IJPSR (2018), Volume 9, Issue 10 (Research Article)

INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES AND RESEARCH

Received on 23 January, 2018; received in revised form, 02 August, 2018; accepted, 31 August, 2018; published 01 October, 2018

# ON SOME TOPOLOGICAL INDICES OF TRIANGULAR SILICATE AND TRIANGULAR OXIDE NETWORKS

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**Keywords:**

Topological index, Triangular oxide network, Triangular silicate network, Harrary index, Wiener index, Forgotten index

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**ABSTRACT:** A topological index is a numeric quantity from the structural graph of a molecule. It has become a very useful tool in the prediction of pharmacological, toxicological and physico - chemical properties of a compound. In this paper, we have computed some topological indices of triangular silicate *TsL (n)* and triangular oxide *TOL (n)* networks.

**INTRODUCTION:** Let G be a simple connected graph with *n* vertices and *m* edges. A simple graph is a molecular graph if its vertices and edges correspond to atoms and bonds respectively. A simple graph is an undirected and un-weighted graph with no multiple edges or loops. If there is a path between all pairs of vertices in a graph, then the graph is called a connected graph. So a molecular graph is always a simple connected graph. Graph theory has found considerable use in modeling chemical structures. Chemical graph theory is an important branch of mathematical chemistry that uses graph theory in the mathematical modeling of chemical phenomena [1, 2, 3].

QUICK RESPONSE CODE

DOI: 10.13040/IJPSR.0975-8232.9(10).4326-31

Article can be accessed online on: www.ijpsr.com

DOI link: http://dx.doi.org/10.13040/IJPSR.0975-8232.9(10).4326-31

Chemical graph theory has an important effect in the development of mathematical chemistry and chemical sciences. Computing topological indices in mathematical chemistry is an important branch.

Topological index has become a very useful tool in the prediction of physiochemical and pharmacological properties of a compound. The number of vertices and edges are the topological index molecular structure matters. The main ingredients of the molecular topological models are topological indices which are the topological characterization of molecules by means of numerical invariants. These models are instrumental in the discovery of new applications of molecules with specific chemical, pharmacological and biological properties. Applications of graph theory have led to the emergence of a number of graph-theoretical indices [4]. These indices are used by various researchers in their studies. The first use of a topological index was made by the chemist Harold Wiener [5] in 1947.

In recent years many researchers have worked on computing topological indices [6, 7, 8, 9, 10, 11, 12, 13, 14]. Bharati R *et al*., have calculated the Zagreb, Randić and ABC index of silicate, honeycomb and hexagonal networks [15].

Kulli introduced the first and second K-Banhatti indices of a graph in [16]. Kulli also defined some properties of these newly defined indices. The coindices of K-Banhatti indices were also defined in his work. Later kulli defined K hyper-Banhatti indices of V-Phenylenic nanotubes and nanotorus [17]. Gutman *et al*., developed relations between Banhatti and Zagreb indices and discussed the lower and upper bounds for Banhatti indices of a connected graph in terms of Zagreb indices [18]. Kulli et al also computed Banhatti indices for certain families of benzenoid systems [19]. Moreover, Kulli introduced multiplicative hyper-Banhatti indices and coindices, Banhatti geometric-arithmetic index connectivity Banhatti indices for certain families of benzenoid systems [20-21]. Fazal Dayan *et al*., [22] computed Banhatti indices for triangular silicate, triangular oxide, rhombus silicate and rhombus oxide networks. Fazal Dayan *et al*., [23] also computed Banhatti indices for hexagonal, honeycomb and derived networks.

In recent years many researchers have worked on computing topological indices [24-26].

In this study, we compute some topological indices of *TsL (n)* and *TOL (n)* networks. Silicates are the largest, the most complicated and the most interesting class of minerals by far. $SiO_4$ tetrahedron is the basic chemical unit of silicates. The silicates sheets are rings of tetrahedrons linked by shared oxygen nodes to other rings in two dimensional planes producing a sheet like structures. A silicate can be obtained by fusing a metal oxide or a metal carbonate with sand. Essentially every silicate contains $SiO_4$ tetrahedron.

The corner and the center vertices represent oxygen and silicon ions respectively. These vertices are called oxygen nodes and silicon node respectively. A Silicate network is obtained in different ways. Paul Manuel has constructed a silicate network from a honeycomb network [5]. In **Fig. 1**, $SiO_4$ tetrahedra is shown where the corner and the center vertices represent oxygen and silicon ions respectively.

In **Fig. 2** and **3**, triangular silicate network of order 3 and 4 are given.

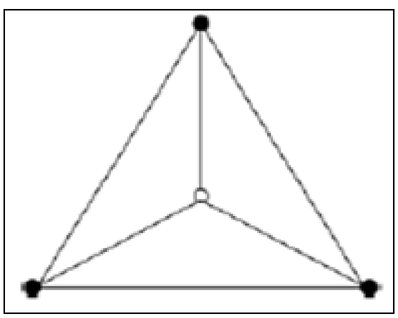

**FIG. 1: $SiO_4$ TETRAHEDRA**

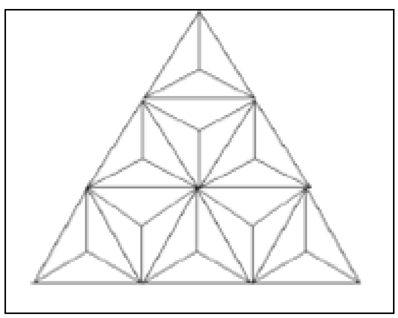

**FIG. 2: TRIANGULAR SILICATE NETWORK OF ORDER 3**

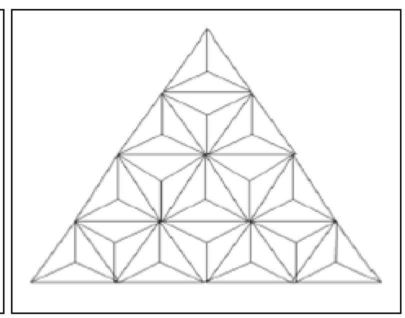

**FIG. 3: TRIANGULAR SILICATE NETWORK OF ORDER 4**

Following are the types of edges based on the degree of the vertices of each edge in a triangular silicate network from level 4. These six types are given in the **Table 1**.

**TABLE 1: TYPES AND NUMBER OF EDGES IN A TRIANGULAR SILICATE NETWORK**

| | **(3, 3)** | **(3, 7)** | **(7, 12)** | **(12, 12)** | **(7, 7)** | **(3, 12)** |
|---|---|---|---|---|---|---|
| Total number of edges | 3 | 33+9 ($n$-4) | 12+6 ($n$-4) | $3\frac{(n-3)(n-2)}{2}$ | 3($n$-1) | $6\frac{(n-2)(n-1)}{2}$ |

Following are the four types of edges based on the degree of the vertices of each edge in a triangular oxide network from level 4. These four types are given in the **Table 2**.

**TABLE 2: TYPES AND NUMBER OF EDGES IN A TRIANGULAR OXIDE NETWORK**

| | **(2, 4)** | **(4, 4)** | **(4, 6)** | **(6, 6)** |
|---|---|---|---|---|
| Total number of edges | 6 | 3($n$-1) | 6($n$-2) | $\frac{3\{(n-3)^2 + (n-2)]}{2}$ |

**Harrary Index, Wiener Index and Forgotten Index:** For a simple graph *G*, the Harrary, Wiener and Forgotten indices are given by:

$$H(G) = \sum_{u,v \in G} \frac{1}{du.dv}$$

$$W(G) = \frac{1}{2} \sum_{u,v \in G} d(u,v)$$

$$F(G) = \sum [d(u)^2 + d(v)^2]$$

Where *du* and *dv* denote the degree of the vertex *u* and *v* in G respectively.

**Main Results:**

**Theorem:** For a triangular silicate network, *TsL* (*n*) of dimension *n*, the Harrary index is given by

$$H(G) = 0.0141666n^2 + 1.0601615595n + 0.048894125$$

**Proof:**

$$H(G) = \sum_{u,v \in E_{3,3}} \frac{1}{9} + \sum_{u,v \in E_{3,7}} \frac{1}{21} + \sum_{u,v \in E_{7,12}} \frac{1}{84} + \sum_{u,v \in E_{12,12}} \frac{1}{144} + \sum_{u,v \in E_{7,7}} \frac{1}{49} + \sum_{u,v \in E_{3,12}} \frac{1}{36}$$

$$= 3\left(\frac{1}{9}\right) + \left(33 + 9(n-4)\right)\frac{1}{21} + \left(12 + 6(n-4)\right)\frac{1}{84} + \frac{3(n-3)(n-2)}{2}\left(\frac{1}{144}\right) + \left(3(n-1)\right)\frac{1}{49} + \left(6\frac{(n-2)(n-1)}{2}\right)\frac{1}{36}$$

$$= \frac{3}{9} + \frac{33}{21} - \frac{36}{21} + \frac{9n}{21} + \frac{12}{84} + \frac{6n}{84} - \frac{24}{84} + \frac{3n^2}{288} - \frac{15n}{288} + \frac{18}{288} + \frac{3n}{49} - \frac{3}{49}$$

$$= 0.0141666n^2 + 1.0601615595n + 0.048894125$$

**Theorem:** For a triangular oxide network, *TOL (n)* of dimension *n*, the Harrary index is given by

$$H(TOL(n)) = 0.04166666n^2 + 0.229166666n + 0.3125$$

**Proof:**

$$H(G) = \sum_{u,v \in E_{2,4}} \frac{1}{8} + \sum_{u,v \in E_{4,4}} \frac{1}{16} + \sum_{u,v \in E_{4,6}} \frac{1}{24} + \sum_{u,v \in E_{6,6}} \frac{1}{36}$$

$$= \frac{1}{8}(6) + \frac{1}{16}(3n-3) + \frac{1}{24}(6n-12) + \frac{1}{36}\left(\frac{3(n-3)^2 + (n-3)}{2}\right)$$

$$= \frac{6}{8} + \frac{3n}{16} - \frac{3}{16} + \frac{6n}{24} - \frac{12}{24} + \frac{1}{36}\left(\frac{3n^2 - 18n + 27 + 3n - 9}{2}\right)$$

$$= \frac{6}{8} - \frac{3}{10} - \frac{12}{24} + \frac{27}{72} - \frac{9}{72} + \frac{3n}{16} + \frac{6n}{24} - \frac{18n}{72} + \frac{3n}{72} + \frac{3n^2}{72}$$

$$= 0.3125 + 0.229166666n + 0.04166666n^2$$

**Theorem:** For a triangular silicate network, *TsL* (*n*) of dimension, the Wiener index is given by

$$W(TsL(n)) = 162n^2 - 331n + 160.5$$

**Proof:**

$$W(G) = \frac{1}{2}\sum_{u,v\in E_{3,3}}(9) + \frac{1}{2}\sum_{u,v\in E_{3,7}}(21) + \frac{1}{2}\sum_{u,v\in E_{7,12}}(84) + \frac{1}{2}\sum_{u,v\in E_{12,12}}(144) + \frac{1}{2}\sum_{u,v\in E_{7,7}}(49) + \frac{1}{2}\sum_{u,v\in E_{3,12}}(36)$$

$$= \frac{9}{2}(3) + \frac{21}{2}(33+9(n-4)) + 42(12+6(n-4)) + 72\left(\frac{3(n^2-5n+6)}{2}\right) + \frac{49}{2}(3(n-1)) + 18\left(\frac{6(n^2-3n+2)}{2}\right)$$

$$= 13.5 + 346.5 + 94.5n - 378 + 504 + 252n - 1008 + 108n^2 - 540n + 648 + 73.5n - 73.5 + 54n^2 - 162n + 108$$

$$= 162n^2 - 331n + 160.5$$

**Theorem:** For a triangular oxide network, *ToL (n)* of dimension n, the Wiener index is given by

$$W(ToL(n)) = 27n^2 - 39n + 34$$

**Proof:**

$$H(G) = \frac{1}{2}\sum_{u,v\in E_{2,4}} 8 + \frac{1}{2}\sum_{u,v\in E_{4,4}} 16 + \frac{1}{2}\sum_{u,v\in E_{4,6}} 24 + \frac{1}{2}\sum_{u,v\in E_{6,6}} 36$$

$$= 4(6) + 8(3(n-1)) + 12(6(n-2)) + 18\left(\frac{3[(n-3)^2+(n-3)]}{2}\right)$$

$$= 24 + 24n - 8 + 72n - 144 + 27(n^2 - 5n + 6)$$

$$= 27n^2 - 39n + 34$$

**Theorem:** For a triangular silicate network, *TsL(n)* of dimension n, the Forgotten index is given by

$$F(TsL(n)) = 891n^2 - 1558n + 4404$$

**Proof:**

$$F(G) = \sum_{u,v\in E_{3,3}}(18) + \sum_{u,v\in E_{3,7}}(58) + \sum_{u,v\in E_{7,12}}(193) + \sum_{u,v\in E_{12,12}}(288) + \sum_{u,v\in E_{7,7}}(98) + \sum_{u,v\in E_{3,12}}(153)$$

$$= 3(18) + (33+9(n-4))58 + (6n-12)193 + \left(\frac{3(n^2-5n-6)}{2}\right)288 + (3n-3)98 + 3(n^2-3n+2)(153)$$

$$= 54 + 1914 + 522n - 2088 + 1158n - 2316 + 432n^2 - 2160n - 2592 + 294n + 459n^2 - 1377n + 918$$

$$= 891n^2 - 1558n + 4404$$

**Theorem:** For a triangular oxide network, *ToL(n)* of dimension n, the Forgotten index is given by

$$F(ToL(n)) = 108n^2 - 132n + 48$$

**Proof:**

$$F(G) = \sum_{u,v\in E_{2,4}} 20 + \sum_{u,v\in E_{4,4}} 32 + \sum_{u,v\in E_{4,6}} 52 + \sum_{u,v\in E_{6,6}} 72$$

$$= 6(20) + (3(n-1))(32) + (6n-12)(52) + \left(\frac{3[(n-3)^2 + (n-3)]}{2}\right)(72)$$

$$= 120 + 96n - 96 + 312n - 624 + 108n^2 - 648n + 972 + 108n - 324$$

$$= 108n^2 - 132n + 48$$

**CONCLUSION:** In this paper, we have computed some topological indices *i.e.* the Harrary Index, the Wiener Index and the Forgotten Index for triangular silicate network and triangular oxide network that will help to understand the physical features, chemical reactivities and biological activities of the triangular silicate and triangular oxide networks. These results can also provide a significant determination in the pharmaceutical industry.

**ACKNOWLEDGEMENT:** The authors are very grateful to the editor and reviewers for their comments and suggestions, which are helpful in improving the paper.

**CONFLICT OF INTEREST:** Nil

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**How to cite this article:**
Dayan F, Ahmad B, Zulqarnain M, Ali U, Ahmad Y and Zia TJ: On some topological indices of triangular silicate and triangular oxide networks. Int J Pharm Sci & Res 2018; 9(10): 4326-31. doi: 10.13040/IJPSR.0975-8232.9(10).4326-31.