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Research Article

Computation of Zagreb Polynomial and Indices for Silicate Network and Silicate Chain Network

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The connection of Zagreb polynomials and Zagreb indices to chemical graph theory is a bifurcation of mathematical chemistry, which has had a crucial influence on the development of chemical sciences. Nowadays, the study of topological indices has become a vast effective research area in chemical graph theory. In this article, we add up eight different Zagreb polynomials for the Silicate Network and Silicate Chain Network. From these Zagreb polynomials, we catch up on degree-based Zagreb indices. We also provide a graphical representation of the outcome that describes the dependence of topological indices on the given parameters of polynomial structure.

1. Introduction

Using chemical graph theory, we can determine a wide range of characteristics such as chemical networks; physical, chemical, and thermal properties; biological activity; and chemical activity. Topological indices, which are molecular descriptors, can characterise these features and specific graphs [1, 2]. In chemical graph theory, vertices represent atoms and edges represent chemical bonding between the atoms [3, 4]. The topological index of a chemical composition is a numerical value or a continuation of a given structure under discussion, which indicates chemical, physical, and biological properties of a chemical molecule, see for details [5–7].

Hayat et al. [8] and Ghani et al. [9] presented valency-based molecular descriptors for p-electronic measurements of lower polycyclic aromatic hydrocarbon energy. As a result of the incomplete combustion of organic matter, cyclic aromatic hydrocarbons ($CPAH_n$) are widely diffused and relocated in the ecosystem. Many $CPAH_n$ and their hydroxyl are very poisonous, toxic, and/or carcinogenic to bacteria as well as higher systems such as humans. 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 parameters of molecules, which is an advantage in the chemical industry. Many researchers have worked on various chemical compounds and computed topological descriptors of various molecular graphs over the last few decades [10, 11].

In chemical graph theory, a molecular graph is a simple connected graph composed of chemical atoms and bonds, which are commonly referred to as vertices and edges, respectively, and there must be linkage between the vertices set $V(G)$ and the edges set $E(G)$. The valency of each atom is actually the total number of atoms linked to v of G, and it is denoted by dv [12].

In 1972, Gutman and Trinajstic initiated the idea of computing the branching of the carbon-atom skeleton, which was, later on, known as the first Zagreb index [13]. In 2004, Gutman and Das adulate characteristics of the first and second Zagreb polynomials for some chemical graphs of a chemical compound, which we studied in the research articles [14, 15]. The first Zagreb polynomial corresponding to the first Zagreb index is defined as

$$M_1(G,y)=\sum_{uv\in E(G)} y^{d_u+d_v} \quad \text{and} \quad M_1(G)=\sum_{u,v\in E(G)} d_u+d_v. \tag{1}$$

The second Zagreb polynomial, which corresponds to the second Zagreb index [14], is written as

$$M_2(G,y)=\sum_{u,v\in E(G)} y^{d_u d_v} \quad \text{and} \quad M_2(G)=\sum_{u,v\in E(G)} d_u d_v. \tag{2}$$

In 2013, Shirdel et al. initiated the concept of the hyper Zagreb index [16]. The hyper Zagreb polynomial and index are defined as

$$HM(G,y)=\sum_{u,v\in E(G)} y^{(d_u+d_v)^2} \quad \text{and} \quad HM(G)=\sum_{u,v\in E(G)} (d_u+d_v)^2. \tag{3}$$

The modified Zagreb polynomial and index [17] are defined as

$$MD(G,y)=\sum_{u,v\in E(G)} y^{1/d_u d_v} \quad \text{and} \quad MD(G)=\sum_{u,v\in E(G)} \frac{1}{d_u d_v}. \tag{4}$$

In 2010, Furtula et al. introduced the augmented Zagreb index [18]. The augmented Zagreb polynomial and index are defined as

$$AZI(G,y)=\sum_{u,v\in E(G)} y^{[(d_u d_v)/(d_u+d_v-2)]^3} \quad \text{and} \quad AZI(G)=\sum_{u,v\in E(G)} \left[\frac{(d_u d_v)}{(d_u+d_v-2)}\right]^3. \tag{5}$$

Ranjini, Lokesha, and Usha introduced a redefined version of the Zagreb indices $ReZG1$, $ReZG2$, and $ReZG3$ in 2013 [19]. The redefined Zagreb polynomial and indices are defined as follows:

$$ReZG_1(G,y)=\sum_{u,v\in E(G)} y^{(d_u+d_v)/d_u d_v} \quad \text{and} \quad ReZG_1=\sum_{u,v\in E(G)} \frac{d_u+d_v}{d_u d_v}, \tag{6}$$

$$ReZG_2(G,y)=\sum_{u,v\in E(G)} y^{d_u d_v/(d_u+d_v)} \quad \text{and} \quad ReZG_2=\sum_{u,v\in E(G)} \frac{d_u d_v}{d_u+d_v}, \tag{7}$$

$$ReZG_3(G,y)=\sum_{u,v\in E(G)} y^{(d_u d_v)(d_u+d_v)} \quad \text{and} \quad ReZG_3=\sum_{u,v\in E(G)} (d_u d_v)(d_u+d_v). \tag{8}$$

A silicate Si is an element of a family of anions (an ion is an atom or molecule with a net-electrical charge) containing silicon and oxygen in industrial chemistry, usually represented by the general formula $[SiO_{4-t}^{(4-2t)-}]_n$, where $0 \le t < 2$. Using this formula, the Orthosilicate family$SiO_4^{4-}(t=0)$, see in [20], Metasilicate$SiO_3^{2-}(t=1)$, see in [21] and Pyrosilicate$Si_2O_7^{6-}(t=1/2, n=2)$, see in [22]. We can extend silicate S_i to any anions containing silicon (atom-bonding with other than O_2), as Hexafluorosilicate SiF_3^{2-}, see in [23]. Here, we discuss only chain of silicates, which is obtained by alternating sequence of tetrahedron SiO_4, see for details [24, 25].

In this article, the above defined eight Zagreb polynomials and Zagreb indices are constructed by the atom-bonds set of Silicate Network $\mathcal{SN}_P$ and Silicate Chain Network $\mathcal{CN}_P$, which partitioned according to the valencies of its S_i and O_2 atoms. We also investigate silicon tetrahedron S_iO_4 in a compound structure and derived the precise formulas of certain essential valency-based Zagreb indices using the approach of atom-bonds partitioning of molecular structure of silicates.

2. Zagreb Polynomials and Indices of Silicate Network $\mathcal{SN}_P$

Metal oxides or metal carbonates are fused with sand to form silicate networks. The basic unit of silicates is the tetrahedron SiO_4, found in almost all silicates. The sides of the tetrahedron SiO_4 represent oxygen atoms, while the middle represents silicon atoms from a chemical perspective [26]. Figure 1 depicts a SiO_4 tetrahedron in a silicate network $\mathcal{SN}_P$, where p is the number of hexagons between the centre and the network's boundary. A silicate sheet network is a collection of SiO_4 linked to other rings in a two-dimensional plane by shared oxygen atoms, resulting in a sheet-like structure, as shown in Figure 1.

Silicon atoms and corner atoms (lying on SiO_4 tetrahedrons in each ring) have valency 3 in the Silicate Network $\mathcal{SN}_P$, whereas all other atoms have valency 6. The numbers of atoms of valency 3 and valency 6 are $6p^2+6p$ and $9p^2-3p$, respectively. Thus, the total number of atoms and the total number of atom-bonds are shown in equation (9).

$$|V(\mathcal{SN}_P)|=3\left(5p^2+1\right) \quad \text{and} \quad |E(\mathcal{SN}_P)|=36p^2. \tag{9}$$

According to the valencies of the atoms, there are three types of atom-bonds in $\mathcal{SN}_P$: (3,3), (3,6) and (6,6). The atom-bonds partition of $\mathcal{SN}_P$ is shown in Table 1.

Theorem 1. *Let $\mathcal{SN}_p$ be a Silicate Network, then the first Zagreb polynomial of $\mathcal{SN}_P$ is $6py^6+6(3p^2+1)y^9+6(3p^2-2p)y^{12}$.*

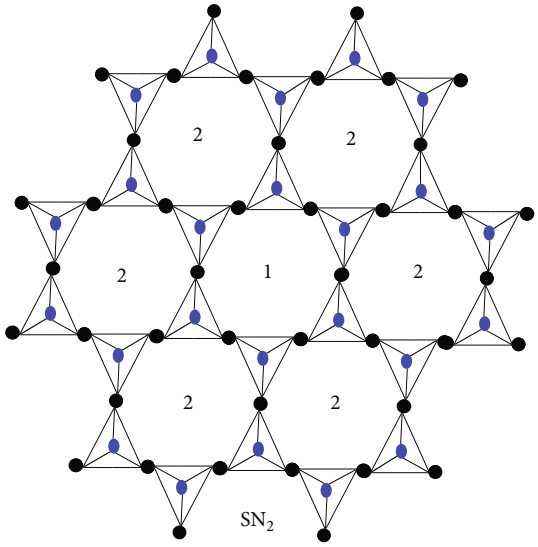

Figure 1: Silicate Network of dimension 2.

Table 1: Atom-bonds partition of $\mathcal{SN}_P$, on the valency based on each atom of *SiO*4.

Types of atom-bonds	$E_{(3,3)}$	$E_{(3,3)}$	$E_{(3,3)}$
Cardinality of atom-bonds	$6p$	$6(3p^2+1)$	$6(3p^2-2p)$

Proof. Using the atom-bonds partition from Table 1 in the formula of the first Zagreb polynomial (1), we obtain

$$M_1(\mathcal{SN}_P, y) = \sum_{E_{(3,3)}} y^6 + \sum_{E_{(3,6)}} y^9 + \sum_{E_{(6,6)}} y^{12}. \quad (10)$$

This gives

$$M_1(\mathcal{SN}_P, y) = 6py^6 + 6(3p^2+1)y^9 + 6(3p^2-2p)y^{12}. \quad (11)$$

□

By taking the first derivative of the polynomial in Theorem 17 at $y = 1$, we get the first Zagreb index of Silicate Network $\mathcal{SN}_P$ as follows:

Corollary 2. *Let $\mathcal{SN}_p$ be a Silicate Network, then the first Zagreb index of $\mathcal{SN}_P$ is $378p^2 - 108p + 54$.*

Theorem 3. *Let $\mathcal{SN}_p$ be a Silicate Network, then the second Zagreb polynomial of $\mathcal{SN}_P$ is $6py^9 + 6(3p^2+1)y^{18} + 6(3p^2-2p)y^{36}$.*

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

$$M_2(\mathcal{SN}_P, y) = \sum_{E_{(3,3)}} y^9 + \sum_{E_{(3,6)}} y^{18} + \sum_{E_{(6,6)}} y^{36}. \quad (12)$$

This gives

$$M_2(\mathcal{SN}_P, y) = 6py^9 + 6(3p^2+1)y^{18} + 6(3p^2-2p)y^{36}. \quad (13)$$

□

By taking the first derivative of the polynomial in Theorem 19 at $y = 1$, we get the second Zagreb index of Silicate Network $\mathcal{SN}_P$ as follows:

Corollary 4. *Let $\mathcal{SN}_p$ be a Silicate Network, then the second Zagreb index of $\mathcal{SN}_P$ is $972p^2 - 378p + 108$.*

Theorem 5. *Let $\mathcal{SN}_p$ be a Silicate Network, then the hyper Zagreb polynomial of $\mathcal{SN}_P$ is $6py^{36} + 6(3p^2+1)y^{81} + 6(3p^2-2p)y^{144}$.*

Proof. Using the atom-bonds partition from Table 1 in the formula of hyper Zagreb polynomial (3), we get

$$H(\mathcal{SN}_P, y) = \sum_{E_{(3,3)}} y^{36} + \sum_{E_{(3,6)}} y^{81} + \sum_{E_{(6,6)}} y^{144}. \quad (14)$$

This gives

$$H(\mathcal{SN}_P, y) = 6py^{36} + 6(3p^2+1)y^{81} + 6(3p^2-2p)y^{144}. \quad (15)$$

□

By taking the first derivative of the polynomial in Theorem 21 at $y = 1$, we get the hyper Zagreb index of Silicate Network $\mathcal{SN}_P$ as follows:

Corollary 6. *Let $\mathcal{SN}_p$ be a Silicate Network, then the hyper Zagreb index of $\mathcal{SN}_P$ is $4050p^2 - 1512p + 486$.*

Theorem 7. *Let $\mathcal{SN}_p$ be a Silicate Network, then the modified Zagreb polynomial of $\mathcal{SN}_P$ is $6py^{1/9} + 6(3p^2+1)y^{1/18} + 6(3p^2-2p)y^{1/36}$.*

Proof. Using the atom-bonds partition from Table 1 in the formula of modified Zagreb polynomial (4), we get

$$MD(\mathcal{SN}_P, y) = \sum_{E_{(3,3)}} y^{1/9} + \sum_{E_{(3,6)}} y^{1/18} + \sum_{E_{(6,6)}} y^{1/36} \quad (16)$$

This gives

$$MD(\mathcal{SN}_P, y) = 6py^{1/9} + 6(3p^2+1)y^{1/18} + 6(3p^2-2p)y^{1/36}. \quad (17)$$

□

By taking the first derivative of the polynomial in Theorem 23 at $y = 1$, we get the modified Zagreb index of Silicate Network $\mathcal{SN}_P$ as follows:

Corollary 8. *Let $\mathcal{SN}_p$ be a Silicate Network, then the modified Zagreb index of $\mathcal{SN}_P$ is $2p^2 + 8/3p + 1/2$.*

Theorem 9. *Let $\mathcal{SN}_p$ be a Silicate Network, then the augmented Zagreb polynomial of $\mathcal{SN}_P$ is $6py^{729/64} + 6(3p^2 + 1)y^{5832/343} + 6(3p^2 - 2p)y^{5832/125}$.*

Proof. Using the atom-bonds partition from Table 1 in the formula of augmented Zagreb polynomial (5), we get

$$AZI(\mathcal{SN}_P, y) = \sum_{E_{(3,3)}} y^{729/64} + \sum_{E_{(3,6)}} y^{5832/343} + \sum_{E_{(6,6)}} y^{4656/1000}. \tag{18}$$

This gives

$$AZI(\mathcal{SN}_P, y) = 6py^{729/64} + 6\left(3p^2 + 1\right)y^{5832/343} + 6\left(3p^2 - 2p\right)y^{5832/125}. \tag{19}$$

□

By taking the first derivative of the polynomial in Theorem 25 at $y = 1$, we get the augmented Zagreb index of Silicate Network $\mathcal{SN}_P$as follows:

Corollary 10. *Let $\mathcal{SN}_p$ be a Silicate Network, then the augmented Zagreb index of $\mathcal{SN}_P$ is $22301/50p^2 - 624/25p + 34392/343$.*

Theorem 11. *Let $\mathcal{SN}_p$ be a Silicate Network, then the first redefined Zagreb polynomial of $\mathcal{SN}_P$ is $6py^{2/3} + 6(3p^2 + 1)y^{1/2} + 6(3p^2 - 2p)y^{1/3}$.*

Proof. Using the atom-bonds partition from Table 1 in the formula of first redefined Zagreb polynomial (6), we get

$$ReZG_1(\mathcal{SN}_P, y) = \sum_{E_{(3,3)}} y^{2/3} + \sum_{E_{(3,6)}} y^{1/2} + \sum_{E_{(6,6)}} y^{1/3}. \tag{20}$$

This gives

$$ReZG_1(\mathcal{SN}_P, y) = 6py^{2/3} + 6\left(3p^2 + 1\right)y^{1/2} + 6\left(3p^2 - 2p\right)y^{1/3}. \tag{21}$$

□

By taking the first derivative of the polynomial in Theorem 27 at $y = 1$, we get the first redefined Zagreb index of Silicate Network $\mathcal{SN}_P$ as follows:

Corollary 12. *Let $\mathcal{SN}_p$ be a Silicate Network, then the first redefined Zagreb index of $\mathcal{SN}_P$ is $15p^2 + 3$.*

Theorem 13. *Let $\mathcal{SN}_p$ be a Silicate Network, then the second redefined Zagreb polynomial of $\mathcal{SN}_P$ is $6py^{3/2} + 6(3p^2 + 1)y^2 + 6(3p^2 - 2p)y^3$.*

Proof. Using the atom-bonds partition from Table 1 in the formula of second redefined Zagreb polynomial (7), we get

$$ReZG_2(\mathcal{SN}_P, y) = \sum_{E_{(3,3)}} y^{3/2} + \sum_{E_{(3,6)}} y^2 + \sum_{E_{(6,6)}} y^3. \tag{22}$$

This gives

$$ReZG_2(\mathcal{SN}_P, y) = 6py^{3/2} + 6\left(3p^2 + 1\right)y^2 + 6\left(3p^2 - 2p\right)y^3. \tag{23}$$

□

By taking the first derivative of the polynomial in Theorem 29 at $y = 1$, we get the second redefined Zagreb index of Silicate Network $\mathcal{SN}_P$ as follows:

Corollary 14. *Let $\mathcal{SN}_p$ be a Silicate Network, then the second redefined Zagreb index of $\mathcal{SN}_P$ is $90p^2 - 27p + 12$.*

Theorem 15. *Let $\mathcal{SN}_p$ be a Silicate Network, then the third redefined Zagreb polynomial of $\mathcal{SN}_P$ is $6py^{54} + 6(3p^2 + 1)y^{196} + 6(3p^2 - 2p)y^{432}$.*

Proof. Using the atom-bonds partition from Table 1 in the formula of third redefined Zagreb polynomial (8), we get

$$ReZG_3(\mathcal{SN}_P, y) = \sum_{E_{(3,3)}} y^{54} + \sum_{E_{(3,6)}} y^{196} + \sum_{E_{(6,6)}} y^{432}. \tag{24}$$

This gives

$$ReZG_3(\mathcal{SN}_P, y) = 6py^{54} + 6\left(3p^2 + 1\right)y^{196} + 6\left(3p^2 - 2p\right)y^{432}. \tag{25}$$

□

By taking the first derivative of the polynomial in Theorem 31 at $y = 1$, we get the third redefined Zagreb index of Silicate Network $\mathcal{SN}_P$ as follows:

Corollary 16. *Let $\mathcal{SN}_p$ be a Silicate Network, then the third redefined Zagreb index of $\mathcal{SN}_P$ is $11304p^2 - 4860p + 1176$.*

3. Comparison

In this section, we present in Table 2 and Figure 2 a numerical and graphical comparison of the Zagreb indices of Zagreb polynomials for $n = 2, 3, 4, \cdots, 12$ for the Silicate Network SN_p.

In the Silicate Network, the formulae for the polynomials M_1, M_2, H, MD, AZI, $ReZG_1$, $ReZG_2$, and $ReZG_3$ show that the degree of the polynomial increases while the coefficients remain constant. As a result, the growing behaviour in each graph of their indices is consistent, although the expansion varies as the degree of the polynomial increases.

Table 2: Zagreb topological indices of Silicate Network SN_p for $p \geq 2$.

n	M_1	M_2	H	MD	AZI	$ReZG_1$	$ReZG_2$	$ReZG_3$
2	1350	3240	13662	13.83	1834.43	63	318	36672
3	3132	7722	32400	26.50	4039.57	138	741	88332
4	5670	14148	59238	43.17	7136.75	243	1344	162600
5	8964	22518	94176	63.83	11125.97	378	2127	259476
6	13014	32832	137214	88.50	16007.23	543	3090	378960
7	17820	45090	188352	117.17	21780.53	738	4233	521052
8	23382	46492	247590	149.83	28445.87	963	5556	685752
9	29700	75438	314928	186.50	36003.25	1218	7059	873060
10	36774	93528	390366	227.17	44452.67	1503	8742	1082976
11	44604	113562	473904	271.83	53794.13	1818	10605	1315500
12	53190	135540	565542	320.50	64027.63	2163	12648	1570632

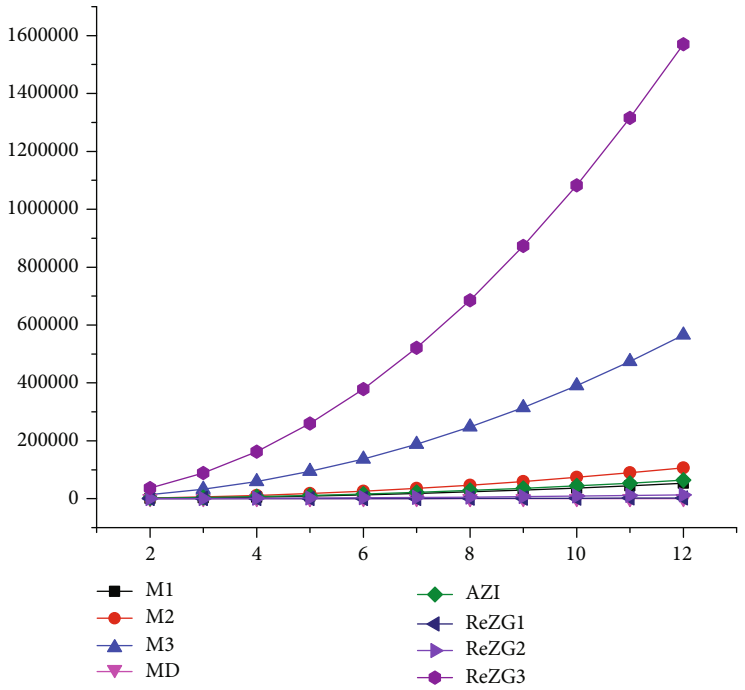

Figure 2: Graphical comparison of Zagreb indices of Silicate Network.

4. Zagreb Polynomials and Indices of Silicate Chain Network $\mathscr{CN}_P$

In this section, we will look at a family of silicate chain networks denoted by $\mathscr{CN}_P$ and obtained by linearly arranging p tetrahedral SiO_4, as shown in Figure 3.

It can be seen in Silicate Chain Network $\mathscr{CN}_P$, see Figure 3, that silicon atoms and corner atoms (lying on $Si O_4$ tetrahedrons in each ring) have valency 3, whereas all other atoms have valency 6 [27]. The number of atoms of valency 3 and valency 6 is $2(p+1)$ and $p-1$, respectively. Thus, the total number of atoms and total number of atom-bonds are shown in equation (26).

$$|V(\mathscr{CN}_P)| = 3p+1 \quad \text{and} \quad |E(\mathscr{CN}_P)| = 6p. \tag{26}$$

According to the valencies of the atoms, there are also three types of atom-bonds in $\mathscr{CN}_P$: (3,3), (3,6), and (6,6). The atom-bonds partition of $\mathscr{CN}_P$ is shown in Table 3.

Theorem 17. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the first Zagreb polynomial of $\mathscr{CN}_P$ is $(p+4)y^6 + 2(2p-1)y^9 + (p-2)y^{12}$.*

Proof. Using the atom-bonds partition from Table 3 in the formula of first Zagreb polynomial (1), we get

$$M_1(\mathscr{CN}_P, y) = \sum_{E_{(3,3)}} y^6 + \sum_{E_{(3,6)}} y^9 + \sum_{E_{(6,6)}} y^{12}. \tag{27}$$

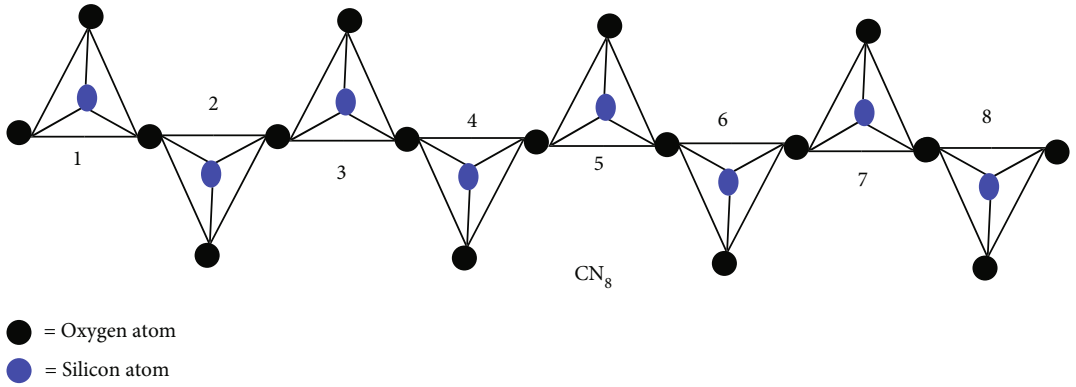

Figure 3: Silicate Chain Network of dimension 8.

Table 3: Atom-bonds partition of $\mathscr{CN}_P$, on the valency based on each atom of SiO_4.

Types of atom-bonds	$E_{(3,3)}$	$E_{(3,3)}$	$E_{(3,3)}$
Cardinality of atom-bonds	$p+4$	$2(2p-1)$	$p-2$

This gives

$$M_1(\mathscr{CN}_P, y) = (p+4)y^6 + 2(2p-1)y^9 + (p-2)y^{12}. \quad (28)$$

□

By taking the first derivative of the polynomial in Theorem 17 at $y=1$, we get the first Zagreb index of Silicate Chain Network $\mathscr{CN}_P$ as follows:

Corollary 18. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the first Zagreb index of $\mathscr{CN}_P$ is $54p-18$.*

Theorem 19. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the second Zagreb polynomial of $\mathscr{CN}_P$ is $(p+4)y^9 + 2(2p-1)y^{18} + (p-2)y^{36}$.*

Proof. Using the atom-bonds partition from Table 3 in the formula of second Zagreb polynomial (2), we get

$$M_2(\mathscr{CN}_P, y) = \sum_{E_{(3,3)}} y^9 + \sum_{E_{(3,6)}} y^{18} + \sum_{E_{(6,6)}} y^{36}. \quad (29)$$

This gives

$$M_2(\mathscr{CN}_P, y) = (p+4)y^9 + 2(2p-1)y^{18} + (p-2)y^{36}. \quad (30)$$

□

By taking the first derivative of the polynomial in Theorem 19 at $y=1$, we get the second Zagreb index of Silicate Chain Network $\mathscr{CN}_P$ as follows:

Corollary 20. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the second Zagreb index of $\mathscr{CN}_P$ is $117p-72$.*

Theorem 21. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the hyper Zagreb polynomial of $\mathscr{CN}_P$ is $(p+4)y^{36} + 2(2p-1)y^{81} + (p-2)y^{144}$.*

Proof. Using the atom-bonds partition from Table 3 in the formula of hyper Zagreb polynomial (3), we get

$$H(\mathscr{CN}_P, y) = \sum_{E_{(3,3)}} y^{36} + \sum_{E_{(3,6)}} y^{81} + \sum_{E_{(6,6)}} y^{144}. \quad (31)$$

This gives

$$H(\mathscr{CN}_P, y) = (p+4)y^{36} + 2(2p-1)y^{81} + (p-2)y^{144}. \quad (32)$$

□

By taking the first derivative of the polynomial in Theorem 21 at $y=1$, we get the hyper Zagreb index of Silicate Chain Network $\mathscr{CN}_P$ as follows:

Corollary 22. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the hyper Zagreb index of $\mathscr{SN}_P$ is $504p-306$.*

Theorem 23. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the modified Zagreb polynomial of $\mathscr{CN}_P$ is $(p+4)y^{1/9} + 2(2p-1)y^{1/18} + (p-2)y^{1/36}$.*

Proof. Using the atom-bonds partition from Table 3 in the formula of modified Zagreb polynomial (4), we get

$$MD(\mathscr{CN}_P, y) = \sum_{E_{(3,3)}} y^{1/9} + \sum_{E_{(3,6)}} y^{1/18} + \sum_{E_{(6,6)}} y^{1/36}. \quad (33)$$

This gives

$$MD(\mathscr{CN}_P, y) = (p+4)y^{1/9} + 2(2p-1)y^{1/18} + (p-2)y^{1/36}. \quad (34)$$

□

Table 4: Zagreb topological indices of Chain Network CN_p for $p \geq 2$.

n	M_1	M_2	H	MD	AZI	$ReZG_1$	$ReZG_2$	$ReZG_3$
2	90	162	702	1	170.35	7	8.5	84
3	144	279	1206	1.36	296.4	10	14.75	648
4	198	396	1710	1.72	422.45	13	21	1212
5	252	513	2214	2.08	548.5	16	27.25	1776
6	306	630	2718	2.44	674.55	19	33.5	2340
7	360	747	3222	2.81	800.6	22	39.75	2904
8	414	864	3726	3.17	926.65	25	46	3468
9	468	981	4230	3.52	1052.7	28	52.25	4032
10	522	1098	4734	3.88	1178.75	31	58.5	4596
11	576	1215	5238	4.25	1304.8	34	64.75	5160
12	630	1332	5742	4.61	1430.85	37	71	5724

By taking the first derivative of the polynomial in Theorem 23 at $y = 1$, we get the modified Zagreb index of Silicate Chain Network $\mathscr{CN}_P$ as follows:

Corollary 24. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the modified Zagreb index of $\mathscr{CN}_P$ is $13/36p + 5/18$.*

Theorem 25. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the augmented Zagreb polynomial of $\mathscr{CN}_P$ is $(p+4)y^{729/64} + 2(2p-1)y^{5832/343} + (p-2)y^{5832/125}$.*

Proof. Using the atom-bonds partition from Table 3 in the formula of augmented Zagreb polynomial (5), we get

$$AZI(\mathscr{CN}_P, y) = \sum_{E_{(3,3)}} y^{729/64} + \sum_{E_{(3,6)}} y^{5832/343} + \sum_{E_{(6,6)}} y^{4656/1000}. \tag{35}$$

This gives

$$AZI(\mathscr{CN}_P, y) = (p+4)y^{729/64} + 2(2p-1)y^{5832/343} + (p-2)y^{5832/125}. \tag{36}$$

□

By taking the first derivative of the polynomial in Theorem 25 at $y = 1$, we get the augmented Zagreb index of Silicate Chain Network $\mathscr{CN}_P$as follows:

Corollary 26. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the augmented Zagreb index of $\mathscr{CN}_P$ is $2521/20p - 327/4$.*

Theorem 27. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the first redefined Zagreb polynomial of $\mathscr{CN}_P$ is $(p+4)y^{2/3} + 2(2p-1)y^{1/2} + (p-2)y^{1/3}$.*

Proof. Using the atom-bonds partition from Table 3 in the formula of first redefined Zagreb polynomial (6), we get

$$ReZG_1(\mathscr{CN}_P, y) = \sum_{E_{(3,3)}} y^{2/3} + \sum_{E_{(3,6)}} y^{1/2} + \sum_{E_{(6,6)}} y^{1/3}. \tag{37}$$

This gives

$$ReZG_1(\mathscr{CN}_P, y) = (p+4)y^{2/3} + 2(2p-1)y^{1/2} + (p-2)y^{1/3}. \tag{38}$$

□

By taking the first derivative of the polynomial in Theorem 27 at $y = 1$, we get the first redefined Zagreb index of Silicate Chain Network $\mathscr{CN}_P$ as follows:

Corollary 28. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the first redefined Zagreb index of $\mathscr{CN}_P$ is $3p + 1$.*

Theorem 29. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the second redefined Zagreb polynomial of $\mathscr{CN}_P$ is $(p+4)y^{3/2} + 2(2p-1)y^2 + (p-2)y^3$.*

Proof. Using the atom-bonds partition from Table 3 in the formula of second redefined Zagreb polynomial (7), we get

$$ReZG_2(\mathscr{CN}_P, y) = \sum_{E_{(3,3)}} y^{3/2} + \sum_{E_{(3,6)}} y^2 + \sum_{E_{(6,6)}} y^3. \tag{39}$$

This gives

$$ReZG_2(\mathscr{CN}_P, y) = (p+4)y^{3/2} + 2(2p-1)y^2 + (p-2)y^3. \tag{40}$$

□

By taking the first derivative of the polynomial in Theorem 29 at $y = 1$, we get the second redefined Zagreb index of Silicate Chain Network $\mathscr{CN}_P$ as follows:

Corollary 30. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the second redefined Zagreb index of $\mathscr{CN}_P$ is $25/4p - 4$.*

Theorem 31. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the third redefined Zagreb polynomial of $\mathscr{CN}_P$ is $(p+4)y^{54} + 2(2p-1)y^{196} + (p-2)y^{432}$.*

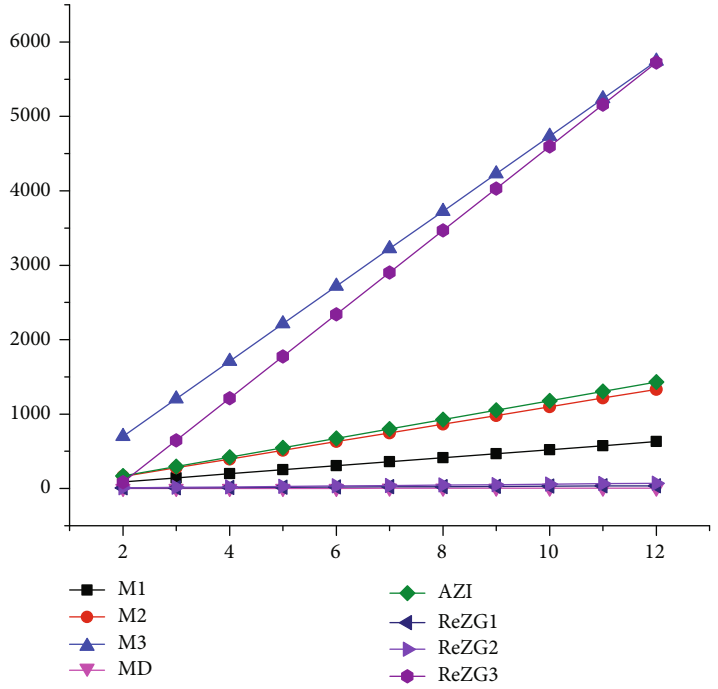

FIGURE 4: Graphical comparison of Zagreb indices of Silicate Chain Network.

Proof. Using the atom-bonds partition from Table 3 in the formula of third redefined Zagreb polynomial (8), we get

$$ReZG_3(\mathscr{CN}_P, y) = \sum_{E_{(3,3)}} y^{54} + \sum_{E_{(3,6)}} y^{196} + \sum_{E_{(6,6)}} y^{432}. \quad (41)$$

This gives

$$ReZG_3(\mathscr{CN}_P, y) = (p+4)y^{54} + 2(2p-1)y^{196} + (p-2)y^{432}. \quad (42)$$

□

By taking the first derivative of the polynomial in Theorem 31 at $y = 1$, we get the third redefined Zagreb index of Silicate Chain Network $\mathscr{CN}_P$ as follows:

Corollary 32. *Let $\mathscr{CN}_p$ be a Silicate Chain Network, then the third redefined Zagreb index of $\mathscr{CN}_P$ is $564p - 1044$.*

5. Comparison

In this section, we present a numerical and graphical comparison of the Zagreb indices of Zagreb polynomials for $n = 2, 3, 4, \cdots, 12$, for the Silicate Chain Network CN_p in Table 4 and Figure 4.

These numerical variables correlate to a graph that is useful in linking the structure with various physicochemical attributes, chemical reactivity, and biological activities. The values of M_1, M_2, H, AZI, and $ReZG_3$ in this graph (Figure 4) are rapidly increasing, while the values of MD, "$ReZG_1$," and "$ReZG_2$" are slowly increasing.

6. Closing Remarks

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-bond partitioning of these molecular structures. Our investigated results, such as the Zagreb indies, are useful for determining physiochemical properties of chemical compounds; as in 2005, Zhou explains in [28], 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.

Data Availability

The data used to support the findings of this study are included in the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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