(8^2 + 2^2)$$
$$F(F_3^4) = 576$$

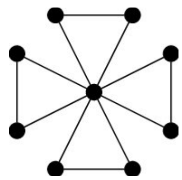

Figure 1: Friendship Graph F_3^4

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 Forgotton 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

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

$$F(F_3^4) = 24(2^2 + 2^2)$$
$$F(F_3^4) = 192$$

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.

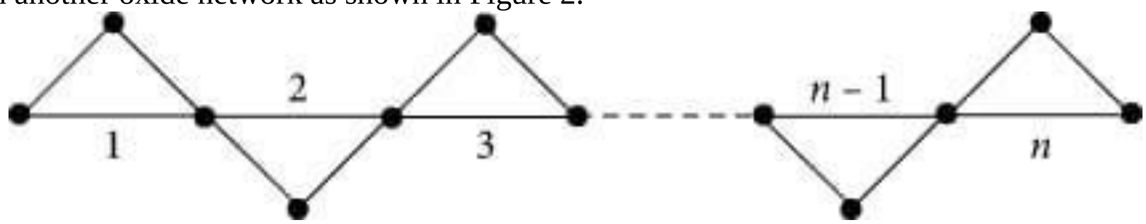

Figure 2: Chain Oxide Network *COXn* of Order n

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≥3

Theorem 4.1. Suppose Q1 is the oxide network of order n then its randic index is:

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

Proof. The oxide chain COXn where n≥3 and n is integer so the formula of RI is

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

By utilizing table 3 we get

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

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

$$R_{\frac{-1}{2}}(Q_1) = 1.45n - 0.957$$

Theorem 4.2. Suppose Q1 is the oxide network of order n then its forgotten index is;

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

Proof. Let Q1=COXn where n is an integer and n≥3 than

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

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 Q1 is oxide chain with n order then its AG1-index is;

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

Proof. We have oxide network with order n and n is an integer than the AG1 index is

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

With the help of Table 3 we have

$$AG_1(Q_1) = (n+1)\times\frac{(2+2)}{2\sqrt{2\times 2}} + (2n-2)\times\frac{(4+2)}{2\sqrt{4\times 2}} + (n-3)\times\frac{(4+4)}{2\sqrt{4\times 4}}$$
$$AG_1(Q_1) = (\frac{3}{\sqrt{2}}+2)n - (2+\frac{3}{\sqrt{2}})$$
$$AG_1(Q_1) = 4.12n - 4.12$$

Theorem 4.4. Consider Q1 is oxide network with n order then GA index is

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

Proof. Q1 is an oxide network with n order than its GA index is

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

By the mean of Table 3 we get

$$GA(Q_1) = (n+1)\times\frac{2\sqrt{2\times 2}}{(2+2)} + (2n-2)\times\frac{2\sqrt{4\times 2}}{(4+2)} + (n-3)\times\frac{2\sqrt{4\times 4}}{(4+4)}$$
$$GA(Q_1) = (\frac{4\sqrt{2}}{3}+2)n - (2+\frac{4\sqrt{2}}{3})$$
$$GA(Q_1) = 3.88n - 3.88$$

Theorem 4.5. Suppose Q1 is oxide network with n order then its zegreb indices are

$$\begin{aligned} M_1(Q_1) &= 24n - 32 \\ M_2(Q_1) &= 36n - 60 \\ HM(Q_1) &= 400n - 880 \\ AM(Q_1) &= (\frac{1160}{27})n - \frac{584}{9} \end{aligned}$$

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

$$M_1(Q_1) = \sum_{uv \varepsilon E(Q_1)} (d(u) + d(v))$$
$$M_2(Q_1) = \sum_{uv \varepsilon E(Q_1)} (d(u) \times d(v))$$
$$HM(Q_1) = \sum_{uv \varepsilon E(Q_1)} (d(u) \times d(v))^2$$
$$AM(Q_1) = \sum_{uv \varepsilon E(Q_1)} (\frac{d(u) \times d(v)}{d(u) + d(v) - 2})^3$$

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

$$AM(Q_1) = (n+1)(\frac{2 \times 2}{2+2-2})^3 + (2n-2)(\frac{4 \times 2}{4+2-2})^3 + (n-3)(\frac{4 \times 4}{4+4-2})^3$$
$$AM(Q_1) = (\frac{1160}{27})n - \frac{584}{9}$$
$$AM(Q_1) = 42.96 - 64.88$$

Which are our required results

4.2 Comparision 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.

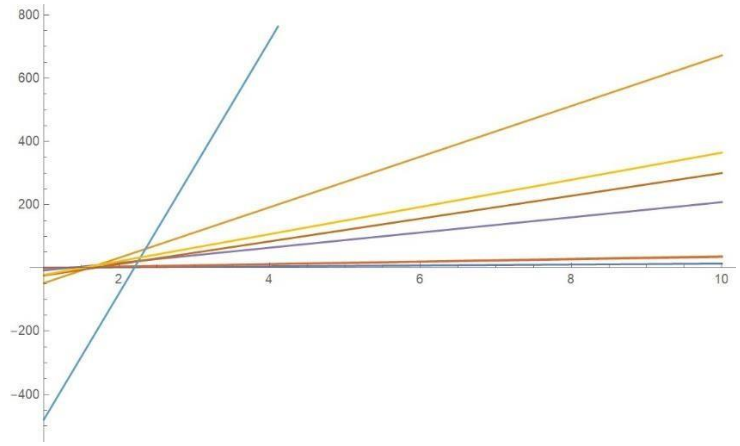

Figure 3: Comparsion of Degree Based Topological Indice for the Oxide Chain

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 Q1 is oxide network with n order then Sanskruti index is;

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

Proof. Let we have oxide chain Q1 ∼= COXn for n≥4 than by definition S(Q1)is;

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

By utilizing table 2 we get

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

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

After some easy and simple calculation we get;

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

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

Which is required result.

Theorem 4.7. Let Q1 is an n order oxide network then its AG2 index is;

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

Proof. A we have Q1 ∼= COXn for n≥4 and n is an integer by the definition of ;

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

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

$$AG_2(Q_1) = 4 \times \frac{(8+6)}{2\sqrt{8 \times 6}} + (n-3) \times \frac{(8+8)}{2\sqrt{8 \times 8}} + 4 \times \frac{(6+12)}{2\sqrt{6 \times 12}} + 2 \times \frac{(8+10)}{2\sqrt{8 \times 10}})$$

$$+(2n-8) \times \frac{(8+12)}{2\sqrt{8 \times 12}} + 2 \times \frac{(10+12)}{2\sqrt{10 \times 12}} + (n-4) \times \frac{(12+12)}{2\sqrt{12 \times 12}}$$

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

$$AG_2(Q_1) = 4.04n + 1.18$$

Theorem 4.8. Suppose Q1 is an oxide of n order than its ABC4 index is

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

Proof. Let Q1=COXn where n is an integer and n≥4 than according to by definition

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

By putting the values in table two we get

$$ABC_4(Q_1) = 4 \times \sqrt{\frac{8+6-2}{8 \times 6}} + (n-3) \times \sqrt{\frac{8+8-2}{8 \times 8}} + 4 \times \sqrt{\frac{6+12-2}{6 \times 12}} + 2 \times (\sqrt{\frac{8+10-2}{8 \times 10}})$$

$$+(2n-8) \times \sqrt{\frac{8+12-2}{8 \times 12}} + 2 \times \sqrt{\frac{10+12-2}{10 \times 12}} + (n-4) \times \sqrt{\frac{12+12-2}{12 \times 12}}$$

After some simple computition we get

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

$$ABC_4(Q_1) = 1.72n + 1.28$$

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.

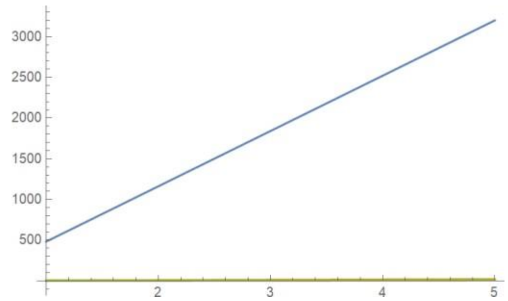

Figure 4: Comparsion of Degree Based Topological Indice for Oxide network

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 5we show that silicate network.

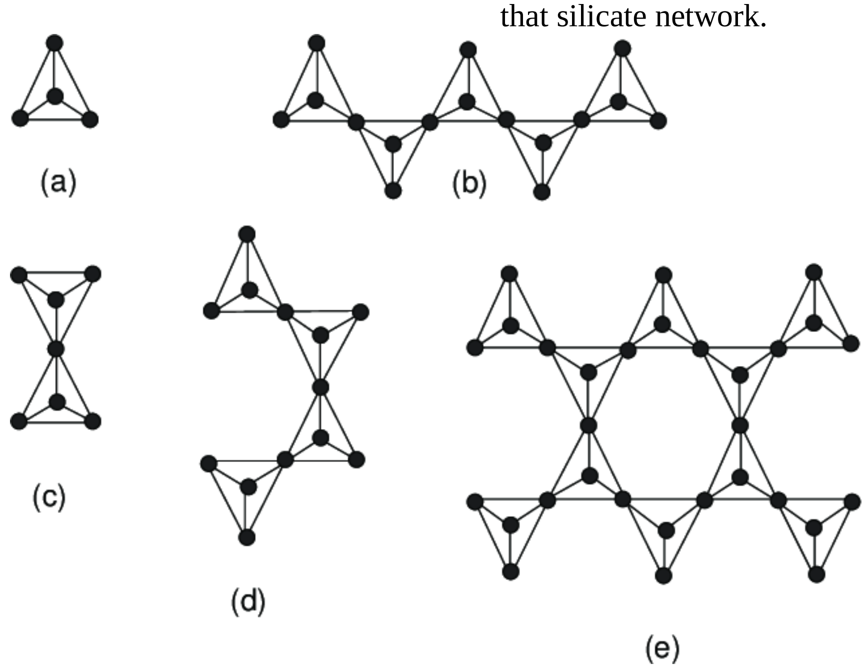

Figure 5: Silicate Network

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 CSn where n≥3.

Theorem 5.1. Suppose Q2 is the chain of silicate network with order n then its Randic index is;

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

Proof. Let Q2∼= COXn where n≥3 and n is integer so by definition;

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

By putting the values from Table 5 we get

$$R_{\frac{-1}{2}}(Q_2) = \frac{4n}{\sqrt{3\times 3}}+\frac{4n-6}{\sqrt{3\times 6}}+\frac{n-3}{\sqrt{6\times 6}}$$

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

$$R_{\frac{-1}{2}}(Q_2) = 2.44n-1.91$$

Theorem 5.2. Consider Q2 is the chain of silicate network with order n then its forgotten index is;

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

Proof. Suppose Q2∼= COXn where n is an integer and n≥3 than

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

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 Q2 is chain of silicate network with n order then its AG1 is

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

Proof. Let Q2 represents the silicate network and by definition AG1 index is

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

With the help of Table 5 we get

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

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

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

Theorem 5.4. Let Q2 is the silicate network given in Figure 5 with n order then GA index is;

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

Proof. As $Q_2 \simeq COX_n$ where n is an integer n≥3 so;

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

From the edge partition Table 5 we get

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

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

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

Theorem 5.5. Consider Q2 is graph of CSn network with n is the number of tetrahedrons then its zegreb indices are;

$$\begin{aligned} M_1(Q_2) &= 72n - 90 \\ M_2(Q_2) &= 144 - 214 \\ HM(Q_2) &= 2916n - 5832 \\ AM(Q_2) &= (\frac{439671564}{2744000})n - \frac{10375128}{42875} \end{aligned}$$

Proof. Let $Q_2 \simeq COX_n$ where n≥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;

$$M_1(Q_2) = \sum_{uv\varepsilon E} (d(u) + d(v))$$
$$M_2(Q_2) = \sum_{uv\varepsilon E} (d(u) \times d(v))$$
$$HM(Q_2) = \sum_{uv\varepsilon E} (d(u) \times d(v))^2$$
$$AM(Q_2) = \sum_{uv\varepsilon E} (\frac{d(u) \times d(v)}{d(u) + d(v) - 2})^3$$

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

$$M_1(Q_2) = (4n)(3+3) + (4n-6)(6+3) + (n-3)(6+6)$$
$$M_1(Q_2) = 72n - 90$$
$$M_2(Q_2) = (4n)(3\times 3) + (4n-6)(6\times 3) + (n-3)(6\times 6)$$
$$M_2(Q_2) = 144n - 216$$
$$HM(Q_2) = (4n)(3\times 3)^2 + (4n-6)(6\times 3)^2 + (n-3)(6\times 6)^2$$
$$HM(Q_2) = 2916n - 5832$$
$$AM(Q_2) = (4n)(\frac{3\times 3}{3+3-2})^3 + (4n-6)(\frac{6\times 3}{6+3-2})^3 + (n-3)(\frac{6\times 6}{6+6-2})^3$$
$$AM(Q) = (\frac{439671564}{2744000})n - \frac{10375128}{42875}$$
$$AM(Q_1) = 160.2n + 241.98$$

Which are our required results.

5.2 Comparision Of Degree Based Topological Indices For CSn

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 vartiation of different TIs with changing the inputs.

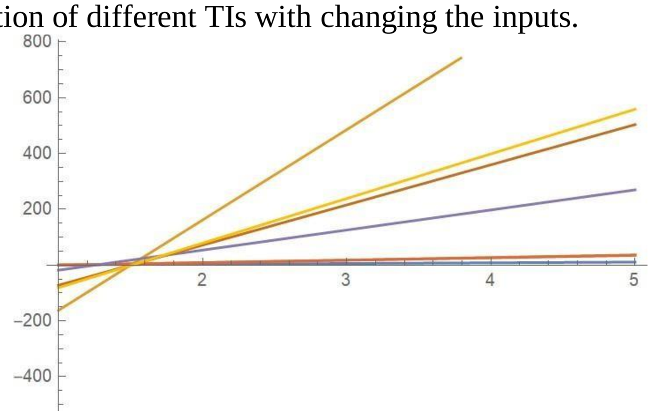

Figure 6: Comparsion of Above Calculated Topological Indices for the Silicate Network

(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 CSn for n≥ 3

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

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

Proof. Suppose $Q_1 \simeq COX_n$ where n≥4 and n is an integer so according to definition

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

By using Table 6 we have

$$AG_2(Q_2)=12\times\frac{(12+15)}{2\sqrt{12\times 15}}+(4n-12)\times\frac{(15+15)}{2\sqrt{15\times 15}}+6\times\frac{(12+24)}{2\sqrt{12\times 24}}+4\times\frac{(15+21)}{2\sqrt{15\times 21}}$$

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

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

$$AG_2(Q_2)=9.11n-8.49$$

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;

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

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

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

By ultilizing Table 6 we get

$$ABC_4(Q_2)=12\times\sqrt{\frac{12+15-2}{12\times 15}}+(4n-12)\times\sqrt{\frac{15+15-2}{15\times 15}}+6\times\sqrt{\frac{12+24-2}{12\times 24}}+4\times\sqrt{\frac{15+21-2}{15\times 21}}$$

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

After some simple compution we get

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

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

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

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

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

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

By ultilizing Table 4 we get

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

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

After some simple computition we get

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

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

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.

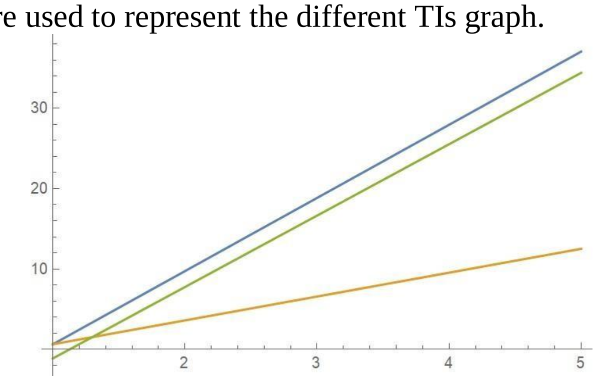

Figure 7: Comparison of above Calculated Topological Indices for the Silicate Network

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	-o.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	3685	270	504	8748	559	35.2	37.06	12.51	34.42

Table 8: Comparison of all TIs for Silicate Network

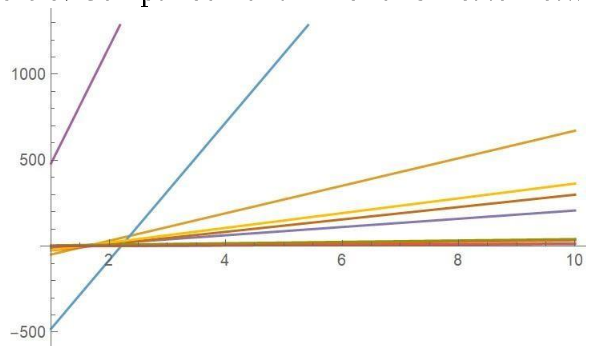

Figure 8: Comparison of Topological Indices for the Oxide Network

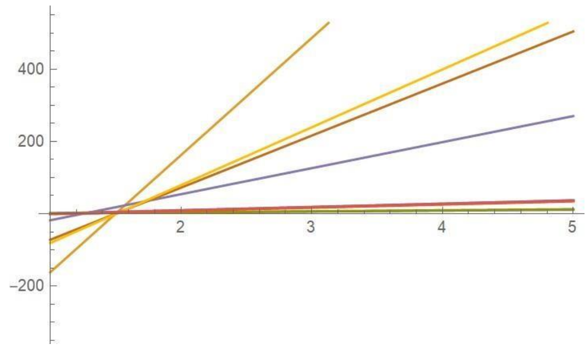

Figure 9: Comparsion of Topological Indices for the Silicate Network

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 are2 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

Any network representing a molecule's structure may be fitted using the mathematical formula of topological indices. Using this index, it is possible to investigate a molecule's physical properties. One use of topological indices is the construction of quantitative structure-activity relationships (QSARs). Quantitative structure-activity relationship (QSAR) models are a kind of statistical method-based prediction model that links chemical activity (including target therapeutic advantages and unwanted side effects) to structural and/or characteristic descriptors. In Bi-distance degree-based topological indices, we are revising the idea of single edge degree-based indices. Topological indices in the Oxide and Silicate Network Chains are being discussed. Our future endeavours will include using Bi-distance edge-based topological indices to the study of molecular structures.

Access to Data

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