GENERALIZATION OF NEW DEGREE BASED TOPOLOGICAL INDICES OF SILICATE NETWORK GRAPH

P. SELVARANI
Assistant Professor, PG & Research Department of Mathematics, Holy Cross College (Autonomous), Trichy – 02.

K. DHANALAKSHMI
Assistant Professor, PG & Research Department of Mathematics, Holy Cross College (Autonomous), Trichy – 02.

J. IRUDAYA MONICA CATHERINE
Assistant Professor, PG & Research Department of Mathematics, Holy Cross College (Autonomous), Trichy – 02.

Abstract. In the fields of chemical graph theory and mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph. Topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) and other properties of molecules are correlated with their chemical structure. In that Silicates are the most common minerals in the Earth’s crust and mantle, it has a wide variety of physical properties which paved way to find the topological indices. In this paper gives us the generalized new form of topological indices such as Arithmetic-Geometric Index (AG Index), SK Index, SK₁ Index and SK₂ Index of Silicate network graphs

1. INTRODUCTION
In chemical graph theory, topological indices play a vital role. The theory consists of two main components such as mathematical chemistry and molecular topology. Topological indices are used to formulate numerical parameters of graphs which give a Quantitative Structure Activity Relationships(QSARs) and molecular properties of certain chemical structures.

The topological indices usually include all the molecular simple graphs. Let $G = (V, E)$ be the set of vertices $V$ and edges $E$ and $d(u)$ be the number of edges which is attached with vertex $u$. The structure of molecular graphs gives the carbon skeleton of the compounds.

In this paper we consider on such chemical compound named as silicate. They are the combination of two minerals silicon and oxygen, it is one of the major components of the earth’s crust. The molecular formula of the silicate in general is $(SiO_4)^{4-}$ tetrahedron. They are held together by 50 percent ionic and 50 percent covalent (i.e.) they are strong silicon-oxygen bonds.

The structure of the silicates is like triangular pyramid shape with four oxygen atoms at the corners and one silicon atom at the center. Thus the aim of this paper is to find generalized form of new degree based topological indices of the silicate network. The nature of this study is to bring out the indices of the chemical compounds without using any software applications.
2. **Definition and Results.**

**Definition 1** *(Arithmetic-Geometric Index (AG(G))):* Let $G = (V, E)$ be a molecular graph and $d(u)$ be the degree of the vertex $u$, then AG index of $G$ is defined as

$$ AG(G) = \sum_{u, v \in E(G)} \frac{d_G(u) + d_G(v)}{2 \sqrt{d_G(u) d_G(v)}} $$

Where AG index is considered for distinct vertices.

The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of $u$ and $v$, where $d_G(u)$ and $d_G(v)$ denote the degree of the vertex $u$ and $v$.

**Definition 2** *(SK index):* The SK index of a graph $G = (V, E)$ is defined as

$$ SK(G) = \sum_{u, v \in E(G)} \frac{d_G(u) + d_G(v)}{2} $$

where $d_G(u)$ and $d_G(v)$ denote the degree of the vertex $u$ and $v$ respectively.

**Definition 3** *(SK$_1$ index):* The SK$_1$ index of a graph $G = (V, E)$ is defined as

$$ SK_1(G) = \sum_{u, v \in E(G)} \left( \frac{d_G(u) d_G(v)}{2} \right) $$

where $d_G(u)$ and $d_G(v)$ are the product of the degree of the vertex $u$ and $v$ respectively.

**Definition 4** *(SK$_2$ index):* The SK$_2$ index of a graph $G = (V, E)$ is defined as

$$ SK_2(G) = \sum_{u, v \in E(G)} \left( \frac{d_G(u) d_G(v)}{2} \right)^2 $$

where $d_G(u)$ and $d_G(v)$ are the degree of the vertex $u$ and $v$ respectively.

**RESULTS:**

- The AG Index for a Path graph ($P_n, n \geq 2$) is given by
  
  $$(r - 1) + \frac{3}{\sqrt{2}} \text{ for } r = 1, 2, 3, ...$$

- The SK Index for Path graph is given by $(2r - 1)$ for $r = 1, 2, ...$
- The $SK_1$ Index of path graph ($P_n, n \geq 2$) is $2r$ for $r = 1, 2, 3, ...$
- The $SK_2$ Index for path graph of ‘k’ vertices be
  
  $$(2r - 1)f or r = 1, 2, 3, ...$$

- The AG Index of a cycle graph is given by
  
  $$(r + 2) f or r = 1, 2, ...$$

- The $SK$ and $SK$ Index for a cycle graph $C_n, n \geq 3$ is found to be
  
  $$(2r + 4) f or all r = 1, 2, ...$$

- The $SK_2$ Index for a cycle graph ($C_n, n \geq 3$) is given by
  
  $$(4r + 8) \forall r = 1, 2, ...$$

**3. Main Result**

**Theorem: 1**

The AG Index for Silicate network graph is given by

$$ \frac{1}{\sqrt{2}} [2n(\sqrt{2} + 3) + 2\sqrt{2} - 3] \text{ for } n \geq 2. $$

**Proof:**
Let $G=S_n$ be a silicate network graph of ‘n’ vertices. Now to find the AG index of silicate network graph.
We consider $n = 1$, \therefore $G = S_1$, the numbers of vertices are $V(G) = \{v_1, v_2, v_3, v_4\}$ and the numbers of edges are $E(G) = \{e_1, e_2, e_3, e_4, e_5, e_6\}$.

Based on the degree of each vertex, we calculate the index of silicate.
$d(v_1) = d(v_2) = d(v_3) = d(v_4) = 3$. We have all the six edges having the degree sequence as (3, 3). The AG Index is given by

$$AG(G) = 6 \left[ \frac{3+3}{2\sqrt{3 \times 3}} \right] = 6(1) = 6$$

Now let us consider for $n = 2$, i.e. $G = S_2$, the numbers of vertices are $V(G) = \{v_1, v_2, v_3, v_4, \ldots, v_7\}$ and the numbers of edges are $E(G) = \{e_1, e_2, e_3, \ldots, e_{12}\}$.

We observe that there are six pairs of vertices having the degree sequence (3,3) and six pairs of vertices having the degree sequence (3,6).

$$AG(G) = 6 \left( \frac{3 + 3}{2\sqrt{3 \times 3}} \right) + 6 \left( \frac{3 + 6}{2\sqrt{3 \times 6}} \right)$$

$$= 6 + 6 \left( \frac{3}{2\sqrt{2}} \right)$$

Similarly we consider for $n = 3$, i.e. $G = S_3$
The numbers of vertices $V(G) = \{v_1, v_2, v_3, \ldots, v_9\}$ and
The numbers of edges $E(G) = \{e_1, e_2, e_3, \ldots \ldots e_{18}\}$

We observe that there are seven pairs of vertices having the degree sequence (3,3), ten pairs of vertices having the degree sequence (3,6) and one pair of vertices having the degree sequence (6,6).

$$\text{AG}(G) = 7\left(\frac{3 + 3}{2\sqrt{3} \times 3}\right) + 10\left(\frac{3 + 6}{2\sqrt{3} \times 6}\right) + 1\left(\frac{6 + 6}{2\sqrt{6} \times 6}\right)$$

Proceeding in this way for $n$ numbers, we get finite chain silicate network $\therefore G = S_n$

Let $V(G) = \{v_1, v_2, v_3, \ldots \ldots v_{3n+1}\}$ and $E(G) = \{v_i v_{i+1}; 1 \leq i \leq 3n\} \cup \{v_1 v_5, v_5 v_7, v_7 v_9, \ldots \ldots v_{3n-1} v_{3n+1}\}$

be the set of vertices and edges of $G$ respectively.

In general for $n \geq 2$

$$\text{AG}(G) = \frac{1}{2\sqrt{2}} \left[2n(\sqrt{2} + 3) + 2\sqrt{2} - 3\right] \text{ for } n \geq 2.$$  

**Theorem: 2**

The SK Index for Silicate network graph is given by $\frac{1}{2} [54n - 18]$ for $n \geq 2$.

**Proof:**

Let $G = S_n$ be a silicate network graph of ‘n’ vertices.

We are going to find the Sk Index of silicate network graph.

Now let us consider $n = 1$, i.e. $G = S_1$

The numbers of vertices are $V(G) = \{v_1, v_2, v_3, v_4\}$ and the numbers of edges are $E(G) = \{e_1, e_2, e_3, e_4, e_5, e_6\}$.

Based on the degree of each vertex, we calculate the index of the silicate $d(v_1) = d(v_2) = d(v_3) = (v_4) = 3$.

We have all the six edges having the degree sequence as (3, 3).
The $SK$ Index of the silicate graph

$$SK(G) = 6 \left( \frac{3+3}{2} \right) = 18.$$ 

Now let us consider for $n = 2$, i.e. $G = S_2$

The numbers of vertices are $V(G) = \{v_1, v_2, v_3, \ldots v_7\}$ and the numbers of edges are $E(G) = \{e_1, e_2, e_3, \ldots, e_{12}\}$.

We observe that there are six pairs of vertices having the degree sequence (3,3) and six pairs of vertices having the degree sequence (3,6).

$$SK(G) = 6 \left( \frac{3+3}{2} \right) + 6 \left( \frac{3+6}{2} \right)$$

$$= 18 + 6 \left( \frac{9}{2} \right)$$

Similarly we consider for $n = 3$, i.e. $G = S_3$

The number of vertices $V(G) = \{v_1, v_2, v_3, \ldots v_9\}$ and the numbers of edges $E(G) = \{e_1, e_2, e_3, \ldots e_{18}\}$

We observe that there are seven pairs of vertices having the degree sequence (3,3), ten pairs of vertices having the degree sequence (3,6) and one pair of vertices having the degree sequence (6,6).

$$SK(G) = 7 \left( \frac{3+3}{2} \right) + 10 \left( \frac{3+6}{2} \right) + 1 \left( \frac{6+6}{2} \right)$$

$$= 27 + 10 \left( \frac{9}{2} \right)$$

Proceeding in this way for $n$ numbers, we get finite chain silicate network i.e $G = S_n$

Let $V(G) = \{v_1, v_2, v_3, \ldots, v_{3n+1}\}$ and $E(G) = \{v_i v_{i+1} : 1 \leq i \leq 3n\} \cup \{v_1 v_3, v_5 v_7, v_9 v_{10}, \ldots, v_{3n-1} v_{3n+1}\}$

$\cup \{v_2 v_4, v_4 v_6, v_6 v_{10}, \ldots, v_{3n-2} v_{3n}\}$

$\cup \{v_1 v_4, v_4 v_7, v_7 v_{10}, \ldots, v_{3n-2} v_{3n+1}\}$

is the set of vertices and edges respectively of $G$.

Hence in general, if $n \geq 2$

$$SK(G) = \frac{1}{2} (54n - 18)$$

**Theorem: 3**

The $SK_1$ Index for silicate network graph is given by

$$\frac{(n+4)^9}{2} + \frac{(n-2)^6}{2} + 9(4n - 2) \text{ for } n \geq 2.$$ 

**Proof:**

Let silicate network graph of $n$ vertices be $G = S_n$

Now to find the $SK_1$ index of silicate network graph we consider $n = 1$ i.e. $G = S_1$.

The vertex set $V(G) = \{v_1, v_2, v_3, v_4\}$ and the edge set $E(G) = \{e_1, e_2, e_3, e_4, e_5, e_6\}$.

We calculate the index of the silicate using the degree of each vertex.

i.e. $d(v_1) = d(v_2) = d(v_3) = d(v_4) = 3$. From this we get that there are six edges having the degree sequence as $(3, 3)$.

The $SK_1$ Index is given as

$$SK_1(G) = 6 \left( \frac{3 \times 3}{2} \right)$$

$$= 27$$

Let us consider for $n = 2$, i.e. $G = S_2$

The vertex set is $\{v_1, v_2, v_3, \ldots, v_7\}$ and the edge set be $\{e_1, e_2, e_3, \ldots, e_{12}\}$. We observe that there are six pairs of vertices and another six pairs of vertices having the degree sequence as $(3, 3)$ and $(3, 6)$ respectively.

Thus the $SK_1$ Index is given by

$$SK_1(G) = 6 \left( \frac{3 \times 3}{2} \right) + 6 \left( \frac{3 \times 6}{2} \right)$$
\[ \text{SK}_1(G) = 7 \left( \frac{3 \times 3}{2} \right) + 10 \left( \frac{3 \times 6}{2} \right) + 1 \left( \frac{6 \times 6}{2} \right) \]

Consequently we consider for \( n = 3 \), i.e. \( G = S_3 \).

We observe that there three pairs of degree sequence (3,3), (3,6) and (6,6). Therefore the index is found to be

\[ \text{SK}_1(G) = 6 \left( \frac{3+3}{2} \right)^2 + 6(9) \]

Proceeding in this way we obtain a chain silicate network for \( n \) vertices.

Let the vertex set and edge set be \( V(G) = \{ v_1, v_2, \ldots, v_{3n+1} \} \) and \( E(G) = \{ v_i v_{i+1} ; 1 \leq i \leq 3n \} \cup \{ v_1 v_3, v_5 v_7, \ldots, v_{3n-1} v_{3n+1} \} \cup \{ v_2 v_4, v_6 v_8, \ldots, v_{3n-2} v_{3n} \} \cup \{ v_1 v_4, v_4 v_7, \ldots, v_{3n-2} v_{3n+1} \} \)

In general if \( n \geq 2 \) we get,

\[ \text{SK}_1(G) = (n + 4) \left( \frac{9}{2} \right) + (n - 2) \left( \frac{6^2}{2} \right) + 9(4n - 2) \text{ for } n \geq 2.\]

Hence the \( \text{SK}_1 \) Index is found.

**Theorem:**

The \( \text{SK}_2 \) Index for silicate network graph is given by

\[ (9n + 36) + 6^2(n - 2) + \left( \frac{9}{2} \right)^2 (4n - 2) \text{ for } n \geq 2 \]

**Proof:**

Let the silicate network graph of \( n \) vertices be \( G = S_n \)

Now let us consider \( n = 1 \), i.e. \( G = S_1 \)

The number of vertices is \( V(G) = \{ v_1, v_2, v_3, v_4 \} \) and the number of edges is \( E(G) = \{ e_1, e_2, e_3, \ldots, e_6 \} \).

The corresponding silicate structure is shown in the figure 3.1, we calculate the index of the silicate

\( d(v_1) = d(v_2) = d(v_3) = d(v_4) = 3 \).

We have all the six edges having the degree sequence as (3, 3).

The \( \text{SK}_2 \) Index given as

\[ \text{SK}_2(G) = 6 \left( \frac{3+3}{2} \right)^2 = 54. \]

Now let us consider for \( n = 2 \). (i.e.) \( G = S_2 \)

The number of vertices \( V(G) = \{ v_1, v_2, v_3, \ldots, v_7 \} \) and the number of edges \( E(G) = \{ e_1, e_2, e_3, \ldots, e_{12} \} \).

We observe that there are six pairs of vertices having the degree sequence (3, 3) and six pairs of vertices having the degree sequence (3, 6).

\[ \text{SK}_2(G) = 6 \left( \frac{3+3}{2} \right)^2 + 6 \left( \frac{3+6}{2} \right)^2 \]

\[ = 54 + 6 \left( \frac{9}{2} \right)^2 \]

Similarly we consider for \( n = 3 \). (i.e) \( G = S_3 \)

The number of vertices \( V(G) = \{ v_1, v_2, \ldots, v_9 \} \) and the number of edges \( E(G) = \{ e_1, e_2, \ldots, e_{18} \} \).

We observe that there are seven pairs of vertices having the degree sequence (3, 3), ten pairs of vertices having the degree sequence (3, 6) and one pair of vertices having the degree sequence (6, 6).

\[ \text{SK}_2(G) = 7 \left( \frac{3+3}{2} \right)^2 + 10 \left( \frac{3+6}{2} \right)^2 + 1 \left( \frac{6+6}{2} \right)^2 \]

\[ = 63 + 10 \left( \frac{9}{2} \right)^2 + 1(6)^2 \]

Continuing in this way for \( n \) numbers, we get a chain silicate network

i.e. \( G = S_n \) Let \( V(G) = \{ v_1, v_2, v_3, \ldots, v_{3n+1} \} \) and

\( E(G) = \{ v_i v_{i+1} ; 1 \leq i \leq 3n \} \cup \{ v_1 v_3, v_5 v_7, v_7 v_9, \ldots, v_{3n-1} v_{3n+1} \} \)
be the set of all vertices and edges respectively of G.

The general index of the silicates,

\[ SK_2(G) = (9n + 36) + \binom{n}{2}(4n - 2) + 6^2(n - 2) \text{ for } n \geq 2. \]

3. CONCLUSION:

This paper examines the idea based on topological indices of some simple graphs. Further this can also be used for other forms of molecular graphs. Thus a new generalized form of topological indices using the AG index, SK index, SK\(_1\) index and SK\(_2\) index for chain silicate network and some simple graphs has been found explicit of any software applications.

REFERENCES:

[1] Stephen S, Rajan B, William A and Grigorious C 2012 On Certain topological indices of silicate, honeycomb and hexagonal networks. J. Comput. Mathematical. Sciences.

[2] Gutman I 2013 Degree-Based topological indicesCroatica Chemica Acta, 86.

[3] Shigehalli V S and Kanabur R 2015 Arithmetic-Geometric indices of Path Graph, Journal of Computer and Mathematical sciences.

[4] Shigehalli V S and Kanabur R 2016 Computation of New Degree-Based Topological Indices of Graphene, Journal of Mathematics, Hindawi Publications.

[5] Shigehalli V S and Kanabur R 2016 Computing Degree-Based Topological Indices of Polyhex Nanotubes, Journal of Mathematical Nanoscience.

[6] Snehal Thabaj and Mallikarjun Hottinnavar 2017 New Version of Degree-Based Topological Indices of Some Class of Graph, RA Journal of Applied Research, 3 (7).