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On SiO4 Molecular Topological Characterization of Chemical Structures

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Abstract

In this paper, our aim is to study valency-based molecular invariants for SiO_4 in a chain network. We compute the harmonic polynomial, atom bond connectivity polynomial, forgotten polynomial, geometric arithmetic polynomial, Randic polynomial, reciprocal Randic polynomial, symmetric division polynomial, inverse symmetric division polynomial, sigma polynomial, Sombor polynomial, and their degree-base topological indices for SiO_4 embedded in a silicate chain network for various conditions. Physio-chemical properties of chemical compounds, such as formation enthalpies, boiling points, chromatographic retention times, vapour pressure, and surface areas, can be determined using our investigated results, such as the H-index, ABC-index, F-index, GA-index, R-index, RR-index, SDD-index, $ISDD$index, S-index, and SO-index. We also create graphical representations of the results that describe the dependence of topological indices on polynomial structure parameters.

Keywords: SiO_4 in a chain, ABC polynomial and ABC index, geometric arithmetic polynomial, Randic index and reciprocal randic polynomial, sigma and Sombor index

2020 Mathematics Subject Classification: 05C07, 05C09, 05C31, 05C76, 05 C 99

Introduction

One of the standard procedures used in the study of structure-property relations is the use of structure descriptors. The ability to correlate and predict physical, chemical, and biological activity (property) from a molecular structure is a challenging problem in theoretical and computational chemistry [1, 2]. A topological index is a number that describes the graph's topology. It is one of the best quantification methods because it can be computed quickly for a large number of molecules and can be obtained directly from molecular structures. Wiener, a chemist, used a topological index for the first time in 1947 while studying the relationship between molecular structure and the physical and chemical properties of certain hydrocarbon compounds [3, 17]. Liu et al. discussed several aspects of graph theory in

[5]-[12].

Mathematical chemistry describes how to use polynomials and functions to offer instructions concealed in the symmetry of molecular graphs, and graph theory has many applications in modern chemistry, particularly organic chemistry. The atoms and bonds of a molecular structure are represented by vertices and edges, respectively, in chemical graph theory. Many applications of topological indices are employed in theoretical chemistry, [13, 14], particularly QSPR/QSAR research. Many famous researchers have studied topological indices to get information about different families of graphs [4, 15]. In qualitative structure-property relationships (QSPR) and qualitative structure-activity relationships (QSAR), topological indices are used directly as simple numerical descriptors in comparison with physical, biological, or chemical characteristics of molecules, which is a benefit. Many researchers have worked on various chemical compounds and computed topological descriptors of various molecular graphs during the last few decades [18].

In chemical graph theory, a molecular graph is a simple connected graph that contains chemical atoms and bonds, which are often referred to as vertices and edges, respectively, and there must be a linkage between the vertices set V_G and edges set E_G.If two atoms have an atom-bond, then it is denoted by $e \sim f$, the valency of every atom of G is actually the total number of atoms connected to f of G and it is denoted by d_f, [16, 19].

Several polynomials closely related to degree-based indices are also introduced.

In 2012, Zhang introduced harmonic index [31]. The harmonic polynomial corresponding to harmonic index is defined as

$$H(G,x) = \sum_{ef\in E(G)} x^{\frac{2}{de+df}} \;\&\; H(G) = \sum_{ef\in E(G)} \frac{2}{d_{e+d_f}} \qquad (1)$$

In 1998, Estrada et.al introduced atom bond connectivity index [21]. The ABC polynomial corresponding to the ABC indices is expressed as

$$ABC(G,x) = \sum_{ef\in E(G)} x^{\sqrt{\frac{d_{e+d_f}-2}{d_{e+d_f}}}} \;\&\; ABC(G) = \sum_{ef\in E(G)} \sqrt{\frac{d_{e+d_f}-2}{d_{e+d_f}}} \qquad (2)$$

In 2015, Formula and Gutmann introduced Forgotten Topological index or F-index [22]. The forgotten polynomial and index are defined as

$$F(G,x) = \sum_{ef\in E(G)} x^{[\,(d_e)^2+[(d_f)^2]} \;\&\; F(G) = \sum_{ef\in E(G)} [\,(d_e)^2 + [(d_f)^2] \qquad (3)$$

The first GA-index was proposed by Vukicevic [23]. The geometric arithmetic polynomial and index are defined as

$$GA(G,x) = \sum_{ef\in E(G)} x^{\frac{2\sqrt{d_{e+d_f}}}{d_{e+d_f}}} \;\&\; GA(G) = \sum_{ef\in E(G)} \frac{2\sqrt{d_{e+d_f}}}{d_{e+d_f}} \qquad (4)$$

The Randic polynomial and index, [24] are defined as

$$R(G,x) = \sum_{ef\in E(G)} x^{\frac{1}{\sqrt{d_{e+d_f}}}} \;\&\; R(G) = \sum_{ef\in E(G)} \frac{1}{\sqrt{d_{e+d_f}}} \qquad (5)$$

The reciprocal Randic polynomial and index [25] are defined as

$$RR(G,x) = \sum_{ef\in E(G)} x^{\sqrt{d_e\ d_f}} \;\&\; RR(G) = \sum_{ef\in E(G)} \sqrt{d_e\ d_f} \qquad (6)$$

The symmetric division degree polynomial and index [26] are defined as

$$SDD(G,x) = \sum_{ef\in E(G)} x^{\frac{[\,(d_e)^2+[(d_f)^2]}{(d_e)(d_f)}} \;\&\; SDD(G) = \sum_{ef\in E(G)} \frac{[\,(d_e)^2 + [(d_f)^2]}{(d_e)(d_f)} \qquad (7)$$

The inverse symmetric Division Degree polynomial and index [27] are defined as

$$ISDD(G,x) = \sum_{ef \in E(G)} x^{\frac{(d_e)(d_f)}{[(d_e)^2+[(d_f)^2]}} \& \quad ISDD(G) = \sum_{ef \in E(G)} \frac{(d_e)(d_f)}{[(d_e)^2+[(d_f)^2]} \quad (8)$$

Sigma polynomial and index [28] are defined as

$$S(G,x) = \sum_{ef \in E(G)} x^{(d_e - d_f)^2} \& \quad S(G) = \sum_{ef \in E(G)} (d_e - d_f)^2 \quad (9)$$

The concept of Sombor index was recently introduced by Gutman [29]. The Sombor polynomial and index are defined as

$$S(G,x) = \sum_{ef \in E(G)} x^{\sqrt{[(d_e)^2+[(d_f)^2]}} \& \quad SO(G) = \sum_{ef \in E(G)} \sqrt{[(d_e)^2+[(d_f)^2]} \quad (10)$$

In this study, the atom-bond partition set of $SiO4$ in a chain network, which is partitioned according to the valencies of their S_i and O_2 atoms, is used to generate the ten polynomials mentioned above and their corresponding indices.

1 Chain of SiO_4

A SiO_4 tetrahedron, the fundamental building block of silicates, is created by fusing metal oxides or mixing metal carbonates with sand. The SiO_4 tetrahedron is present in almost all silicates. As shown in Figure 1, a tetrahedron SiO_4 is a pyramid with a triangular base (a single tetrahedron SiO_4), and the silicon atom Si is bonded with evenly spaced oxygen atoms. The resulting SiO_4, a silicate tetrahedron that connects with other SiO_4 horizontally, forms a single chain. Similar to this, when two SiO4 molecules join corner to corner, each one shares its O_2 atoms with the other, as shown in Figure 1. These two molecules of SiO_4 can be joined with two other molecules once this sharing process is finished. We now have a silicate chain, SC_q^p, where p and q stand for the total number of SiO_4 atoms in one silicate chain and the number of silicate chains that were formed, respectively. The pq number of SiO_4 tetrahedrons used in the chain of SiO_4 SC_q^p is shown in Figure 1.

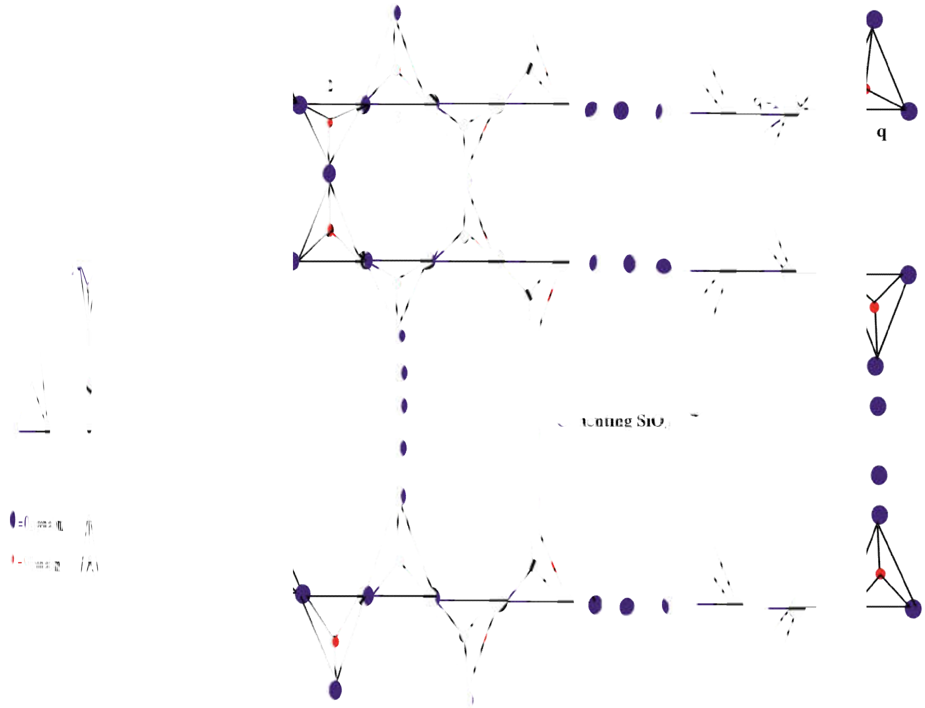

Figure 1: 1

1.1 Result and discussion

Here, we have observed that there are three types of atom bonds on the bases of the valency of each atom of SC_q^p in a chain of SiO_4 SC_q^p. As a result, there are two different types of atoms, v_i and v_j, with valencies of $\forall\ v_i, v_j \in \mathcal{SC}_q^p$ and $d_{v_i} = 3$ and $d_{v_j} = 6$, respectively. Three different types of atom-bonds $(3 \sim 3)$, $(3 \sim 6)$, and $(6 \sim 6)$ in SC_q^p are based on the valencies (3 and 6) of atoms. Table 1 provides the division of the set of atom bonds based on valency.

Table 1: Atom-bond partition of SC_q^p, for $p = q$

Type of atom-bond	$3 = d_e \sim d_f = 3$	$3 = d_e \sim d_f = 6$	$6 = d_e \sim d_f = 6$
Number of atom bonds	$3p + 2$	$3(pq + q) - 4$	$3(pq - 2q) + 2$

Theorem 2.1. *For $p > 1$ and $p = q$, the harmonic polynomial of* SC_q^p, is $(3P + 2)y^{\frac{1}{3}} + (3p^2 + 3p - 4)y^{\frac{2}{9}} + (3p^2 - 6p + 2)y^{\frac{1}{6}}$

Proof.

Using Table"1" enter the following formula harmonic polynomial (1), we get

$$H(\mathrm{SC}_p^p, y) = \sum_{3=d_e\sim d_f=3} y^{\frac{2}{3+6}} + \sum_{3=d_e\sim d_f=6} y^{\frac{2}{3+6}} + \sum_{3=d_e\sim d_f=6} y^{\frac{2}{6+6}}$$

This gives

$$H(\mathrm{SC}_p^p, y) = (3p+2)y^{\frac{1}{3}} + (3p^2+3p-4)y^{\frac{2}{9}} + (3p^2-6p+2)y^{\frac{1}{6}}$$

□

By taking the first derivative of the polynomial in Theorem 2.1 at $y = 1$, we get the harmonic index of Silicate Network SC_p^pas follows:

Corollary 2.2. *For p >1 and p = q, the harmonic index of* SC_p^p *is* $\frac{21p^2+12p+2}{18}$

Theorem 2.3. *For p >1 and p = q, the ABS polynomial of* SC_p^p is $(3p+2)y^{\frac{4}{9}} + 3p^2 + 3p - 4)y^{\frac{7}{18}} + (3p^2-6p+2)y^{\frac{5}{18}}$

Proof. Using Table"1" enter the following formula *ABC* polynomial (2), we get

$$ABC(\mathrm{SC}_p^p, y) = \sum_{3=d_e\sim d_f=3} y^{\sqrt{\frac{3+3-2}{(3)(3)}}} + \sum_{3=d_e\sim d_f=6} y^{\sqrt{\frac{3+6-2}{(3)(6)}}} + \sum_{3=d_e\sim d_f=6} y^{\sqrt{\frac{6+6-2}{(6)(6)}}}$$

This gives

$$ABC(\mathrm{SC}_p^p, y) = (3p+2)y^{\frac{4}{9}} + (3p^2+3p-4)y^{\frac{7}{18}} + (3p^2-6p+2)y^{\frac{5}{18}}$$

□

By taking the first derivative of the polynomial in Theorem 2.3 at $y = 1$, we get the *ABC* index of chain SiO_4 (SC_p^p) of as follows:

Corollary 2.4. *For p >1 and p = q, the ABC index of* $\frac{36p^2+15p-2}{18}$

Theorem 2.5. *For p >1 and p = q, the forgotten topological polynomial of* SC_p^p *is* $(3p + 2)$ $y18$+ $(3p^2 + 3p - 4)$ $y45$+ $(3p^2 - 6p + 2)$ y^{72}.

Proof. Using Table"1" enter the following formula forgotten topological polynomial (3), weget

$$F\left(SC_p^p, y\right) = \sum_{3=d_e\sim d_f=3} y^{[3^2+3^2]} + \sum_{3=d_e\sim d_f=6} y^{[3^2+6^2]} + \sum_{3=d_e\sim d_f=6} y^{[6^2+6^2]}$$

This gives

$$F\left(SC_p^p, y\right) = (3p+2)y^{18} + (3p^2+3p-4)y^{45} + (3p^2-6p+2)y^{72}$$

□

By taking the first derivative of the polynomial in Theorem 2.5 at $y = 1$, we get the forgotten index of chain of SiO_4 ($SC_p{}^p$) as follows:

Corollary 2.6. *For p >1 and p = q, the forgotten topological index of* SC_p^p *is* $351p^2 - 243p$.

Theorem 2.7. *For p >1 and p = q, the geometric arithmetic polynomial of* $SC_p^p(3p+2)y^{\frac{\sqrt{6}}{3}} + (3p^2+3p-4)y^{\frac{2}{3}} + (3p^2-6p+2)y^{\frac{1}{\sqrt{3}}}$

Proof. Using Table"1" enter the following formula geometric arithmetic polynomial (4), we get

$$GA\left(SC_p^p, y\right) = \sum_{3=d_e\sim d_f=3} y^{\frac{2\sqrt{3+3}}{3+3}} + \sum_{E_{3\sim 6}} y^{\frac{2\sqrt{3+6}}{3+6}} + \sum_{3=d_e\sim d_f=6} y^{\frac{2\sqrt{6+6}}{6+6}}$$

This gives

$$GA\left(SC_p^p, y\right) = (3P+2)y^{\frac{\sqrt{6}}{3}} + (3p^2+3p-4)y^{\frac{2}{3}} + (3p^2-6p+2)y^{\frac{1}{\sqrt{3}}}$$

□

By taking the first derivative of the polynomial in Theorem 2.7 at $y = 1$, we get the geometric arithmetic index of chain of SiO_4 (SC_p^p) as follows:

Corollary 2.8. *For p >1 and p = q, the geometric arithmetic index of*SC_p^p *is* $(3P+2)y^{\frac{\sqrt{6}}{3}} + (3p^2+3p-4)y^{\frac{2}{3}} + (3p^2-6p+2)y^{\frac{1}{\sqrt{3}}}$

Theorem 2.9. *For p >1 and p = q, the randic polynomial of* SC_p^p *is* $(3P+2)y^{\frac{1}{3}} + (3p^2+3p-4)y^{\frac{1}{3\sqrt{2}}} + (3p^2-6p+2)y^{\frac{1}{6}}$

Proof. Using Table"1" enter the following formula randic polynomial polynomial (5), we get

$$R(SC_p^p, y) = \sum_{3=d_e\sim d_f=3} y^{\frac{1}{\sqrt{(3)(3)}}} + \sum_{3=d_e\sim d_f=6} y^{\frac{1}{\sqrt{(3)(6)}}} + \sum_{3=d_e\sim d_f=6} y^{\frac{1}{\sqrt{(6)(6)}}}$$

This gives

$$R(SC_p^p, y) = (3P+2)y^{\frac{1}{3}} + (3p^2+3p-4)y^{\frac{1}{3\sqrt{2}}} + (3p^2-6p+2)y^{\frac{1}{6}}$$

□

By taking the first derivative of the polynomial in Theorem 2.9 at y = 1, we get the randic polynomial index of chain of SiO_4 (SC_p^p) as follows:

Corollary 2.10. *For p >1 and p = q, the randic polynomial index of*SC_p^p is $\frac{\sqrt{2}p^2+3p^2+3.\sqrt{2}p \quad +6-4.\sqrt{2}}{6}$

Theorem 2.11. *For p >1 and p = q, the reciprocal randic polynomial of*SC_p^p is$(3P+2)y^3+$
$(3p^2+3p-4)y^{3\sqrt{2}} + (3p^2-6p+2)y^{\sqrt{6}}$.

Proof. Using Table "1" enter the following formula reciprocal randic polynomial polynomial

(6), we get

$$RR(SC_p^p, y) = \sum_{3=d_e\sim d_f=3} y^{\sqrt{(3)(3)}} + \sum_{E_3\sim 6} y^{\sqrt{(3)(6)}} + \sum_{3=d_e\sim d_f=6} y^{\sqrt{(6)(6)}}$$

This gives

$$RR(SC_p^p, y) = (3P+2)y^3 + (3p^2+3p-4)y^{3\sqrt{2}} + (3p^2-6p+2)y^{\sqrt{6}}.$$

□

By taking the first derivative of the polynomial in Theorem 2.11 at y = 1, we get the reciprocal randic polynomial index of chain of SiO_4 (SC_p^p) as follows:

Corollary 2.12. *For p >1 and p = q, the reciprocal randic polynomial index of*$3(3P+2)+3\sqrt{2}(3p^2+3p-4)+\sqrt{6}(3p^2-6p+2)$.

Theorem 2.13. For p>1 and p=q. the symmetric degree polynomial of $SC_p^p$is$(3p^2-3p+4)y^2+(3p^2+3p-4)y^{\frac{15}{4}}$

Proof. Using Table enter the following formula symmetric division degree polynomial (7), we get

$$SDD(\mathrm{SC}_p^p, y) = \sum_{3=d_e \sim d_f=3} y^{\frac{[(3)^2+(3)^2]}{(3)(3)}} + \sum_{3=d_e \sim d_f=6} y^{\frac{[(3)^2+(6)^2]}{(3)(6)}} + \sum_{E_6 \sim 6} y^{\frac{[(6)^2+(6)^2]}{(6)(6)}}$$

This gives

$$SDD(\mathrm{SC}_p^p, y) = (3p+2)y^2 + (3p^2+3p-4)y^{\frac{15}{4}} + (3p^2-6p+2)y^2$$
$$= (3p^2-3p+4)y^2 + (3p^2+3p-4)y^{\frac{15}{4}}$$

□

By taking the first derivative of the polynomial in Theorem 2.19 at y = 1, we get the symmetric division degree index of chain of SiO_4 (SC_p^p as follows:

Corollary 2.14. *For p >1 and p = q, the symmetric division degree index of* SC_p^p *is* $2(3p^2 - 3p + 4) + \frac{15(3p^2-3p+4)}{4}$

Theorem 2.15. *For p >1 and p = q, the inverse symmetric division polynomial of* SC_p^p *is* $(3p^2-3p+4)y^{\frac{1}{2}} + (3p^2+3p-4)y^{\frac{4}{15}}$

Proof. Using Table "1" enter the following formula inverse symmetric division degree polynomial (8), we get

$$ISDD(\mathrm{SC}_p^p, y) = \sum_{3=d_e \sim d_f=3} y^{\frac{[(3) \quad +(3) \quad]}{(3)^2+(3)^2}} + \sum_{E_3 \sim 6} y^{\frac{[(3)^2+(6)^2]}{(3)(6)}} + \sum_{6=d_e \sim d_f=6} y^{\frac{[(6)^2+(6)^2]}{(6)(6)}}$$

This gives

$$SDD(\mathrm{SC}_p^p, y) = (3p+2)y^{\frac{1}{2}} + (3p^2+3p-4)y^{\frac{4}{15}} + (3p^2-6p+2)y^{\frac{1}{2}}$$
$$= (3p^2-3p+2)y^{\frac{1}{2}} + (3p^2+3p-4)y^{\frac{4}{15}}$$

□

By taking the first derivative of the polynomial in Theorem 2.15 at y = 1, we get the inverse symmetric division degree index of chain of SiO_4 SC_p^p as follows:

Corollary 2.16. *For p >1 and p = q, the inverse symmetric division degree index of* SC_p^p *is* $\frac{69p^2-21p+28}{30}$.

Theorem 2.17. *For p >1 and p = q, the sigma polynomial of* SC_p^p *is* $(3p^2+3p-4)y^9+3p^2-3p+4$.

Proof. Using Table "1" enter the following formula sigma polynomial (7), we get

$$S(\mathrm{G},x)(\mathrm{SC}_p^p,y)=\sum_{3=d_e\sim d_f=3}y^{(3-3)^2}+\sum_{3=d_e\sim d_f=6}y^{(3-6)^2}+\sum_{E_6\sim 6}y^{(6-6)^2}$$

This gives

$$SDD(\mathrm{SC}_p^p,y)=(3p+2)+(3p^2+3p-4)y^9+(3p^2-6p+2)$$
$$=(3p^2+3p-4)y^9+3p^2-3p+4$$

□

By taking the first derivative of the polynomial in Theorem 2.19 at *y* = 1, we get the sigma index of chain of$SiO_4(\mathcal{SC}_p^p)$ as follows:

Corollary 2.18. *For p >1 and p = q, the sigma index of* SC_p^p*p is* 9(3*p*² + 3*p* − 4).

Theorem2.19. *For p >1 and√ p = q, the somber polynomial of* SC_p^p*is* $(3p+2)y^{3\sqrt{2}}+(3p^2+3p-4)y^{3\sqrt{5}}+(3p^2-6p+2)y^{6\sqrt{2}}$

Proof. Using Table "1" enter the following formula somber polynomial (7), we get

$$SO(\mathrm{SC}_p^p,y)=\sum_{3=d_e\sim d_f=3}y^{\sqrt{(3)^2+(3)^2}}+\sum_{3=d_e\sim d_f=6}y^{\sqrt{(3)^2+(6)^2}}+\sum_{E_6\sim 6}y^{\sqrt{(6)^2+(6)^2}}$$

This gives

$$SO(\mathrm{SC}_p^p,y)=(3p+2)y^{3\sqrt{2}}+(3p^2+3p-4)y^{3\sqrt{5}}+(3p^2-6p+2)y^{6\sqrt{2}}$$

□

By taking the first derivative of the polynomial in Theorem 2.19 at *y* = 1, we get the somber index of chain of$SiO_4(\mathcal{SC}_p^p)$ as follows:

Corollary 2.20. *For p >1 and p = q, the somber index of*SC_p^p *is* $9(2p^2-3p+2)\sqrt{2}+3(3p^2+3p-4)\sqrt{5}$.

1.2 Results for $p<q$ and p is odd

Here, in chain of SiO_4 (SC_q^p), we observed for $p < q$ and p is odd, atom-bonds on the bases of valency of every atom of SC_q^pchanged. So, on the base of valency, Table 2 provides the partition of the set of atom-bonds.

Table 2: Atom-bond partition of SC_q^p, for p is odd and $p < q$

Type of atom-bond	$3 = d_e \sim d_f = 3$	$3 = d_e \sim d_f = 6$	$6 = d_e \sim d_f = 6$
Number of atom bonds	$3(p + 1)$	$3pq + p + 2q - 5$	$3pq - 2(2p + q - 1)$

Theorem 2.21. *Let p be odd and p < q. Then the harmonic polynomial of*SC_q^p *is* $3(p+1)y^{\frac{1}{3}} + (3pq + p + 2q - 5)y^{\frac{2}{9}} + (3pq - 2(2p + q - 1)y^{\frac{1}{6}}$

Proof. Using the atom-bond partition from Table 2, in the formula of harmonic polynomial (1), we get

$$H(SC_p^p, y) = \sum_{3=d_e\sim d_f=3} y^{\frac{2}{3+3}} + \sum_{E_3\sim 6} y^{\frac{2}{3+6}} + \sum_{6=d_e\sim d_f=6} y^{\frac{2}{6+6}}$$

This gives

$$H(SC_p^p, y) = 3(p+1)y^{\frac{1}{3}} + (3pq + p + 2q - 5)y^{\frac{2}{9}} + (3pq - 2(2p + q - 1)y^{\frac{1}{6}}$$

□

By taking the first derivative of the polynomial in Theorem 2.21 at $y = 1$, we get the harmonic index of Silicate Network SC_q^pas follows:

Corollary 2.22. *Let p be odd and p < q. Then the harmonic index of* SC_q^p *is* $a + \frac{21pq - 8p + 2q - 14}{18} + 1.$

Theorem 2.23. *Let p be odd and p < q. Then the ABC polynomial of*SC_q^p *is* $3(p+1)y^{\frac{4}{9}}(3pq + p + 2q - 5)y^{\frac{7}{18}} + (3pq - 2(2p + q - 1)y^{\frac{5}{18}}$

Proof. Using the atom-bond partition from Table 2, in the formula of *ABC* polynomial (2) , we get

$$ABC(SC_p^p, y) = \sum_{3=d_e\sim d_f=3} y^{\sqrt{\frac{3+3-2}{(3)(3)}}} + \sum_{3=d_e\sim d_f=6} y^{\sqrt{\frac{3+6-2}{(3)(6)}}} + \sum_{6=d_e\sim d_f=6} y^{\sqrt{\frac{6+6-2}{(6)(6)}}}$$

This gives

$$ABC\left(\mathrm{SC}_p^q, y\right) = 3(p+1)y^{\frac{4}{9}} + (3pq + p + 2q - 5)y^{\frac{7}{18}} + (3pq - 2(2p + q - 1)y^{\frac{5}{18}}$$

By taking the first derivative of the polynomial in Theorem 2.23 at y = 1, we get the ABC index of chain of SiO_4 (SC_p^q) as follows:

Corollary 2.24. *Let p be odd and p < q. Then the ABC index of*(SC_p^q) *is* $\frac{36pq+11p+4q-1}{18}$

Theorem 2.25. *Let p be odd and p < q. Then the forgotten topological polynomial of* $\mathrm{SC}_q{}^p$ *is* $3(p + 1)y^{18} + (3pq + p + 2q - 5)y^{45} + (3pq - 2(2p + q - 1))y^{72}$.

Proof. Using the atom-bond partition from Table 2, in the formula of forgotten topological polynomial (3), we get

$$F\left(\mathrm{SC}_p^p, y\right) = \sum_{3=d_e\sim d_f=3} y^{[3^2+3^2]} + \sum_{3=d_e\sim d_f=6} y^{[3^2+6^2]} + \sum_{6=d_e\sim d_f=6} y^{[6^2+6^2]}$$

This gives

$$F\left(\mathrm{SC}_p^p, y\right) = 3(p+1)y^{18} + (3pq + p + 2q - 5)y^{45} + 2\left(3pq - 2(2p + q - 1)\right)y^2$$

□

By taking the first derivative of the polynomial in Theorem 2.25 at y = 1, we get the forgotten topological index of chain of SiO_4 $\mathrm{SC}_q{}^p$ as follows:

Corollary 2.26. *Let p be odd and p < q. Then the forgotten topological index of* $\mathcal{SC}_q^p$ *is* $351pq - 189p - 54q - 27$.

Theorem 2.27. *Let p be odd and p < q. Then the geometric arithmetic polynomial of* $\mathcal{SC}_q^p$*is*

$$3(p+1)y^{\frac{\sqrt{6}}{3}} + (3pq + p + 2q - 5)y^{\frac{2}{3}} + 2(2p + q - 1)y^{\frac{1}{\sqrt{3}}}$$

Proof. Using the atom-bond partition from Table 2, in the formula of geometric arithmetic polynomial (4), we get

$$ABC\left(\mathrm{SC}_p^q, y\right) = \sum_{3=d_e\sim d_f=3} y^{\frac{2\sqrt{3+3}}{3+3}} + \sum_{E_3\sim 6} y^{\frac{2\sqrt{3+6}}{3+6}} + \sum_{6=d_e\sim d_f=6} y^{\frac{2\sqrt{6+6}}{6+6}}$$

This gives

$$GA(\mathrm{SC}_p^p, y) = 3(p+1)y^{\frac{\sqrt{6}}{3}} + (3pq+p+2q-5)y^{\frac{2}{3}} + 2(3pq-2(2p+q-1))y^{\frac{1}{\sqrt{3}}}$$

By taking the first derivative of the polynomial in Theorem 2.27 at $y = 1$, we get the □ geometric arithmetic index of chain of SiO_4 SC_p^p as follows:

Corollary 2.28. *Let p be odd and p < q. Then the geometric arithmetic index of* SC_p^p *is*

$$\frac{2(p+3pq+2q-5)+\sqrt{3}(3pq-2(2p+q-1))+3\sqrt{6}\,p+3\sqrt{6}}{3.}$$

Theorem 2.29. *Let p be odd and p < q. Then the randic polynomial polynomial of* SC_q^p *is*

$$3(p+1)y^{\frac{1}{3}} + (3pq+p+2q-5)y^{\frac{2}{3\sqrt{2}}} + 2(3pq-2(2p+q-1))y^{\frac{1}{6}}$$

Proof. Using the atom-bond partition from Table 2, in the formula of randic polynomial polynomial (5), we get

$$R(\mathrm{SC}_p^p, y) = \sum_{3=d_e\sim d_f=3} y^{\frac{1}{\sqrt{(3)(3)}}} + \sum_{3=d_e\sim d_f=6} y^{\frac{1}{\sqrt{(3)(6)}}} + \sum_{6=d_e\sim d_f=6} y^{\frac{1}{\sqrt{(6)(6)}}}$$

This gives

$$R(\mathrm{SC}_p^p, y) = 3(p+1)y^{\frac{1}{3}} + (3pq+p+2q-5)y^{\frac{2}{3\sqrt{2}}} + 2(3pq-2(2p+q-1))y^{\frac{1}{6}}$$

□

By taking the first derivative of the polynomial in Theorem 2.29 at $y = 1$, we get the randic polynomial index of chain of SiO_4 (SC_p^p)as follows:

Corollary 2.30. *Let p be odd and p < q.Then the randic polynomial index of* SC_p^p *is*

$$(3pq+p+2q-5)y^{\frac{2}{3\sqrt{2}}} + 2(3pq-2(2p+q-1))y^{\frac{1}{6}}.$$

Theorem 2.31. *Let p be odd and p < q. Then the reciprocal randic polynomial Polynomial of* SC_p^p *is* $3(p+1)y^3 + (3pq+p+2q-5)y^{3\sqrt{2}} + (3pq-2(2p+q-1))y^6$

Proof. Using the atom-bond partition from Table 2, in the formula of reciprocal randic polynomial polynomial (6), we get

$$R(\mathrm{SC}_p^p, y) = \sum_{3=d_e\sim d_f=3} y^{\sqrt{(3)(3)}} + \sum_{E_3\sim 6} y^{\sqrt{(3)(6)}} + \sum_{6=d_e\sim d_f=6} y^{\sqrt{(6)(6)}}$$

$$R\left(\mathrm{SC}_p^p, y\right) = 3(p+1)y^3 + (3pq+p+2q-5)y^{3\sqrt{2}} + \left(3pq - 2(2p+q-1)\right)y^6$$

□

By taking the first derivative of the polynomial in Theorem 2.31 at $y = 1$, we get the reciprocal randic polynomial index of chain of SiO_4 SC_p^p *as* follows:

Corollary 2.32. *Let p be odd and p < q. Then the reciprocal randic polynomial index of* SC_p^p *is* $9\sqrt{2pq} + 18pq + 3\sqrt{2p} - 15p + 6\sqrt{2b} + 21 - 12q - 15\sqrt{2}.$

Theorem 2.33. *Let p be odd and p < q. Then the sigma polynomial of* SC_p^p *is* $(3pq - p - 2q + 1)y^2 + (4pq + p + 2q - 5)y^{\frac{15}{4}}$

Proof. Using the atom-bond partition from Table 2, in the formula of symmetric division degree polynomial (7), we get

$$SDD\left(\mathrm{SC}_p^p, y\right) = \sum_{3=d_e\sim d_f=3} y^{\frac{[(3)^2+(3)^2]}{(3)(3)}} + \sum_{3=d_e\sim d_f=6} y^{\frac{[(3)^2+(6)^2]}{(3)(6)}} + \sum_{E_6\sim 6} y^{\frac{[(6)^2+(6)^2]}{(6)(6)}}$$

This gives

$$SDD\left(\mathrm{SC}_p^p, y\right) = 3(p+1)y^2 + (3pq+p+2q-5)y^{\frac{15}{4}} + (3pq - 2(2p+q-1))y^2$$
$$= (3pq - p - 2q + 1)y^2 + (3pq + p + 2q - 5)y^{\frac{15}{4}}$$

□

By taking the first derivative of the polynomial in Theorem 2.33 at $y = 1$, we get the symmetric division degree index of chain of SiO_4 (SC_p^p) as follows:

Corollary 2.34. *Let p be odd and p < q. Then the symmetric division degree index of* SC_p^p *is* $\frac{1}{4}(69pq + 7p + 14q - 567).$

Theorem 2.35. *Let p be odd and p < q. Then the inverse symmetric division polynomial of* SC_p^p *is* $(3pq - p - 2q + 1)y^{\frac{1}{2}} + (3pq + p + 2q - 5)y^{\frac{4}{15}}.$

Proof. Using the atom-bond partition from Table 2, in the formula of inverse symmetric division polynomial (8), we get

$$ISDD(\mathrm{SC}_p^p, y) = \sum_{3=d_e\sim d_f=3} y^{\frac{(3)(3)}{[(3)^2+(3)^2]}} + \sum_{E_3\sim 6} y^{\frac{(3)(6)}{[(3)^2+(6)^2]}} + \sum_{6=d_e\sim d_f=6} y^{\frac{(6)(6)}{[(6)^2+(6)^2]}}$$

This gives

$$\begin{aligned} ISDD(\mathrm{SC}_p^p, y) &= 3(p+1)y^{\frac{1}{2}} + (3pq+p+2q-5)y^{\frac{4}{15}} + (3pq-2(2p-2(2p+q-1))y^{\frac{1}{2}} \\ &= (3pq-p-2q+1)y^{\frac{1}{2}} + (3pq+p+2q-5)y^{\frac{4}{15}}. \end{aligned}$$

□

By taking the first derivative of the polynomial in Theorem 2.39 at y = 1, we get the inverse symmetric division index of chain of SiO_4 SC_p^pas follows:

Corollary 2.36. *Let p be odd and p < q. Then the inverse symmetric division index of* $\mathcal{SC}_q^p$*is*

$\frac{1}{30}(69pq - 7p - 14q - 25)$.

Theorem 2.37. *Let p be odd and p < q. Then the sigma polynomial of* SC_p^p*is* (3*pq* + *p* + 2*q* − 5) *y*9+ 3*pq* − *p* − 2*q* + 1*.*

Proof. Using the atom-bond partition from Table 2, in the formula of sigma polynomial (8), we get

$$S(\mathrm{SC}_p^p, y) = \sum_{3=d_e\sim d_f=3} y^{(3-3)^2} + \sum_{3=d_e\sim d_f=6} y^{(3-6)^2} + \sum_{E_6\sim 6} y^{(6-6)^2}$$

This gives

$$\begin{aligned} SDD(\mathrm{SC}_p^p, y) &= 3(p+1) + (3pq+p+2q-5)y^9 + (3pq-2(2p-2(2p+q-1)) \\ &= (3pq+p+2q-5)y^9 + 3pq-p-2q+1. \end{aligned}$$

□

By taking the first derivative of the polynomial in Theorem 2.39 at y = 1, we get the sigma index of chain ofSiO_4 SC_q^p as follows:

Corollary 2.38. *Let p be odd and p < q. Then the sigma index of* SC_p^p*is* (3*pq* + *p* + 2*q* − 5)*.*

Theorem 2.39. *Let p be odd and p < q. Then the somber polynomial of* SC_p^p *is* $3(p+1)y^{3\sqrt{2}} + (3pq+p+2q-5)y^{3\sqrt{5}} + (3pq-2(2p+q-1)y^{6\sqrt{2}}$.

Proof. Using the atom-bond partition from Table 2, in the formula of somber polynomial (8), we get

$$SO(\mathrm{SC}_p^p, y) = \sum_{3=d_e\sim d_f=3} y^{\sqrt{(3)^2+(3)^2}} + \sum_{3=d_e\sim d_f=6} y^{\sqrt{(3)^2+(6)^2}} + \sum_{E_6\sim 6} y^{\sqrt{(6)^2+(6)^2}}$$

This gives

$$SO(\mathrm{SC}_p^p, y) = 3(p+1)y^{3\sqrt{2}} + (3pq+p+2q-5)y^{3\sqrt{5}} + (3pq-2(2p+q-1)y^{6\sqrt{2}}$$

□

By taking the first derivative of the polynomial in Theorem 2.39 at $y = 1$, we get the somber index of chain of SiO_4 ($\mathrm{SC}_q{}^p$) as follows:

Corollary 2.40. *Let p be odd and p < q. Then the somber index of* SC_p^p *is* $(3pq+p+2q-5)3\sqrt{5} + (6pq-5p-4q+5))3\sqrt{2}$

Conclusion

In this article, two important silicon tetrahedron compound structures are considered, and the accurate formulas of some important valency-based topological indices are calculated using the technique of atom-bonds partitioning of these molecular structures. Our investigated results, such as the *H*-index, *ABC*-index, *F*-index, *GA*-index, *R*-index, *RR*- index, *SDD*-index, *ISDD*-index, *S*-index and *SO*-index are useful for determining physio-chemical properties of chemical compounds, as in 2005, Zhou explain in [34], such as formation enthalpies, boiling points, chromatographic retention times, vapour pressure, and surface areas. The obtained results are also innovative and noteworthy contributions to network science, providing a foundation for understanding the deep topology of these important networks. These findings, may also be useful in determining the role of silicon-carbon in electronics and industry. We also present a numerical comparison of topological characterizations for $p = q$ for the SiO_4 chain in ($\mathrm{SC}_q{}^p$) in Table 3 and a graphical comparison in Figure 2.

Table 3: Topological characterizations of $SC_q^p \text{ for } p < q$ and *p* is odd

p=q	H	ABC	F	GA	R	RR	SDD	ISDD	SO
2	6.11	9.56	918	17.02	6.30	88.30	72.5	8.73	144.83
3	12.61	20.39	2430	36.66	13.04	195.71	164	19.53	354.67
4	21.44	35.22	4644	63.78	22.20	343.27	290	34.93	655.67
5	32.61	54.06	7560	98.34	33.77	530.99	450.5	54.93	1047.84
6	46.11	76.89	11178	140.38	47.76	758.86	645.5	79.53	1531.16
7	61.94	103.72	15498	189.89	64.16	1026.89	875	108.73	2105.65
8	80.11	134.56	20520	246.86	82.97	1335.07	1139	142.53	2771.30
9	100.61	169.39	26244	311.29	104.20	1683.39	1437.5	180.93	3528.11
10	123.44	208.22	32670	383.18	127.84	2071.88	1770.5	223.93	4376.08

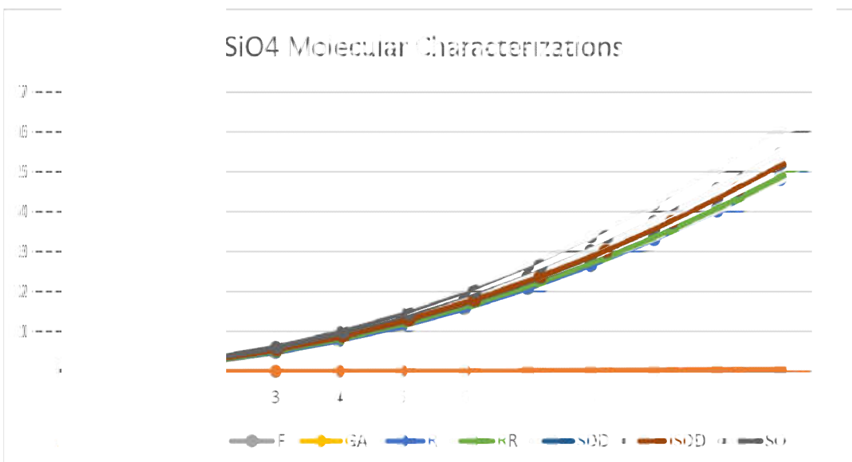

Figure 2: Graphical comparison

Open problems For the characterization of the chain of SiO_4 the followers are invited to discuss or research the these open problems.

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