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Generalized Zagreb indices for some silicate networks

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Abstract

Graph theory received a great attention in chemical graph theory which is a branch of mathematical chemistry to model a molecule through a graph where vertices are considered as the atoms of the molecule and edges are considered as the bonds between

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them. A topological index or molecular descriptor of a graph is a numeric quantity obtained mathematically which characterizes its topology and it is invariant under graph isomorphisms. In chemical graph theory, various topological indices play important role in predicting physicochemical properties of chemical compounds. In this paper, we compute the general Zagreb index of some silicate networks and hence obtain some degree based topological indices such as Zagreb indices, forgotten topological index, redefined Zagreb index, general first Zagreb index, general Randić index and symmetric division deg index of silicate networks.

Subject Classification: *05C35, 05C07, 05C40.*

Keywords: *General Zagreb index, Degree-based topological indices, Silicate networks.*

1. Introduction

A new branch of mathematical chemistry is called chemical graph theory which deals with applications of graph theory to solve problems of molecules. A graph is used to represent a chemical structure by considering atoms as vertices and edges as bonds between them. A chemical graph is simple, connected and finite and is defined as $G = (V(G), E(G))$ where $V(G)$ denotes the set of vertices and $E(G)$ denotes the set of edges of G, respectively. The degree of a vertex $h \in V(G)$ is the number of edges incident to it and denoted by $d_G(h)$. A topological index gives a real number for a given graph which characterizes its topology and usually a graph invariant. In chemical graph theory, various topological indices are used to develop some quantitative structure-activity relationships (QSAR) and quantitative structure property relationships (QSPR) in which the biological activity and physiochemical properties of the molecules are correlated with their chemical structures. To study the structure-dependency of total π-electron energy (ε), Gutman and Trinajstić in 1972 [13], noticed that ε depends on the terms of the form

$$M_1(G) = \sum_{h \in V(G)} d_G(h)^2 = \sum_{hk \in E(G)} [d_G(h) + d_G(k)];$$

$$M_2(G) = \sum_{hk \in E(G)} d_G(h) d_G(k).$$

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Thus this quantity provides a measure of the branching of the carbon-atom skeleton of the underlying molecule. Later, these two indices are considered as molecular structure descriptors and named as first Zagreb index and second Zagreb index respectively. We encourage the reader to see [5, 17, 23] for further study about this index. In the same paper [13], where Zagreb indices were introduced, the term of the sum of cubes of degrees of vertices of the molecular graph was shown to influence (ε), but this topological index was never again investigated and was left to oblivion. In 2015 [9], Furtula and Gutman reinvestigated this index again and shown that it can significantly enhance the physicochemical applicability of the first Zagreb index. They named this index as forgotten topological index or *F*-index and it is defined as

$$F(G) = \sum_{h \in V(G)} d_G(h)^3 = \sum_{hk \in E(G)} [d_G(h)^2 + d_G(k)^2].$$

We refer the reader to [6-8, 21] for further study about this index. In [18], Ranjini et al. introduced the redefined first Zagreb index as

$$\mathrm{Re}\, ZM(G) = \sum_{hk \in E(G)} d_G(h)\, d_G(k) [d_G(h) + d_G(k)].$$

See [14, 15, 25] for some recent study about this index. A general version of the first Zagreb index and F-index was introduced by Li and Zheng in [16]. They defined this index as

$$M^{\alpha}(G) = \sum_{h \in V(G)} d_G(h)^{\alpha}$$

where $\alpha \neq 0, 1$ and $\alpha \in IR$. Gutman and Lepović in [11], generalized the Randić index as

$$R_a = \sum_{hk \in E(G)} \{d_G(h) . d_G(k)\}^a$$

where, $a \neq 0, a \in IR$. Vukičević et al. [12], first introduced the symmetric division deg index as a remarkable predictor of total surface area of polychlorobiphenyls. It is one of discrete Adriatic indices that showed good predictive properties on the testing sets provided by International Academy of Mathematical Chemistry. They defined this index as

$$SDD(G) = \sum_{hk \in E(G)} \left[\frac{d_G(h)}{d_G(k)} + \frac{d_G(k)}{d_G(h)} \right].$$

We encourage the reader to [1, 10] for further study about this index. Followed by Zagreb indices, Azari et al. [3], first proposed the general Zagreb index or (a, b)-Zagreb index in 2011. They, defined this index by

Table 1

Correspondence between general Zagreb index and some other vertex degree based topological indices [24]

Topological index	Corresponding general Zagreb index
M_1	$Z_{1,0}$
M_2	$\frac{1}{2}Z_{1,1}$
F	$Z_{2,0}$
$\mathrm{Re}\,ZM$	$Z_{2,1}$
M^a	$Z_{a-1,0}$
R_a	$\frac{1}{2}Z_{a,a}$
SDD	$Z_{1,-1}$

$$Z_{a,b}(G) = \sum_{hk \in E(G)} (d_G(h)^a d_G(k)^b + d_G(h)^b d_G(k)^a).$$

See [19, 20, 22], for some recent work on this index. Table 1 shows the correspondence between general Zagreb index and some other vertex degree based topological indices for some particular values of *a* and *b*.

1.1 *Silicates and their applications*

The silicates are largest, quite interesting and more complicated minerals than any other minerals. Nearly 30% of minerals are silicates and various geologists discovered that 90% of earth's crust is made up of silicates, SiO_4^{4-} based material. Thus for the earth's crust, oxygen and silicon are two most plentiful elements. Silicate (SiO_4^{4-}) is tetrahedron shaped and silicon is the central element of silicates. The central silicon atom has $(+ve)$ charge equal to 4 while each oxygen has $(-ve)$ charge equal to 2. Thus the silicat tetrahedron has a net charge of -4 and the energy of every silicon-oxygen bond is equal to half of the total bond energy of oxygen. In silicate minerals, these tetrahedron are arranged and linked together in different ways.

The simplest silicate structure, olivine, is composed of isolated tetrahedra bond with iron or magnesium atoms. In olivine, the -4 charge of each silica tetrahedron is balanced by two divalent (that is $+2$) iron or magnesium cations. It can be either Mg_2SiO_4 or Fe_2SiO_4 or some combination of the two $(Mg, Fe)_2SiO_4$. For some interesting properties of silicates including capacity to conduct electricity, it causes a high-frequency vibration and give thermal insulation.

Silicates are hard crystals that can be sliced into little pieces. Therefore silicon is the authentic material to make microchips which run in PDA, PC and other game tools. SiO_4^{4-} shares each oxygen atom with other units to form a three dimensional system. Quartz is such a structure which has an exceptional ability to create rhythmic high-frequency vibrations. Because of these attributes quartz are used to make oscillators which are used in radios and watches. Silicates are also used to make ceramics hard, flammable and inert. For this reason ceramics can be used in high temperature for corrosive and tribological applications.

1.2 *Silicate networks*

A honeycomb network can be constructed in various ways from a hexagon. The honeycomb network HC_1 is a hexagon. If we add six hexagons to the boundary edges of HC_1, then we get the honeycomb network HC_2. An n dimensional honeycomb network HC_n is derived from HC_{n-1} by adding a layer of hexagons around the boundary of HC_{n-1}. An example of honeycomb network of dimension four is shown in Figure 1.

Similarly, an n dimensional silicate network is constructed from the n dimensional honeycomb network HC_n by replacing silicon atoms with all the vertices of HC_n, then inserting an oxygen atom into each edge of HC_n and adding $6n$ new pendant edges, each one at the 2-degree silicon atoms of HC_n and placing oxygen atoms at the pendent vertices as shown in Figure 2(a). Thus each silicon atom which is related to the three adjacent oxygen atoms form a tetrahedron as shown in Figure 2(b). The resulting network is called a silicate network of dimension n and is denoted by SL_n.

An n dimensional chain silicate network is derived by arranging n tetrahedra linearly and is denoted by CS_n (see Figure 3). Some Zagreb type calculations are done in [2, 4]. There exist three regular plane tilings which consist of the same regular polygons such as triangular, hexagonal and square. In hexagonal networks, the triangular tilings are used. They are denoted by HX_n where the parameter n denotes the dimension of HX_n. The figure of a hexagonal network of dimension 6 is illustrated in Figure 4. If we delete all the silicon nodes from a silicate network, then we obtain a new network named as oxide network and is denoted by OX_n (see Figure 7 for an oxide network of dimension 5).

Table 2

Edge partition of oxide networks

$(d(h), d(k)) : hk \in E(HC_n)$	Total number of edges
(2, 2)	6
(2, 3)	$12n$ - 12
(3, 3)	$9n^2 - 15n + 16$

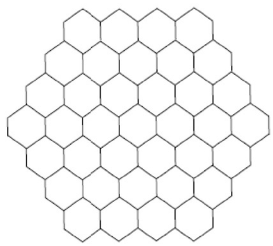

Figure 1

The honeycomb network HC_4 of dimension four

2. Main results

In this section, we compute general Zagreb index or (a, b)-Zagreb index of some silicate networks such as honeycomb networks, silicate networks, chain silicate networks, hexagonal networks and oxide networks. First, we consider the honeycomb networks HC_n. Based on the degrees of the end vertices of each edge, the edge partition of HC_n is shown in Table 2. Note that $|V(HC_N)| = 6n^2$ and $|E(HC_n)| = 9n^2 - 3n$.

Theorem 1 : *The general Zagreb index of the honeycomb network HC_n is given by*

$$Z_{a,b}(HC_n) = 3 \cdot 2^{a+b+2} + 12(n-1)(2^a 3^b + 2^b 3^a) + 2(3n^2 - 5n + 2) 3^{a+b+1}. \quad (1)$$

Proof : From the definition of general Zagreb index, we get

$$\begin{aligned} Z_{a,b}(HC_n) &= \sum_{hk \in E(HC_n)} [d_{HC_n}(h)^a d_{HC_n}(k)^b + d_{HC_n}(h)^b d_{HC_n}(k)^a] \\ &\quad + \sum_{hk \in E_3(HC_n)} (3^a.3^b + 3^b.3^a) \\ &= |E_1(HC_n)|(2^a.2^b + 2^b.2^a) + |E_2(HC_n)|(2^a.3^b + 2^b.3^a) \\ &\quad + |E_3(HC_n)|(3^a.3^b + 3^b.3^a) \\ &= 3.2^{a+b+2} + (12n-12)(2^a.3^b + 2^b.3^a) + (9n^2 - 15n + 6)2.3^{a+b}. \end{aligned}$$

Hence, the result follows.

By Eqn. (1), we have

Corollary 1 : *Some generalized Zagreb indices of HC_n are as follows* :

$$
\begin{aligned}
(i)\quad & M_1(HC_n) &&= Z_{1,0}(HC_n) = 54n^2 - 30n, \\
(ii)\quad & M_2(HC_n) &&= \frac{1}{2} Z_{1,1}(HC_n) = 81n^2 - 63n + 6, \\
(iii)\quad & F(HC_n) &&= Z_{2,0}(HC_n) = 162n^2 - 84n, \\
(iv)\quad & \operatorname{Re} ZM(HC_n) &&= Z_{2,1}(HC_n) = 486n^2 - 450n + 60, \\
(v)\quad & M^a(HC_n) &&= Z_{a-1,0}(HC_n) = 3.2^{a+1} + (n-1)(2^{a+1} \cdot 3 + 4 \cdot 3^a) \\
& && \quad +(3n^2 - 5n + 2).2.3^a, \\
(vi)\quad & R_a(HC_n) &&= \frac{1}{2} Z_{a,a}(HC_n) = 3.2^{2a+1} + (n-1).2^{a+2}.3^{a+1} \\
& && \quad +(3n^2 - 5n + 2).3^{2a+1}, \\
(vii)\quad & SDD(HC_n) &&= Z_{1,-1}(HC_n) = 18n^2 - 4n - 2.
\end{aligned}
$$

Now, we consider the silicate networks SL_n of dimension n such that $|V(SL_n)| = 15n^2 + 3n$ and $|E(SL_n)| = 36n^2$. Based on degree of the end vertices of each edge, the edge partition of silicate networks SL_n is shown in Table 3 [26].

Table 3

Edge partition of silicate networks

$(d(h), d(k)) : hk \in E(SL_n)$	Total number of edges
(3,3)	$6n$
(3,6)	$18n^2 + 6n$
(6,6)	$18n^2 - 12n$

Theorem 2 : *The general Zagreb index of silicate network SL_n is as follows* :

$$Z_{a,b}(SL_n) = 12n \cdot 3^{a+b} + 6n(3n+1)(3^a \cdot 6^b + 3^b \cdot 6^a) + 12(3n^2 - 2n) \cdot 6^{a+b} \qquad (2)$$

Proof : From the definition of general Zagreb index, we get

$$
\begin{aligned}
Z_{a,b}(SL_n) &= \sum_{hk \in E(SL_n)} (d_{SL_n}(h)^a d_{SL_n}(k)^b + d_{SL_n}(h)^b d_{SL_n}(k)^a) \\
&\quad + \sum_{hk \in E_3(SL_n)} 2 \cdot 6^{a+b}
\end{aligned}
$$

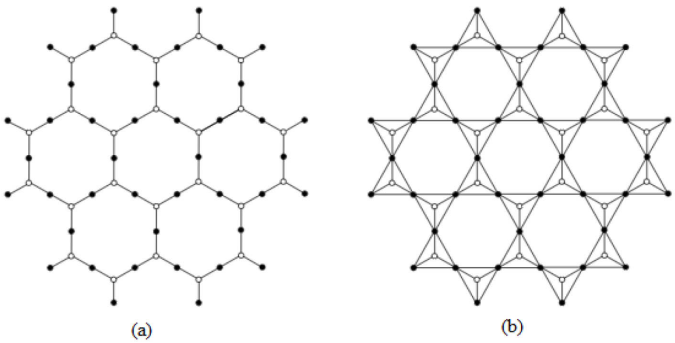

Figure 2

The silicate network of dimension two

$$\begin{aligned} &= |E_1(SL_n)|(3^a.3^b+3^b.3^a)+|E_2(SL_n)|(3^a.6^b+3^b.6^a) \\ &\quad +2|E_3(SL_n)|6^{a+b} \\ &= 6n(3^a\cdot 3^b+3^b\cdot 3^a)+6(3n^2+n)(3^a\cdot 6^b+3^b\cdot 6^a) \\ &\quad +12(3n^2-2n)6^{a+b}. \end{aligned}$$

Hence, the theorem.

By Eqn. (2), we have

Corollary 2 : *Some general Zagreb indices of SL_n are as follows* :

$$\begin{aligned} &(i) && M_1(SL_n) &&= Z_{1,0}(SL_n)=378n^2+234n, \\ &(ii) && M_2(SL_n) &&= \frac{1}{2}Z_{1,1}(SL_n)=18(54n^2-15n), \\ &(iii) && F(SL_n) &&= Z_{2,0}(SL_n)=9(234n^2-54n), \\ &(iv) && \operatorname{Re}ZM(SL_n) &&= Z_{2,1}(SL_n)=10692n^2-3888n, \\ &(v) && M^a(SL_n) &&= Z_{a-1,0}(SL_n)=12n\cdot 3^{a-1}+6n(3n+1)(3^{a-1}+6^{a-1}) \\ &&&&& \quad +12(3n^2-2n)6^{a-1}, \\ &(vi) && R_a(SL_n) &&= \frac{1}{2}Z_{a,a}(SL_n)=6n\cdot 3^{2a}+6n(3n+1)\cdot 3^a\cdot 6^a \\ &&&&& \quad +6n(3n-2)6^{2a}, \\ &(vii) && SDD(SL_n) &&= Z_{1,-1}(SL_n)=81n^2. \end{aligned}$$

Here, we consider chain silicate networks and compute general Zagreb index of them. A chain silicate network consists of a chain of n complete graphs K_4 and is denoted by CS_n, $n \geq 2$. Here $|V(CS_n)| = 3n+1$

and $|E(CS_n)| = n.$ Based on degrees of the end vertices of each edge, the edge partition of a chain silicate network CS_n is shown in Table 4 [26].

Theorem 3 : *The general Zagreb index of chain silicate network* (CS_n) $n \geq 2$ *is given by*

$$Z_{a,b}(CS_n) = 2(n+4)3^{a+b} + 2(2n-1)(3^a \cdot 6^b + 3^b \cdot 6^a) + 2(n-2) \cdot 6^{a+b} \quad (3)$$

Table 4

Edge partition of chain silicate network

$(d(h), d(k)) : hk \in E(CS_n)$	Total number of edges
(3, 3)	$n + 4$
(3, 6)	$4n$ - 2
(6, 6)	n - 2

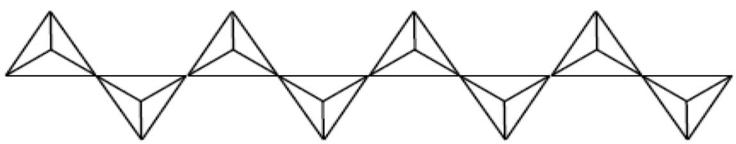

Figure 3

An example of chain silicate network of dimension n

Proof **:** From the definition of general Zagreb index, we get

$$\begin{aligned} Z_{a,b}(CS_n) &= \sum_{hk \in E(CS_n)} (d_{CS_n}(h)^a d_{CS_n}(k)^b + d_{CS_n}(h)^b d_{CS_n}(k)^a) \\ &= 2 \sum_{hk \in E_1(CS_n)} 3^{a+b} + \sum_{hk \in E_2(CS_n)} (3^a \cdot 6^b + 3^b \cdot 6^a) \\ &\quad +2 \sum_{hk \in E_3(CS_n)} 6^{a+b} \\ &= 2|E_1(CS_n)|3^{a+b} + |E_2(CS_n)|(3^a \cdot 6^b + 3^b \cdot 6^a) \\ &\quad +2|E_3(CS_n)|6^{a+b} \\ &= 2(n+4)3^{a+b} + (4n-2)(3^a \cdot 6^b + 3^b \cdot 6^a) \\ &\quad +2(n-2)6^{a+b}. \end{aligned}$$

Hence, the result follows.

Corollary 3 : *We compute the following topological indices by using Eqn.* (3)

$$
\begin{array}{lrcl}
(i) & M_1(CS_n) & = & Z_{1,0}(CS_n) = 54n - 18, \\
(ii) & M_2(CS_n) & = & \frac{1}{2} Z_{1,1}(CS_n) = 117n - 72, \\
(iii) & F(CS_n) & = & Z_{2,0}(CS_n) = 270n - 162, \\
(iv) & \operatorname{Re} ZM(CS_n) & = & Z_{2,1}(CS_n) = 1134n - 972, \\
(v) & M^a(CS_n) & = & Z_{a-1,0}(CS_n) = 2(n+4).3^{a-1} + 2(2n-1)(3^{a-1} + 6^{a-1}) \\
 & & & +2(n-2).6^{a-1}, \\
(vi) & R_a(CS_n) & = & \frac{1}{2} Z_{a,a}(CS_n) = (n+4).3^{2a} + 2(2n-1).3^a.6^a + (n-2).6^{2a}, \\
(vii) & SDD(CS_n) & = & Z_{1,-1}(CS_n) = 14n - 1.
\end{array}
$$

Now, we compute general Zagreb index of hexagonal networks HX_n. For a hexagonal network HX_n, the edge set is divided into five based on the degrees of the end vertices of each edge and is shown in Table 5 [26]. Note that $|V(HX_n)| = 3n^2 - 3n + 1$ and $|E(HX_n)| = 9n^2 - 15n + 6$.

Table 5

Edge partition of hexagonal network HX_n

$(d(h), d(k)) : hk \in E(HX_n)$	Total number of edges
(3, 4)	12
(3, 6)	6
(4, 4)	6*n* - 18
(4, 6)	12*n* - 24
(6, 6)	$9n^2 - 33n + 30$

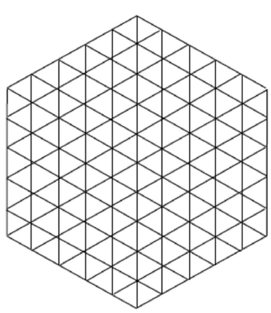

Figure 4

An example of a hexagonal network of dimension 6

Theorem 4 : *The general Zagreb index of chain silicate networks* HX_n *is given by*

$$\begin{aligned} Z_{a,b}(HX_n) &= 12(3^a \cdot 4^b + 3^b \cdot 4^a) + 6(3^a \cdot 6^b + 3^b \cdot 6^a) + 6(n-3)2^{2(a+b)+1} \\ &\quad +12(n-2)(4^a \cdot 6^b + 4^b \cdot 6^a) + 6(3n^2 - 11n + 10)6^{a+b}. \end{aligned} \tag{4}$$

Proof **:** From the definition of general Zagreb index, we get

$$\begin{aligned} Z_{a,b}(HX_n) &= \sum_{hk \in E(HX_n)} (d_{HX_n}(h)^a d_{HX_n}(k)^b + d_{HX_n}(h)^b d_{HX_n}(k)^a) \\ &= \sum_{hk \in E_1(HX_n)} (3^a \cdot 4^b + 3^b \cdot 4^a) + \sum_{hk \in E_2(HX_n)} (3^a 6^b + 3^b.6^a) \\ &\quad + 2 \sum_{hk \in E_3(HX_n)} 4^{a+b} + \sum_{hk \in E_4(HX_n)} (4^a.6^b + 4^b.6^a) \\ &\quad + 2 \sum_{hk \in E_5(HX_n)} 6^{a+b} \\ &= |E_1(HX_n)|(3^a.4^b + 3^b.4^a) + |E_2(HX_n)|(3^a.6^b + 3^b.6^a) \\ &\quad + 2|E_3(HX_n)|4^{a+b} + |E_4(HX_n)|(4^a.6^b + 4^b.6^a) \\ &\quad + 2|E_5(HX_n)|6^{a+b} \\ &= 12(3^a.4^b + 3^b.4^a) + 6(3^a.6^b + 3^b.6^a) + 6(n-3)2^{2(a+b)+1} \\ &\quad +12(n-2)(4^a.6^b + 4^b.6^a) + 6(3n^2 - 11n + 10)6^{a+b} \end{aligned}$$

which is the required result.

In Figures 5 and 6, respectively, graphical representations of several indices are compared for all silicate networks.

Corollary 4: *Using Eqn. (4), we obtain the following topological indices:*

$$\begin{aligned} &(i)\ M_1(HX_n) &&= Z_{1,0}(HX_n) = 108n^2 - 228n + 154, \\ &(ii)\ M_2(HX_n) &&= \tfrac{1}{2} Z_{1,1}(HX_n) = 324n^2 - 1000n + 252, \\ &(iii)\ F(HX_n) &&= Z_{2,0}(HX_n) = 648n^2 - 2460n + 906, \\ &(iv)\ ReZM(HX_n) &&= Z_{2,1}(HX_n) = 3888n^2 - 10608n + 6876, \\ &(v)\ M^a(HX_n) &&= Z_{a-1,0}(HX_n) = 12(3^{a-1} + 4^{a-1}) + 6(3^{a-1} + 6^{a-1}) \\ &&&\quad + 6(n-3).2^{2a-1} + 12(n-2)(4^{a-1} + 6^{a-1}) \\ &&&\quad +3(3n^2 - 11n + 10) \cdot 2 \cdot 6^{a-1}, \\ &(vi)\ R_a(HX_n) &&= \tfrac{1}{2} Z_{a,a}(HX_n) = 12 \cdot 3^a \cdot 4^a + 6 \cdot 3^a \cdot 6^a + 6(n-3) \cdot 2^{4a} \\ &&&\quad +12(n-2) \cdot 4^a \cdot 6^a + 3(3n^2 - 11n + 10) \cdot 6^{2a}, \\ &(vii)\ SDD(HX_n) &&= Z_{1,-1}(HX_n) = 18n^2 - 28n + 12. \end{aligned}$$

Finally, we compute the general Zagreb index of oxide network OX_n, such that $|V(OX_n)| = 9n^2 + 3n$ and $|E(OX_n)| = 18n^2$. The edge partition of an oxide network with respect to the degrees of the end vertices of each edge is shown in Table 6 [26], as follows:

The comparative illustrations of the four graph indices discussed above for all considered silicate networks are given in Figure 5.

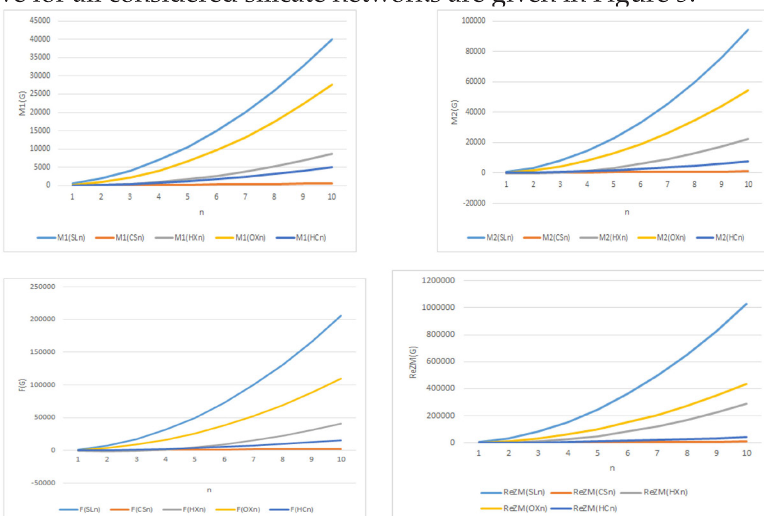

Figure 5

Comparative graphical representations of first Zagreb index, second Zagreb index, $F-$index and reformulated Zagreb index for all silicate networks

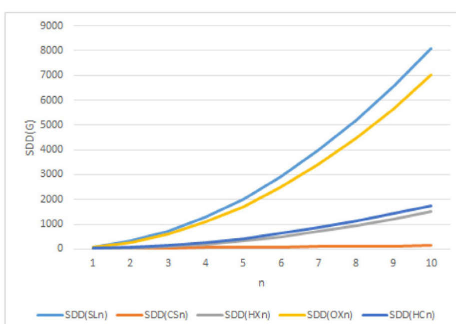

Figure 6

Comparative graphical representations of symmetric division deg index for all silicate networks

The comparative illustration of symmetric division deg index for all considered silicate networks is given in Fig. 6.

Corollary 4 : *Using Eqn.* (4), *we obtain the following topological indices*:

(*i*) $M_1(HX_n) = Z_{1,0}(HX_n) = 108n^2 - 228n + 154,$

(*ii*) $M_2(HX_n) = \frac{1}{2}Z_{1,1}(HX_n) = 324n^2 - 1000n + 252,$

(*iii*) $F(HX_n) = Z_{2,0}(HX_n) = 648n^2 - 2460n + 906,$

(*iv*) $\operatorname{Re} ZM(HX_n) = Z_{2,1}(HX_n) = 3888n^2 - 10608n + 6876,$

(*v*) $M^a(HX_n) = Z_{a-1,0}(HX_n) = 12(3^{a-1} + 4^{a-1}) + 6(3^{a-1} + 6^{a-1})$
$+6(n-3).2^{2a-1} + 12(n-2)(4^{a-1} + 6^{a-1})$
$+3(3n^2 - 11n + 10)\cdot 2\cdot 6^{a-1},$

(*vi*) $R_a(HX_n) = \frac{1}{2}Z_{a,a}(HX_n) = 12\cdot 3^a\cdot 4^a + 6\cdot 3^a\cdot 6^a + 6(n-3)\cdot 2^{4a}$
$+12(n-2)\cdot 4^a\cdot 6^a + 3(3n^2 - 11n + 10)\cdot 6^{2a},$

(*vii*) $SDD(HX_n) = Z_{1,-1}(HX_n) = 18n^2 - 28n + 12.$

Finally, we compute the general Zagreb index of oxide network OX_n, such that $|V(OX_n)| = 9n^2 + 3n$ and $|E(OX_n)| = 18n^2$. The edge partition of an oxide network with respect to the degrees of the end vertices of each edge is shown in Table 6 [26], as follows:

Table 6

Edge partition of oxide network

$(d(h), d(k)) : hk \in E(OX_n)$	Total number of edges
(2, 4)	$12n$
(4, 4)	$180^2 - 12n$

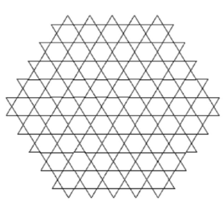

Figure 7

The example of an oxide network OX_n of dimension 5

Theorem 5 : *The general Zagreb index of oxide network* OX_n *is given by*

$$Z_{a,b}(OX_n) = 12n(2^a.4^b + 2^b.4^a) + 3(3n^2 - 2n)2^{2(a+b)+3}. \quad (5)$$

Proof : From the definition of (a, b)-Zagreb index, we get

$$\begin{aligned} Z_{a,b}(OX_n) &= \sum_{hk\in E(OX_n)} [d_{OX_n}(h)^a d_{OX_n}(k)^b + d_{OX_n}(h)^b d_{OX_n}(k)^a] \\ &= \sum_{hk\in E_1(OX_n)} (2^a \cdot 4^b + 2^b \cdot 4^a) + \sum_{hk\in E_2(OX_n)} (4^a \cdot 4^b + 4^b \cdot 4^a) \\ &= |E_1(OX_n)|(2^a \cdot 4^b + 2^b \cdot 4^a) + |E_2(OX_n)|(4^a \cdot 4^b + 4^b \cdot 4^a) \\ &= 12n(2^a \cdot 4^b + 2^b \cdot 4^a) + 3(3n^2 - 2n)2^{2(a+b)+3}. \end{aligned}$$

Hence, the result follows.

Corollary 5 : *From Eqn.* 5, *we compute the following topological indices as follows*:

(*i*) $M_1(OX_n) = Z_{1,0}(OX_n) = 288n^2 - 120n,$

(*ii*) $M_2(OX_n) = \frac{1}{2}Z_{1,1}(OX_n) = 576n^2 - 288n,$

(*iii*) $F(OX_n) = Z_{2,0}(OX_n) = 1152n^2 - 528n,$

(*iv*) $\operatorname{Re}ZM(OX_n) = Z_{2,1}(OX_n) = 4608n^2 - 2496n,$

(*v*) $M^a(OX_n) = Z_{a-1,0}(OX_n) = 12n(2^{a-1} + 4^{a-1}) + 3n(3n-2)2^{2a+1},$

(*vi*) $R_a(OX_n) = \frac{1}{2}Z_{a,a}(OX_n) = 12n \cdot 2^{3a} + 3n(3n-2)2^{4a+2},$

(*vii*) $SDD(OX_n) = Z_{1,-1}(OX_n) = 72n^2 - 18n.$

3. Conclusions

In this paper, we compute the general Zagreb index of four types of chemical networks such as chain silicate network, silicate network, oxide network and hexagonal network with their chemical significance and hence we obtain some other degree based topological indices such as Zagreb indices, general first Zagreb index, forgotten topological index, general Randić index, redefined Zagreb index, and symmetric division deg index for some particular values of *a* and *b*. For future study, some other chemical structures can be considered for studying this general Zagreb index.

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