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Ghani Mersenne Temperature Indices For Silicate Network and Silicate Chain Network

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Abstract One of chemistry's most fundamental ideas is the chemical bond. It explains why chemical reactions take place or why atoms are drawn to one another. Several features of chemical compounds in a molecular structure can be identified using the mathematical language offered by several types of topological indices. In actuality, a topological index links the molecular structure of chemical compounds to some of its physical characteristics, such as boiling point and stability energy. Such an index specifies the topology of the structure and is an invariant understructure that maintains mappings. It is produced by transforming a chemical network into a numerical value related to a molecular graph. The Ghani Mersenne temperature molecular descriptors, are suggested in this article by fusing the central ideas of the Mersenne number of silicate and silicate chain network. We compute the of first and second temperature, hyper temperature indices, the sum connectivity Ghani mersenne temperature index, the product connectivity Ghani mersenne temperature index, the reciprocal product connectivity Ghani mersenne temperature index and the F Ghani mersenne temperature index of by using the new temperature $T(Gm)_{u_i} = \frac{2^{d_{u_i}-1}}{|V_G|-2^{d_{u_i}-1}}$ of temperature of a molecular graph Silicate network and Silicate chain network.

Index Terms Ghani mersenne temperature indices, silicate and silicate chain network, ghani mersenne index, temperature indices

I. Introduction

In graph theory, the structural formula of every chemical compound is known as a molecular graph, with atoms and bonds representing the graph's vertices and edges, respectively. If two atoms have an atom-bond then it is denoted by $u \sim v$, the valency of every atom of G is actually the total number of atoms connected to v of G and it is denoted by d_v, [1]. Chemical graph is a field of mathematics that applies graph theory concepts to chemical molecules. Chemistry generates molecular graphs, and vice versa [2]. Chemical graph theory is utilised in the modelling of chemical substances [3], [4]. Topological indices are numerical numbers that indicate a graph's topology and invariants [5], [6]. Topological indices are critical in identifying the physical and chemical properties of a molecule. Topological indices are commonly employed for relationship analysis in theoretical chemistry, environmental chemistry, and toxicology. In chemical graph theory, the study of topological indices of a molecular graph has been particularly popular in the medical field recently Topological indicators [7]–[9] of several chemical structures used in the treatment of COVID-19 patients [10], Drugs' forgotten topological index of chemical structure [11]. Recent work proposes a new molecular descriptor, the atom-bond sum-connectivity (ABS) index [12].

An issue occurs when we study the intrinsic links between structural features and some invariant molecular networks. Topological indices are classified into three types: distance-based, spectrum-based, and degree-based indices [13]–[15]. Many indices, however, have both distance and degree bases. When trying to determine the boiling point of paraffin, Harold Wiener created the first topological index, known as the Wiener index, in 1947. Ali et al. drawn to examine outstanding foundations based on their vast spectrum of utility [17].

Some of the previously defined topological indices do not provide precise values for their indices; rather, they always provide an approximation. According to Randić, the branching index of an (molecular) graph also known as the Randić index [18], [19], the atom-bond sum connectivity index, geometric index and fourth version of the ABC index etc. All these indices, and other indices which have square root in their formulae, always give us an approximate value, and their equations are not in polynomial form.

We only consider finite, simple, connected graphs in this

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paper. Assume that G is a graph with the vertex set V_G and the edge set ξ_G. The number of vertices adjacent to a vertex u determines its degree d_u. For fundamental notations and terminologies, we refer the reader to [20].

Fajtlowicz put forward the follow definition of the temperature of any vertex u_i of a graph G [21]:

$$T_{u_i} = \frac{du_i}{|V_G| - du_i} \qquad \text{where} \qquad \forall\ u_i \in V_G.$$

Mersenne numbers are numbers with the form $M_n = 2^n - 1$, where n is a positive integer. The searching for Mersenne primes is a popular topic in number theory and computer science. It is also one of the most important applications for distributed computing [2], which is a technique in which hundreds of computers are linked over the Internet and work together to solve a problem. Using the Mersenne number definition, we defined the temperature of vertex u of a graph G as follows:

$$GMT_{u_i} = \frac{2^{d_{u_i}-1}}{|V_G| - 2^{d_{u_i}-1}} \qquad \text{where} \qquad \forall\ u_i \in V_G. \quad (1)$$

The first Ghani mersenne temperature index [16] is introduced as follows:

$$GMT_1 = \sum_{u_i,v_j \in \xi(G)} \left(GMT_{u_i} + GMT_{v_j}\right). \quad (2)$$

In 2020, Kulli introduced second Ghani mersenne temperature index [22], which is given by

$$GMT_2 = \sum_{u_i,v_j \in \xi(G)} \left(GMT_{u_i} \times GMT_{v_j}\right). \quad (3)$$

Kulli investigated the first and second hyper temperature indices in [22], which are defined as

$$GMHT_1 = \sum_{u_i,v_j \in \xi(G)} \left(GMT_{u_i} + GMT_{v_j}\right)^2, \quad (4)$$

$$GMHT_2(GM) = \sum_{u_i,v_j \in \xi(G)} \left(GMT_{u_i} \times GMT_{v_j}\right)^2. \quad (5)$$

The sum connectivity Ghani mersenne temperature index, the product connectivity Ghani mersenne temperature index, and the reciprocal product connectivity index are defined respectively as:

$$GMST(G) = \sum_{u_i,v_j \in \xi(G)} \frac{1}{\sqrt{\left(GMT_{u_i} + GMT_{v_j}\right)}}, \quad (6)$$

$$GMPT(G) = \sum_{u_i,v_j \in \xi(G)} \frac{1}{\sqrt{\left(T_u \times T_v\right)}}, \quad (7)$$

$$GMRPT(G) = \sum_{u_i,v_j \in \xi(G)} \sqrt{\left(GMT_{u_i} \times GMT_{v_j}\right)}. \quad (8)$$

Kulli also studied the F-Ghani mersenne temperature index and general Ghani mersenne temperature index of a graph G as:

$$GMFT(G) = \sum_{u_i,v_j \in \xi(G)} \left(T_u^2 + T_v^2\right). \quad (9)$$

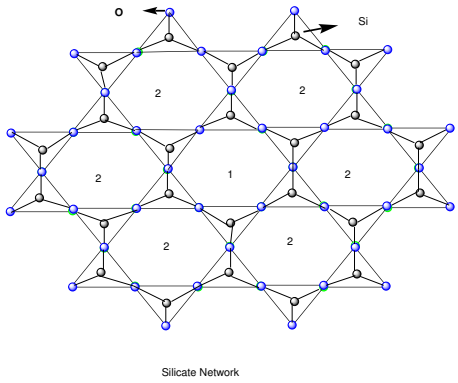

Figure 1: Silicate network SN_n

II. Silicate Network

We will calculate the temperature indices for the silicate network in this section. Sand is combined with metal oxides or metal carbonates to create silicate networks. The tetrahedron SiO_4 is the fundamental unit of silicates and is present in nearly all silicates. From a chemical standpoint, silicon atoms are represented by the middle of the tetrahedron SiO_4, whereas oxygen atoms are represented by its sides. A tetrahedron of SiO_4 in the Silicate network SN_n is shown in Figure 1, where n is the number of hexagons separating SN_P's centre and border. A grouping of SiO_4 connected to other rings on a two-dimensional plane by common oxygen atoms forms a silicate sheet network, which has a structure like a sheet., as shown in Figure 1.

It can be seen in Silicate Network SN_P, see Figure 1 that silicon atoms and corner atoms (lying on SiO_4 tetrahedrons in each ring) have degree 3, where as all other atoms have degree 6. The number of atoms of degree 3 and degree 6 are $6n^2+6n$ and $9p^2-3p$ respectively. Thus, the total number of atoms and total number of atom-bonds are $|V(SN_P)| = 3(5p^2+1)$ and $|E(SN_P)| = 36n^2$. According to the degree of the atoms, there are three types of atom-bonds in SN_P: (3,3), (3,6) and (6,6), that is

$$\xi_{(3,3)} = \left\{e = u_i \sim v_j, \forall\ u_i, v_j \in V(\mathcal{SN}_p) \middle| d_{u_i} = 3, d_{v_j} = 3\right\},$$
$$\xi_{(3,6)} = \left\{e = u_i \sim v_j, \forall\ u_i, v_j \in V(\mathcal{SN}_p) \middle| d_{u_i} = 3, d_{v_j} = 6\right\},$$
$$\xi_{(6,6)} = \left\{e = u_i \sim v_j, \forall\ u_i, v_j \in V(\mathcal{SN}_p) \middle| d_{u_i} = 6, d_{v_j} = 6\right\},$$

such that

$$|\xi_{(3,3)}| = 6n,$$
$$|\xi_{(3,6)}| = (18n^2 + 6),$$
$$|\xi_{(6,6)}| = (18n^2 - 12n).$$

By using this partition of SN_P, there are three types of edges based on the temperature of end vertices of each edge as given in Table 1.

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Theorem 1. *For silicate network, the Ghani mersenne temperature index is*
$\frac{84n}{15n^2-4}+\left(18n^2+6\right)\left(\frac{7}{15n^2-4}+\frac{21}{5(n+2)(n-2)}\right)+\frac{42\left(18n^2-12n\right)}{5(n+2)(n-2)}$.

Proof. Using the Atom-bonds partition from Table 1 in the formula of the first Ghani mersenne temperature index (2), we obtain our desired result. □

Theorem 2. *For silicate network, the second Ghani mersenne temperature index is*
$\frac{294n}{(15n^2-4)^2}+\frac{147\left(18n^2+6\right)}{5(15n^2-4)(n+2)(n-2)}+\frac{441\left(18n^2-12n\right)}{25(n+2)^2(n-2)^2}$.

Proof. Using the Atom-bonds partition from Table 1 in the formula of the second Ghani mersenne temperature index (3), we obtain our desired result. □

Theorem 3. *For silicate network, the first hyper Ghani mersenne temperature index is*
$\frac{1176n}{(15n^2-4)^2}+\frac{\left(18n^2+6\right)\left(350n^2-224\right)^2}{25(n+2)^2(n-2)^2(15n^2-4)^2}+\frac{1764\left(18n^2-12n\right)}{25(n+2)^2(n-2)^2}$.

Proof. Using the Atom-bonds partition from Table 1 in the formula of the first hyper Ghani mersenne temperature index (4), we obtain our desired result. □

Theorem 4. *For silicate network, the second hyper Ghani mersenne temperature index is*
$\frac{14406n}{(15n^2-4)^4}+\frac{21609\left(18n^2+6\right)}{25(15n^2-4)^2(n+2)^2(n-2)^2}+\frac{194481\left(18n^2-12n\right)}{625(n+2)^4(n-2)^4}$.

Proof. Using the Atom-bonds partition from Table 1 in the formula of the second Ghani mersenne temperature index (5), we obtain our desired result. □

Theorem 5. *For silicate network, the sum connectivity Ghani mersenne temperature index is*
$\frac{6n}{\sqrt{\frac{14}{15n^2-4}}}+\frac{3\sqrt{5}\left(3n^2+1\right)\sqrt{(n+2)(n-2)\left(\sqrt{15}n+2\right)\left(\sqrt{15}n-2\right)}\sqrt{350n^2-224}}{7\left(25n^2-16\right)}+\frac{\sqrt{210}n(3n-2)\sqrt{n^2-4}}{7}$.

Proof. Using the Atom-bonds partition from Table 1 in the formula of the sum connectivity Ghani mersenne temperature index (6), we obtain our desired result. □

Theorem 6. *For silicate network, the product connectivity Ghani mersenne temperature index is*
$\frac{6n\left(15n^2-4\right)}{7}+\frac{2\sqrt{15}\left(3n^2+1\right)\sqrt{(15n^2-4)(n^2-4)}}{7}+\frac{10n\left(n^2-4\right)(3n-2)}{7}$.

Proof. Using the Atom-bonds partition from Table 1 in the formula of the product connectivity Ghani mersenne temperature index (7), we obtain our desired result. □

Theorem 7. *For silicate network, the reciprocal product Ghani mersenne temperature index is*
$\frac{42n}{15n^2-4}+\frac{7\sqrt{15}\left(18n^2+6\right)\sqrt{15n^4-64n^2+16}}{75n^4-320n^2+80}+\frac{21\left(18n^2-12n\right)}{5(n^2-4)}$.

Proof. Using the Atom-bonds partition from Table 1 in the formula of the second Ghani mersenne temperature index (8), we obtain our desired result. □

Theorem 8. *For silicate network, the F-Ghani mersenne temperature index is*

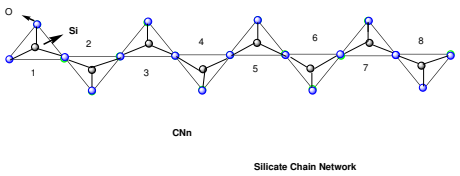

Figure 2: Silicate chain network CN_n

$\frac{588n}{(15n^2-4)^2}+\left(18n^2+6\right)\left(\frac{49}{(15n^2-4)^2}+\frac{441}{25(n+2)^2(n-2)^2}\right)+\frac{882\left(18n^2-12n\right)}{25(n+2)^2(n-2)^2}$.

Proof. Using the Atom-bonds partition from Table 1 in the formula of the F-Ghani mersenne temperature index (9), we obtain our desired result. □

III. Silicate Chain Network CN_n

This section will study a family of silicate chain networks, CN_n, which may be formed by linearly arranging p tetrahedral SIO_4, as Figure 2 illustrates. As can be observed in Silicate Chain Network CN_n, all other atoms have valency 6, whereas silicon and corner atoms (lying on SIO_4 tetrahedrons in each ring) have valency 3. Valency 3 and valency 6 have $2(n+1)$ and $n-1$ atoms, respectively. Now, $|V(CN_P)| = 3P+1$ and $|E(CN_P)| = 6n$. Moreover

$$\xi_{(3,3)} = \left\{e = u_i \sim v_j, \forall\, u_i, v_j \in V(\mathcal{CN}_p) \middle| d_{u_i} = 3, d_{v_j} = 3\right\},$$
$$\xi_{(3,6)} = \left\{e = u_i \sim v_j, \forall\, u_i, v_j \in V(\mathcal{CN}_p) \middle| d_{u_i} = 3, d_{v_j} = 6\right\},$$
$$\xi_{(6,6)} = \left\{e = u_i \sim v_j, \forall\, u_i, v_j \in V(\mathcal{CN}_p) \middle| d_{u_i} = 6, d_{v_j} = 6\right\},$$

such that

$$|\xi_{(3,3)}| = (n+4),$$
$$|\xi_{(3,6)}| = (4n-2),$$
$$|\xi_{(6,6)}| = p-2.$$

By using equation (1) and above partition of CN_n, three types of edges on the basis of the temperature of end vertices of an edge can be identified. They are described in Table 2.

Theorem 9. *For chain of silicate the first Ghani mersenne temperature index is* $\frac{14(n+4)}{3(n-2)}+\frac{(4n-2)(210n-812)}{3(n-2)(3n-62)}+\frac{126(n-2)}{3n-62}$.

Proof. Using the Atom-bonds partition from Table 2 in the formula of the first Ghani mersenne temperature index (2), we obtain our desired results. □

Theorem 10. *For chain of silicate the second Ghani mersenne temperature index is* $\frac{49(n+4)}{(3n-6)^2}+\frac{147(4n-2)}{(n-2)(3n-62)}+\frac{3969(n-2)}{(3n-62)^2}$.

Proof. Using the Atom-bonds partition from Table 2 in the formula of the second Ghani mersenne temperature index (3), we obtain our desired results. □

Theorem 11. *For chain of silicate the first hyper Ghani mersenne temperature index is* $\frac{196(n+4)}{(3n-6)^2}+\frac{(4n-2)(210n-812)^2}{9(n-2)^2(3n-62)^2}+\frac{15876(n-2)}{(3n-62)^2}$.

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(GMT_{u_i}, GMT_{v_j})	$\left(\frac{7}{(15n^2+3)-7}, \frac{7}{(15n^2+3)-7}\right)$	$\left(\frac{7}{(15n^2+3)-7}, \frac{63}{(15n^2+3)-63}\right)$	$\left(\frac{63}{(15n^2+3)-63}, \frac{63}{(15n^2+3)-63}\right)$
Frequency	$6n$	$(18n^2+6)$	$(18n^2-12n)$

Table 1: Atom-bond partition of SN_n

(GMT_{u_i}, GMT_{v_j})	$\left(\frac{7}{(3n+1)-7}, \frac{7}{(3n+1)-7}\right)$	$\left(\frac{7}{(3n+1)-7}, \frac{63}{(3n+1)-63}\right)$	$\left(\frac{63}{(3n+1)-63}, \frac{63}{(3n+1)-63}\right)$
Frequency	$(n+4)$	$(4n-2)$	$n-2$

Table 2: Atom-bond partition of CN_n, for $p = q$

Proof. Using the Atom-bonds partition from Table 2 in the formula of the first hyper Ghani mersenne temperature index (4), we obtain our desired results. □

Theorem 12. *For chain of silicate the second hyper Ghani mersenne temperature index is* $\frac{2401(n+4)}{(3n-6)^4} + \frac{21609(4n-2)}{(n-2)^2(3n-62)^2} + \frac{15752961(n-2)}{(3n-62)^4}$.

Proof. Using the Atom-bonds partition from Table 2 in the formula of the second Ghani mersenne temperature index (5), we obtain our desired results. □

Theorem 13. *For chain of silicate the sum connectivity Ghani mersenne temperature index is* $\frac{\sqrt{14}(n+4)\sqrt{3n-6}}{14} + \frac{\sqrt{3}(2n-1)\sqrt{(n-2)(3n-62)}\sqrt{210n-812}}{7(15n-58)} + \frac{\sqrt{14}(n-2)\sqrt{3n-62}}{42}$.

Proof. Using the Atom-bonds partition from Table 2 in the formula of the sum connectivity Ghani mersenne temperature index (6), we obtain our desired results. □

Theorem 14. *For chain of silicate the product connectivity Ghani mersenne temperature index is* $\frac{(3n-6)(n+4)}{7} + \frac{\sqrt{3}(4n-2)\sqrt{(n-2)(3n-62)}}{21} + \frac{(3n-62)(n-2)}{63}$.

Proof. Using the Atom-bonds partition from Table 2 in the formula of the product connectivity Ghani mersenne temperature index (7), we obtain our desired results. □

Theorem 15. *For chain of silicate the reciprocal product Ghani mersenne temperature index is* $\frac{7(n+4)}{3n-6} + \frac{7\sqrt{3}(4n-2)\sqrt{(n-2)(3n-62)}}{3n^2-68n+124} + \frac{63(n-2)}{3n-62}$.

Proof. Using the Atom-bonds partition from Table 2 in the formula of the second Ghani mersenne temperature index (8), we obtain our desired results. □

Theorem 16. *For chain of silicate the F-Ghani mersenne temperature index is* $\frac{18(n+4)}{(3n-2)^2} + \frac{6(2p-1)(135p^2-243p+123)}{(3n-2)^2(3p-5)^2} + \frac{72(n-2)}{(3p-5)^2}$.

Proof. Using the Atom-bonds partition from Table 2 in the formula of the F-Ghani mersenne temperature index (9), we obtain our desired results. □

IV. Conclusion

In QSPR/QSAR research, topological indices including the Zagreb index, Randic index, and atom-bond connectivity index are utilised to predict chemical compound bioactivity. We propose computing the first Ghani mersenne temperature index, second Ghani mersenne temperature index, first hyper Ghani mersenne temperature index, second hyper Ghani mersenne temperature index, sum Ghani mersenne temperature index, product temperature, reciprocal product Ghani mersenne temperature index, and F-Ghani mersenne temperature index of Silicate network and Silicate chain network, which correlates well with entropy, acentric factor, enthalpy of vaporisation, and standard enthalpy of vaporisation.

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