Computing Some Topological Indices of Triangular Silicate Network

M. Rosary, C.J. Deeni, D. Antony Xavier

Abstract--- *A topological index is a numeric quantity from the structural graph of a molecule. This model has become an important tool in the prediction of physico - chemical, pharmacological and toxicological properties of a compound directly. Graph theory has found considerable use in Chemistry, particularly in modelling chemical structures. Topological indices are designed basically by transforming a molecular graph into a number. In this paper, we compute certain topological indices of Triangular silicate network and Triangular oxide network.*

Keywords--- *Some Topological Indices, Triangular Oxide Network, Triangular Silicate Network*

I. Introduction

LET G be a simple graph, the vertex and edge sets of which are represented by V(G) and E(G) respectively. The degree of the vertex u of graph G is denoted by d_u. Essentially, all the silicates contain SiO4 tetrahedra. In Chemistry, the corner vertices of SiO_4 tetrahedron represents oxygen ions and the centre vertex represents the silicon ion. In graph theory, we call the corner vertices as oxygen-nodes and the centre vertex as silicon node. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [14],[12],[9].

This theory had an important effect on the development of the chemical sciences. Let P be the class of finite graphs. A topological index is a function Top from P into real numbers with this property that Top (G) = Top (H), if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological index molecular structure matters. Its scope is the topological characterization of molecules by means of numerical invariants, called topological indices, which are the main ingredients of the molecular topological models. These are statistical models that are instrumental in the discovery of new applications of naturally occurring molecules, as well as in the design of synthetic molecules with specific chemical, biological, or pharmacological properties. In this review, we focus on pharmacology, which is a novel field of application of molecular topology. Besides summarizing some recent developments, we also seek to bring closer this interesting biomedical application of mathematics to an interdisciplinary readership.

Application of graph theory to chemical and to structure-property-activity (QSPR/QSAR) relationships has led to the emergence of several critical graph-theoretical indices [1]. Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstic [14]. Let G be a simple graph. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of G are defined in [14] respectively as

$$M_1(G) = \sum_{u \in E(G)} (du)^2;$$

$$M_2(G) = \sum_{u,v \in E(G)} (d(u)d(v))$$

where d(u) denotes the degree of the vertex u in G and d(v) denotes the degree of the vertex v in G. The Zagreb indices are used by various researchers in their Quantitative Structure – Property Relationship [QSPR] and Quantitative Structure - Activity Relationship [QSAR] studies [10]. The connectivity index introduced in 1975 by Milan Randic [13] , who has shown this index to reflect molecular branching .
Randic index was defined as follows

$$R(G) = \sum_{u,v \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$$

Randic index has a good correlation with several physicochemical properties of alkanes: boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapour pressure, surface areas, etc.[4]. We also call it as, the product-connectivity index. Motivated by Randic's definition of the product-connectivity index, the sum- connectivity index of a graph G was proposed in [5], which is defined as

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

The applications of the sum-connectivity index have been investigated in [3]. Another topological index namely, Geometric-arithmetic index (GA index) defined by Vukicevic and Furtula as follows

$$GA(G) = \sum_{uv \in E(G)} \frac{2(\sqrt{d_u d_v})}{d_u + d_v}$$

Recently Ernesto Estrada et al. [6], introduced atom - bond connectivity (ABC) index, which it has been applied up until

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now to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows

$$\text{ABC(G)} = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

A molecular graph is a simple graph such that its vertices correspond to the atoms and edges to the bonds. The simplest topological indices do not recognize double bonds and atom types (C,N,O etc) and ignore hydrogen atoms ("hydrogen suppressed") and defined for connected undirected molecular graphs only [8]. In this paper, we compute these indices for the triangular silicate network and triangular oxide network.

II. SILICATE NETWORKS

The silicates are the largest, the most interesting and the most complicated class of minerals by far. The basic chemical unit of silicates is the (SiO_4) tetrahedron. A silicate sheet is a ring of tetrahedrons which are linked by shared oxygen nodes to other rings in a two dimensional plane that produces a sheet-like structure.

Silicates are obtained by fusing metal oxides or metal carbonates with sand. Essentially all the silicates contain SiO_4 tetrahedron. In chemistry, the corner vertices of SiO_4 tetrahedron represent oxygen ions and the centre vertex represents the silicon ion. In graph theory, we call the corner vertices as oxygen nodes and the centre vertex as silicon node. (See Figure 1).

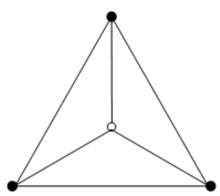


Figure 1

SiO_4 tetrahedra where the corner vertices represent oxygen ions and the centre vertex represent the silicon ion.

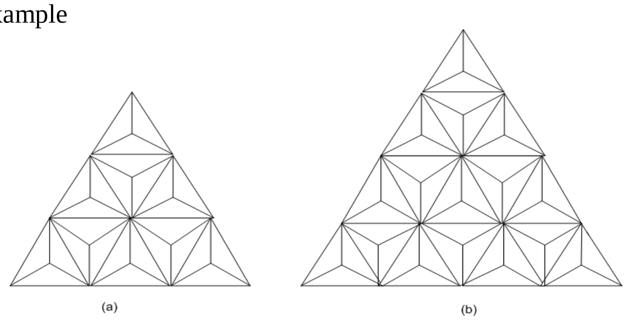
A Silicate network can be constructed in different ways. Paul Manuel described the construction of a silicate network from a honeycomb network [13].

Example

III. TRIANGULAR SILICATE NETWORKS

In this paper we describe the construction of a silicate network from a triangular network.

Example



Triangular Silicate network of level 3 and 4

An n - dimensional triangular silicate network is denoted by TSL(n).

Theorem 3.1

The number of nodes in Triangular Silicate Network TSL(n) is $\left[\frac{(n-1)(n-2)}{2}\right] + 3(n-1) + n^2 + 3$

Theorem 3.2

The number of edges in Triangular Silicate Network TSL(n) is

$$3n\left[\frac{3n+1}{2}\right].$$

TSL(n) is a 3 - regular graph.

In a triangular silicate network, from level 4 there are six types of edges based on the degree of the vertices of each edges. The following table gives the six types and gives the number of edges in each type.

From this table we have the following theorems.

(d_u,d_v) where u,v $\in$ E(G)	Total Number Of edges
(3,3)	3
(3,7)	33+9(n-4)
(7,12)	12+6(n-4)
(12,12)	$\frac{3(n-3)(n-2)}{2}$
(7,7)	3(n-1)
(12,3)	$\frac{6(n-2)(n-1)}{2}$

Theorem 3.3

Let G be the Triangular Silicate network TSL(n) of dimension n. Then the ABC index is given by

$$ABC(G) = 2.389077608n^2 + 1.398905047n + 0.388695452$$

Proof:

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

$$= \sum_{uv\in e_{3,3}} \frac{2}{3} + \sum_{uv\in e_{3,7}} \sqrt{\frac{8}{21}} + \sum_{uv\in e_{3,12}} \frac{\sqrt{13}}{6} + \sum_{uv\in e_{7,12}} \sqrt{\frac{17}{84}} + \sum_{uv\in e_{12,12}} \sqrt{\frac{11}{72}} + \sum_{uv\in e_{7,7}} \frac{\sqrt{12}}{7}$$

$$= 3\left(\frac{2}{3}\right) + \; 33 + 9(n-4) \; \sqrt{\frac{8}{21}} + \left[\frac{6(n-2)(n-1)}{2}\right]\frac{\sqrt{13}}{6} +$$

$$12 + 6(n-4) \; \sqrt{\frac{17}{84}} + \left[\frac{3(n-3)(n-2)}{2}\right]\sqrt{\frac{11}{72}} + \; 3(n-1) \; \frac{\sqrt{12}}{7}$$

$$ABC(G) = 2.389077608n^2 + 1.398905047n + 0.388695452$$

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Theorem 3.4

Let G be the Triangular Silicate network TSL(n) of dimension n. Then the Randic index is given by R(G) = 0.625 n^2 + 0.92218611 n + 0.357467561

Proof:

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

$$= \sum_{uv\in e_{3,3}} \frac{1}{3} + \sum_{uv\in e_{3,7}} \frac{1}{\sqrt{21}} + \sum_{uv\in e_{3,12}} \frac{1}{6} + \sum_{uv\in e_{7,12}} \frac{1}{2(\sqrt{21})} + \sum_{uv\in e_{12,12}} \frac{1}{12} + \sum_{uv\in e_{7,7}} \frac{1}{7}$$

$$= 3\left(\frac{1}{3}\right) + 33+9(n-4)\ \frac{1}{\sqrt{21}} + \left[\frac{6(n-2)(n-1)}{2}\right]\frac{1}{6} +$$

$$12+6(n-4)\ \frac{1}{2(\sqrt{21})} + \left[\frac{3(n-3)(n-2)}{2}\right]\frac{1}{12} + \ 3(n-1)\ \frac{1}{7}$$

R(G) = 0.625 n^2 + 0.92218611 n + 0.357467561

Theorem 3.5

Let G be the Triangular Silicate network TSL(n) of dimension n. Then the Sum connectivity index is given by

$R^+(G)$=1.080782886n^2+1.169606925 n + 0.107599687

Proof:

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

$$\sum_{uv\in e_{3,3}} \frac{1}{\sqrt{6}} + \sum_{uv\in e_{3,7}} \frac{1}{\sqrt{10}} + \sum_{uv\in e_{3,12}} \frac{1}{\sqrt{15}} + \sum_{uv\in e_{7,12}} \frac{1}{\sqrt{19}} + \sum_{uv\in e_{12,12}} \frac{1}{\sqrt{24}} + \sum_{uv\in e_{7,7}} \frac{1}{\sqrt{14}}$$

$$= 3\left(\frac{1}{\sqrt{6}}\right) + [33+9(n-4)]\frac{1}{\sqrt{10}} + [\frac{6(n-2)(n-1)}{2}]\frac{1}{\sqrt{15}} +$$

$$[12+6(n-4)]\frac{1}{\sqrt{19}} + [\frac{3(n-3)(n-2)}{2}]\frac{1}{\sqrt{24}} + [3(n-1)]\frac{1}{\sqrt{14}}$$

$R^+(G)$ = 1.080782886n^2+1.169606925n+ 0.107599687

Theorem 3.6

Let G be the Triangular Silicate network TSL(n) of dimension n. Then the Geometric arithmetic index is given by GA(G) = 3.9n^2 + 2.3371 n - 0.526533

Proof:

$$GA(G) = \sum_{uv\in E(G)} \frac{2\ \sqrt{d_u d_v}}{d_u + d_v}$$

$$= \sum_{uv\in e_{3,3}} 9 + \sum_{uv\in e_{3,7}} 9 + \sum_{uv\in e_{3,12}} 144 + \sum_{uv\in e_{7,12}} 144 + \sum_{uv\in e_{12,12}} 144 + \sum_{uv\in e_{7,7}} 49$$

$$3(1) + [33+9(n-4)]\frac{\sqrt{21}}{5} + [\frac{6(n-2)(n-1)}{2}]\frac{12}{15} +$$

$$[12+6(n-4)]\frac{4(\sqrt{21})}{19} + [\frac{3(n-3)(n-2)}{2}](1) + [3(n-1)](1)$$

GA(G) = 3.9n^2 + 2.3371 n - 0.526533

Theorem 3.7

Let G be the Triangular Silicate network TSL(n) of dimension n. Then the First zagreb index is given by $M_1(G)$ = 648n^2 - 1284 n + 285

Proof:

$$M_1(G) = \sum_{uv\in E(G)} d(u)^2$$

$$\sum_{uv\in e_{3,3}} 9 + \sum_{uv\in e_{3,7}} 9 + \sum_{uv\in e_{3,12}} 144 + \sum_{uv\in e_{7,12}} 144 + \sum_{uv\in e_{12,12}} 144 + \sum_{uv\in e_{7,7}} 49$$

$$3(9) + [33+9(n-4)]9 + [\frac{6(n-2)(n-1)}{2}]144 +$$

$$[12+6(n-4)]144 + [\frac{3(n-3)(n-2)}{2}](144) + [3(n-1)](49)$$

$M_1(G)$ = 648n^2 - 1284 n + 285

Theorem 3.8

Let G be the Triangular Silicate network TSL(n) of dimension n. Then the second zagreb index is given by $M_2(G)$ = 324n^2 - 564 n + 321

Proof:

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

$$\sum_{uv\in e_{3,3}} 9 + \sum_{uv\in e_{3,7}} 21 + \sum_{uv\in e_{3,12}} 36 + \sum_{uv\in e_{7,12}} 84 + \sum_{uv\in e_{12,12}} 144 + \sum_{uv\in e_{7,7}} 49$$

$$3(9) + [33+9(n-4)]21 + [\frac{6(n-2)(n-1)}{2}]36 +$$

$$[12+6(n-4)]84 + [\frac{3(n-3)(n-2)}{2}](144) + [3(n-1)](49)$$

$M_2(G)$ = 324n^2 - 564 n + 321

Levels ↓	ABC	Randic	Sum Connectivity	GA	First Zagreb	Second Zagreb
4	44	14	22	71	5517	3249
5	67	21	33	109	10065	5601
6	95	28	46	154	15909	8601
7	127	37	61	207	23049	12249
8	164.5	48	79	268	31485	16545
9	206.5	59	98	336	41217	21489
10	253	72	120	413	52245	27081

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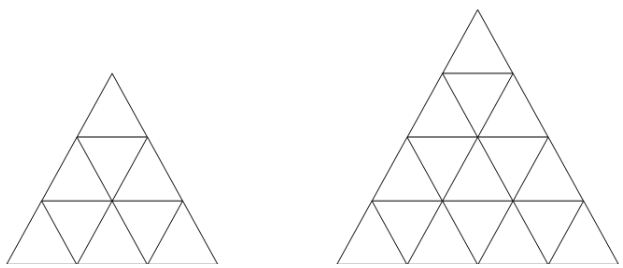
OBSERVATION

The relationship between these indices of a triangular silicate network are M1 > M2 > GA > ABC > R+ > R

IV. TRIANGULAR OXIDE NETWORK

When all the silicon nodes are deleted from a triangular silicate network, we obtain a new network which we shall call as a triangular oxide network (see Figure 3)

Example



(a) (b)

Figure 3

An n - Dimensional Triangular Oxide Network is denoted by TOX(n)

Theorem 4.1

The number of nodes in a triangular oxide network TOX(n) is $\frac{1}{2}\left[n^2-3n+2\right]+3(n-1)+3$

Theorem 4.2

The number of edges in triangular oxide network TOX(n) is $\frac{3n}{2}\ n+1\ \ \frac{3n}{2}\ n+1$.

TOX(n) is a 3-regular graph.

In a triangular oxide network, from level 4 there are four types of edges based on the degree of the vertices of each edge. The following table gives the four types and gives the number of edges in each type.

(d_u,d_v) where $u,v \in E(G)$	Total number of edges
(2,4)	6
(4,4)	3(n-1)
(4,6)	6(n-2)
(6,6)	$\frac{3[(n-3)^2+(n-3)]}{2}$

From this table we have the following theorems.

Theorem 4.3

Let G be the Triangular Oxide network TOX(n) of dimension n. Then the ABC index is given by ABC(G) = 0.790569415 n^2 + 1.348371847n + 0.22073664

Proof:

$$ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$$

$$=\sum_{uv\in e_{2,4}}\sqrt{\frac{1}{2}}+\sum_{uv\in e_{4,4}}\sqrt{\frac{3}{8}}+\sum_{uv\in e_{4,6}}\sqrt{\frac{1}{3}}+\sum_{uv\in e_{6,6}}\sqrt{\frac{5}{18}}$$

$$6\left(\sqrt{\frac{1}{2}}\right)+[3(n-1)]\sqrt{\frac{3}{8}}+[6(n-2)]\sqrt{\frac{1}{3}}+3[(n-3)^2+(n-3)]\sqrt{\frac{5}{18}}$$

ABC(G)=0.790569415n^2+1.348371847n+ 0.22073664

Theorem 4.4

Let G be the Triangular Oxide network TOX(n) of dimension n. Then the GA index is given by

GA(G) = 1.5n^2 + 1.378775383 n - 0.100696521

Proof:

$$GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_ud_v}}{d_u+d_v}$$

$$=\sum_{uv\in e_{2,4}}\frac{\sqrt{8}}{3}+\sum_{uv\in e_{4,4}}1+\sum_{uv\in e_{4,6}}\frac{\sqrt{24}}{5}+\sum_{uv\in e_{6,6}}1$$

$$6\left(\frac{\sqrt{8}}{3}\right)+[3(n-1)]1+[6(n-2)]\frac{\sqrt{24}}{5}+3[(n-3)^2+(n-3)]1$$

GA(G) = 1.5n^2 + 1.378775383 n - 0.100696521

Theorem 4.5

Let G be the Triangular Oxide network TOX(n) of dimension n. Then the Randic index is given by

R(G) = 0.25 n^2 + 0.724744871 n + 0.421830601

Proof:

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

$$=\sum_{uv\in e_{2,4}}\frac{1}{\sqrt{8}}+\sum_{uv\in e_{4,4}}\frac{1}{4}+\sum_{uv\in e_{4,6}}\frac{1}{\sqrt{24}}+\sum_{uv\in e_{6,6}}\frac{1}{6}$$

$$6\left(\frac{1}{\sqrt{8}}\right)+[3(n-1)]\frac{1}{4}+[6(n-2)]\frac{1}{24}+3[(n-3)^2+(n-3)]\frac{1}{6}$$

R(G) = 0.25 n^2 + 0.724744871 n + 0.421830601

Theorem 4.6

Let G be the Triangular Oxide network TOX(n) of dimension n. Then the Sum Connectivity index is given by

R+(G)= 0.433012701n^2+0.792963258n+ 0.19217259

Proof:

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

$$=\sum_{uv\in e_{2,4}}\frac{1}{\sqrt{6}}+\sum_{uv\in e_{4,4}}\frac{1}{\sqrt{8}}+\sum_{uv\in e_{4,6}}\frac{1}{\sqrt{10}}+\sum_{uv\in e_{6,6}}\frac{1}{\sqrt{12}}$$

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$$6\left(\frac{1}{\sqrt{6}}\right)+[3(n-1)]\frac{1}{\sqrt{8}}+[6(n-2)]\frac{1}{\sqrt{10}}+$$
$$3[(n-3)^2+(n-3)]\frac{1}{\sqrt{12}}$$

R+(G)=0.433012701n^2+0.792963258n+ 0.19217259

Theorem 4.7

Let G be the Triangular Oxide network TOX(n) of dimension n. Then the First zagreb index is given by $M_1(G) = 54n^2 - 6n - 132$

Proof:

$$M_1(G) = \sum_{uv\in E(G)} d(u)^2$$
$$= \sum_{uv\in e_{2,4}} 4 + \sum_{uv\in e_{4,4}} 16 + \sum_{uv\in e_{4,6}} 36 + \sum_{uv\in e_{6,6}} 36$$
$$6\ \ 4\ +[3(n-1)]16+[6(n-2)]36+3[(n-3)^2+(n-3)]36$$
$$M_1(G) = 54n^2 - 6n - 132$$

Theorem 4.8

Let G be the Triangular Oxide network TOX(n) of dimension n. Then the Second zagreb index is given by $M_2(G) = 54n^2 - 78n + 36$

Proof:

$$M_2(G) = \sum_{uv\in E(G)} (d(u))(d(v))$$
$$= \sum_{uv\in e_{2,4}} 8 + \sum_{uv\in e_{4,4}} 16 + \sum_{uv\in e_{4,6}} 24 + \sum_{uv\in e_{6,6}} 36$$
$$6\ \ 8\ +[3(n-1)]16+[6(n-2)]24+3[(n-3)^2+(n-3)]36$$
$$M_2(G) = 54n^2 - 78n + 36$$

Levels ↓	ABC	Randic	Sum Connectivity	GA	First Zagreb	Second Zagreb
4	18	29	7	10	708	588
5	27	44	10	15	1188	996
6	37	62	14	21	1776	1512
7	48	83	18	27	2472	2136
8	62	107	22	34	3276	2868
9	76	134	27	42	4188	3708
10	93	164	34	51	5208	4656

V. Observation

The relationship between these indices of a triangular oxide network are M1 > M2 > GA > ABC > R^+ > R

VI. Conclusion

In this paper, we determine the Atom Bond Connectivity index, Zagerb index, Geometric Arithmetic index, Randic index, and Sum connectivity index for triangular silicate network and triangular oxide network.

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