



OPEN Exponential Wiener index of some silicate networks

G. Subashini¹, K. Kannan^{1✉} & A. Menaga²

Any graph that depicts a particular molecular structure can be given a topological graph index, also known as a molecular descriptor. This index can be used to examine numerical data and discover more about specific physical properties of molecules. Silicates are hard crystals that can be sliced into little pieces. Therefore, silicon play a vital role in many real time applications. It is the authentic material to make microchips which run in PDA, PC and other game tools. In the current study, we have determined the new topological index for a few silicate structures, including cyclic, single-chain, and Pyro silicates by grouping the vertices of the corresponding molecular graphs based on their distance sums. This index is known as the exponential Wiener index. It is expanded to include their line graphs as well. The numerical values of exponential Wiener index and multiplicative exponential Wiener index for the molecular graphs of cyclic silicates, single chain silicates and their line graphs with n vertices where $n = 3, 4, 5$ are explored.

The fundamental graphs examined in this work are loop-free, finite, undirected, and have a single edge. The degree of a vertex v in a graph G is indicated by $deg(v)$, which is the number of edges that intersect it. Chemical graph theory is a branch of mathematics that combines graph theory and chemistry. In order to mathematically represent molecules and reveal the physical characteristics of these chemical substances, graph theory is applied. Using discrete mathematics, chemical graph theory is a well-established field of study in chemistry that represents the physical and biological properties of chemical substances. A type of graph invariant known as a molecular structure index links the chemical and physical characteristics of a molecular graph to a numerical value. Some of topological indices are vertex-degree-based, the others are distance or eccentricity-based. The most widely known topological indices are the first and second Zagreb indices, which are the first vertex degree based indexes.

It was defined by $M_1(G) = \sum_{v \in V(G)} deg(v)^2$ and $M_2(G) = \sum_{uv \in E(G)} deg(u)deg(v)$ to be the oldest and most

thoroughly investigated graph invariant, respectively^{32,44}. Estrada et al.⁴³ proposed the atom-bond connectivity index (ABC), a brand-new graph theoretical index based on the connectivity between atoms and bonds in a molecule. This structural descriptor is computed using the vertex and edge degrees, but Randić's initial connectivity index is not²². According to Todeschini et al.⁶, the multiplicative variants of the conventional Zagreb indices are defined as follows: $\prod_1(G) = \prod_{v \in V(G)} deg(v)^2$ and $\prod_2(G) = \prod_{uv \in E(G)} deg(u)deg(v)$, respectively.

These two graph invariants are referred to as multiplicative Zagreb indices by Gutman⁹. The upper bounds of the multiplicative Zagreb indices for join, Cartesian product, Corona product, Composition, and Disjunction of Graphs are calculated by Das et al.²⁶.

The Wiener index is a well-known distance-based topological index introduced as structural descriptor for acyclic organic molecules⁷. It is defined as the sum of distances between all unordered pairs of vertices of a simple graph G . That is, The Wiener index for the graph G is given by the formula $W(G) = \frac{1}{2} \sum_{u \in V(G)} d_G(u)$, where

$d_G(u)$ is the sum of all vertices' distances from $u \in V(G)$. Wiener coined this word to describe a chemical problem. For graphs of order n , the asymptotically sharp upper bound on W_e is $W_e(G) \leq \left(\frac{2n}{5}\right)^5 + O\left(n^{\frac{9}{2}}\right)$

where the edge-Wiener index W_e of G is the sum of the distances between all pairs of edges²⁵. In 2011⁴, the

¹Department of Mathematics, Srinivasa Ramanujan Centre, SASTRA Deemed to be University, Kumbakonam, Tamil Nadu 612001, India. ²Department of Computer Science and Engineering, Srinivasa Ramanujan Centre, SASTRA Deemed to be University, Kumbakonam, Tamil Nadu 612001, India. ✉email: anbukannan@rediffmail.com

precise equations for the Wiener indices of a novel class of carbon nanojunctions ($O_p(Q_{2,0}(T)) - TU(3, 0)$) are provided. The capacity to sum the Wiener indices of weighted quotient graphs with respect to any given collection of Θ^* -classes to represent the Wiener index of a weighted graph (G, w) is demonstrated². In this case, Θ^* represents the transitive closure of the Djokovic-Winkler relation Θ .

According to Liu et al.³⁹, which expands and corrects Yang's discovery¹², a graph must satisfy certain conditions in order to be traceable and Hamiltonian. These conditions are based on the Wiener index and the complement of the graph. Kuang et al.²⁷ give the essential conditions for a connected graph to be Hamiltonian, traceable, and for a connected bipartite graph to be Hamiltonian in terms of the Wiener-type invariants. Carbon atoms form the atomic-scale honeycomb lattice known as graphene. Exact expressions for a number of degree based topological indices of carbon compound graphene, including the augmented Zagreb index, harmonic index, hyper-Zagreb index, first multiple Zagreb index, second multiple Zagreb index, and second Zagreb index, have been presented by Jegadeesh et al.⁴⁰.

The hyper-Wiener indicator $WW(G)$ of a graph G is defined as $WW(G) = \frac{1}{2} \sum_{u \in V(G)} [d_G(u) + d_G^2(u)]$ where $d_G(u)$

is the sum of all vertices' distances from $u \in V(G)$ and $d_G^2(u) = [d_G(u)]^2$. According to Cai et al.⁴², a connected graph must meet certain criteria in terms of the hyper-Wiener index in order to be traceable, Hamiltonian, and Hamilton connected, respectively. Jia et al.¹⁵ discuss the Wiener and Harary indices on Hamilton connected and traceable graphs. The requirements for a connected general graph to be Hamilton-connected and traceable from every vertex, or for a bipartite graph to be Hamiltonian, are given by Qiannan et al.⁴⁵ in terms of the complement of its Wiener-type invariants. A nearly balanced bipartite graph must have certain criteria in order to be traceable with the help of the Wiener, hyper-Wiener and Harary indices with a specified minimum degree, according to Yu et al.¹⁷ Rada¹⁰ has examined the extremal tree graphs for the exponential first and second indices, with the exception of the maximal tree graph of the exponential second Zagreb index. For several Zagreb indices, including the first and second exponential Zagreb indices, which are defined by $EM_1(G)$

$= \sum_{v \in V(G)} e^{deg(v)^2}$ and $EM_2(G) = \sum_{uv \in E(G)} e^{deg(u)deg(v)}$, respectively, new graph invariants known as exponential

Zagreb indices are presented in 2021¹⁸.

In order to explore the utility of topological indices for graphs statistically, Yuede Ma and colleagues' work²¹ assigns a feature vector to a graph with "useful" features represented by certain measurements. Signed graphs have been used for a long time in social network analysis to simultaneously model opposite relationships. In a signed graph, each edge is assigned either a positive or negative sign, referred to as valence. To define the concept of Wiener indices for signed graphs, Sam Spiro worked³. If $|V(G)| > k$ and G has a spanning tree T always such that S is indeed the set of pendant vertices (leaves) of T , given any subset $S \subseteq V(G)$ with $|S| = k$, then a graph G is said to be k -leaf-connected²³. As a result, a graph is only 2-leaf-connected and Hamilton-connected together. The Wiener-type invariant condition for a graph to be a k -leaf-connected and the corresponding results were extended on Hamilton connected graph by Ao et al.³³. Recently, the task of creating graphs with a large proportion of vertices such that removing any one of them does not change the Wiener index of a graph was examined by Akhmejanova et al.¹⁹. As the main result, they built an infinite series of graphs with the proportion of such vertices tending to $\frac{1}{2}$.

For $n = p^\alpha, pq, p^2q, p^2q^2, pqr, p^3q, p^2qr, pqr s$, where p, q, r and s are distinct primes, the Wiener index and forgotten topological index of the prime ideal sum graph of Z_n are calculated and a Sage math code is built for building the graph and calculating the indices¹⁴. Hypergraphs can be handled with the cut method. More specifically, the Wiener index of k -uniform partial cube-hypergraphs is the way for which the method is developed. The technique is used with hypertrees and cube-hypergraphs³¹. The computation of a productive sum based topological index associated to the physical parameters of fullerene was the focus of Umber Sheikh et al.'s work³⁷. In terms of multiple topological indices of graphs, including the general Randić index, the general zeroth-order Randić index, the redefined Zagreb indices, the atom-bond connectivity index, and the first general multiplicative Zagreb index, Akbar Jahanbani et al. provided a variety of lower and upper bounds for the energy of graphs¹. In two-dimensional (2D) multiband systems, Fernando and Cao²⁸ have presented a novel gauge-invariant, quantized interband index. It overcomes challenges in characterizing topology of submanifolds by offering a bulk topological classification of a submanifold of parameter space (e.g., an electron valley in a Brillouin zone). The effectiveness of degree-based topological indices of dominating David derived networks (DDDN) has been examined and evaluated by Zaman et al. In many disciplines, including biology, the social sciences, and computer science, DDDNs are extensively employed for the structural and functional analysis of complex networks¹⁶.

Javid et al.³⁰ compute various topological indices for the rhombus silicate and rhombus oxide networks and comparison between them were also investigated by them. Arockiaraj⁴¹ have developed a new method based on vertex decomposition and computing the degree and distance-based topological indices for polymeric chains, cyclic and double chain silicates, silicate and oxide networks as a function of n , the order of circumscribing. Sarkar et al.⁵ studied the (a, b)-Zagreb index of line graphs of the subdivision graphs of some chemical structures. Sarkar and Pal³⁵ computed some new degree-based topological indices of benzene ring implanted in the P-type-surface in the 2D network and its line subdivision of graph.

Sarkar et al.³⁸ mainly focused on some well-known degree-based topological indices and the corresponding QSPR studies in polycyclic aromatic hydrocarbons. Sarkar et al.³⁴ mainly concerned with some neighborhood degree-based multiplicative topological indices for some line graphs of subdivision graphs of some union graphs of hexagons. Sarkar et al.³⁶ computed the general Zagreb index and some degree based topological indices of some silicate networks recently.

The characterization of molecular graphs by means of parameters calculated for their derived structures is the one of the most important approaches in mathematical chemistry researches¹³. Line graphs is one of the good examples for the derived structure since they reflect the branches of initial graphs. Several researches have been found in the literature of invariants of line graphs which are applied to evaluate the structural complexity of molecular graphs, to order the structures and to design novel topological indices^{20–24}.

In this sequel, in this paper, we build and investigate the exponential Wiener index ($EW(G)$)-a novel variation for some silicate networks by grouping the vertices of the corresponding molecular graphs based on their distance sums $d_G(u)$. The numerical examples are examined for few graphs with $n = 3, 4, 5$ vertices at the end.

Exponential Wiener index and multiplicative exponential wiener index of various silicate structures

In this section, we calculated and examined the exponential Wiener indices for some silicate networks, which is the distance-based topological indices.

Definition 2.1 For the graph G , the exponential Wiener index is defined by

$$EW(G) = \frac{1}{2} \sum_{u \in V(G)} e^{d_G(u)} \quad (1)$$

Ortho silicates (or neso or island silicates)

The minerals known as silicates are composed of silicon and oxygen in the form of tetrahedral SiO_4^{4-} units that are connected in various ways. The Fig. 1 shows the fundamental structural unit and graph structure (top view) of silicates.

These are some instances of ortho silicates: (1) Phenacite or Phenakite (Be_2SiO_4), (2) Willemite (Zn_2SiO_4), (3) Olivine ($(Fe/Mg)_2SiO_4$) and (4) Zirconium oxide ($ZrSiO_4$).

There are 4 vertices in ortho silicates (Fig. 2a) and each of them is adjacent to the other three vertices and hence $d_{OS}(u) = 3$ and the Exponential Wiener Index of ortho silicate is $EW(OS) = \frac{1}{2} \sum_{u \in V[OS]} e^{d_{OS}(u)} = 2e^3$. The

multiplicative Exponential Wiener Index of ortho silicate is $\prod EW(OS) = \frac{1}{2} \prod_{u \in V[OS]} e^{d_{OS}(u)} = \frac{1}{2} e^{12}$. Further,

there are 6 vertices in the line graph $L[OS]$ of ortho silicates (Fig. 2b) and each of them is adjacent to the other 4 vertices and with distance 2 with the remaining one vertex and hence $d_{L[OS]}(u) = 6$ and the Exponential Wiener Index of the line graph $L[OS]$ of ortho silicates is $EW(L[OS]) = \frac{1}{2} \sum_{u \in V[L[OS]]} e^{d_{L[OS]}(u)} = 3e^6$. Finally,

the multiplicative Exponential Wiener Index of the line graph $L[OS]$ of ortho silicates is $\prod EW(L[OS]) = \frac{1}{2} \prod_{u \in V[L[OS]]} e^{d_{L[OS]}(u)} = \frac{1}{2} e^{36}$.

Pyro silicate (or soro silicate or disilicate)

Pyro silicate is composed of $Si_2O_7^{6-}$ ions, which are created by connecting two tetrahedral SiO_4^{4-} molecules, each of which shares an oxygen atom at one corner (one oxygen is subtracted during joining). The pyrosilicate's structure and its line graph is depicted below (Fig. 3).

Compared to the orthosilicate ion, the pyrosilicate ion is less basic. Pyrosilicate ions are only present in one mineral in nature. Thortveitite, $Sc_2Si_2O_7$, is the most straightforward type of pyro silicate.

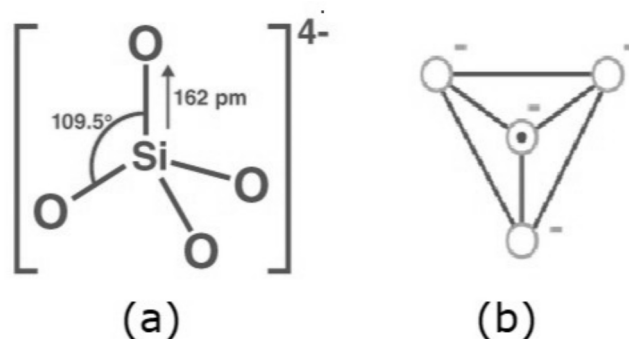


Figure 1. (a) Silicate structure SiO_4^{4-} , (b) basic graph structure of silicates.

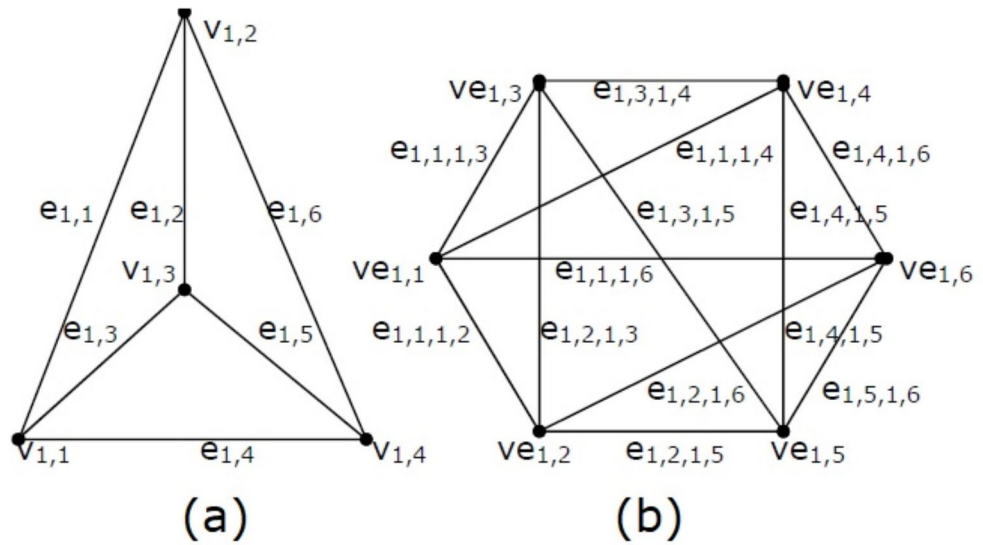


Figure 2. (a) Chain silicate network $CS(1)$, (b) its line graph $L(CS(1))$.

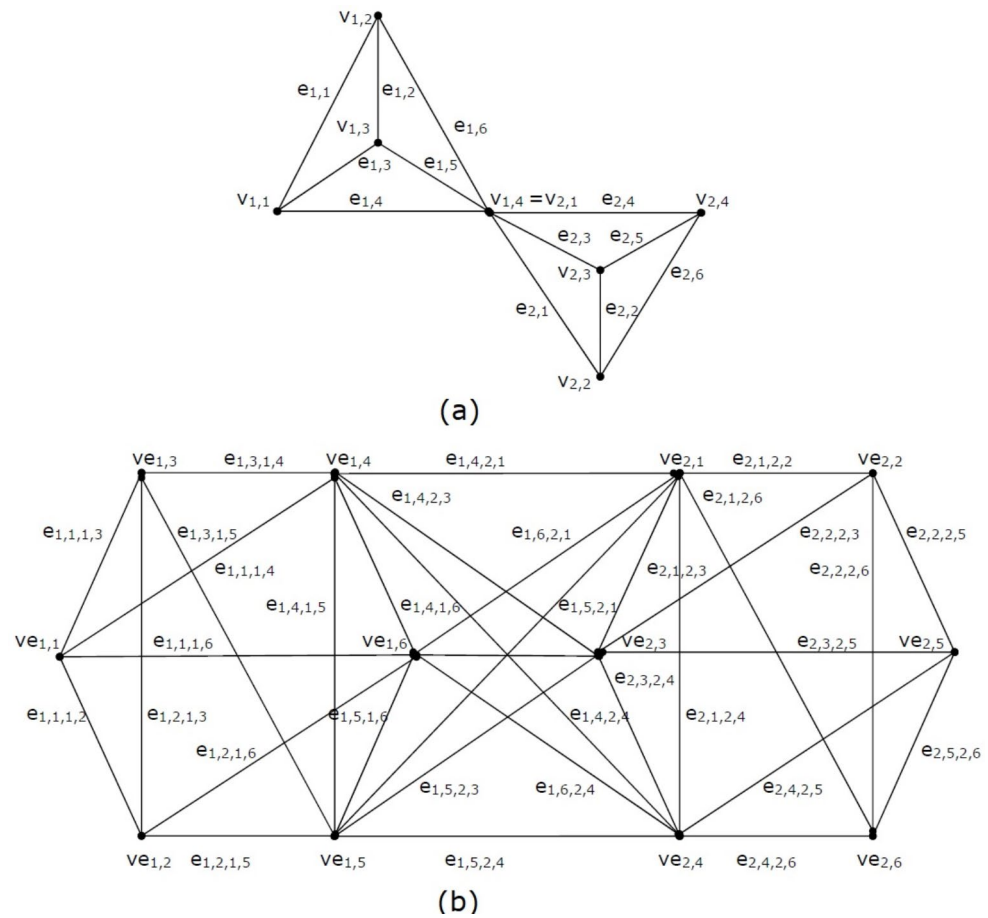


Figure 3. (a) Chain silicate network $CS(2)$, (b) its line graph $L(CS(2))$.

Theorem 2.2 For the Pyro Silicate networks $CS(2)$, the exponential Wiener index is $EW [CS(2)] = \frac{e^6}{2} (1 + 6e^3)$ and the multiplicative exponential Wiener index $\prod EW [CS(2)] = \frac{1}{2}e^{60}$.

Proof There are two vertices corresponding to 2 silicon irons and four vertices corresponding to 4 non-shared Oxygen irons and 1 vertex corresponding to shared Oxygen iron and hence seven vertices in total in the Pyro silicate network $CS(2)$. Hence there are three groups created from these vertices.

- The common oxygen atoms are represented by the vertices of the form $v_{2,1}$ which is at distance from all other vertices and hence $d_{CS(2)}(v_{2,1}) = 6$.
- The nonshared oxygen atoms are represented by the vertices $v_{1,1}, v_{1,2}, v_{2,2}$ and $v_{3,1}$. Corresponding to each of these vertices there are 3 vertices with the distance 1 and the remaining 3 vertices with the distances 2. Hence, $d_{CS(2)}(v_{1,1}) = 3(1) + 3(2) = 9 = v_{1,2} = v_{2,2} = v_{3,1}$.
- The nonshared silicon atoms are represented by the vertices of the form $v_{1,3}, v_{2,3}$. It is similar with the previous case and hence $d_{CS(2)}(v_{1,3}) = 9 = v_{2,3}$. Now, the exponential Wiener index of $CS(2)$ is

$$\begin{aligned} EW [CS(2)] &= \frac{1}{2} \sum_{u \in V[CS(2)]} e^{d_{CS(2)}(u)} \\ &= \frac{1}{2} (e^6 + 4e^9 + 2e^9) \\ &= \frac{e^6}{2} (1 + 6e^3). \end{aligned}$$

The multiplicative exponential Wiener index of $CS(2)$ is

$$\begin{aligned} \prod EW [CS(2)] &= \frac{1}{2} \prod_{u \in V[CS(2)]} e^{d_{CS(2)}(u)} \\ &= \frac{1}{2} (e^6 e^{4(9)} e^{2(9)}) \\ &= \frac{1}{2} e^{60}. \end{aligned}$$

□

Theorem 2.3 For the line graphs $L[CS(2)]$ of pyro silicate networks $CS(2)$, the exponential Wiener index is $EW \{L[CS(2)]\} = 3e^{15} (1 + e^6)$ and the multiplicative exponential Wiener index is $\prod EW \{L[CS(2)]\} = \frac{1}{2}e^{216}$.

Proof There are 12 vertices in the line graphs $L[CS(2)]$ of pyro silicate networks $CS(2)$. There are two groups created from these vertices of which the first group contains 6 vertices, say $ve_{i,1}, ve_{i,2}, ve_{i,3}, i = 1, 2$ and the second group contains 6 vertices, say $ve_{i,4}, ve_{i,5}, ve_{i,6}, i = 1, 2$.

- Now, any vertex $ve_{i,j}, i = 1, 2, j=1, 2, 3$, (i) There are four vertices with distance 1 and one vertex with distance 2 within the set of vertices $\{ve_{i,k}, k=1, 2, 3, 4, 5, 6, k \neq j\}$, (ii) The vertices $ve_{2,l}, i \neq 2, l=1, 2, 3$, have the distances 2, (iii) The vertices $ve_{2,l}, i \neq 2, l=4, 5, 6$, have the distances 3, (iv) The vertices $ve_{1,l}, i \neq 1, l=1, 2, 3$, have the distances 2, (v) The vertices $ve_{1,l}, i \neq 1, l=4, 5, 6$, have the distances 1. Hence, $d_{L[CS(2)]}(ve_{1,j}) = 4+2+3(2) + 3(3) = 21$, $d_{L[CS(2)]}(ve_{2,j}) = 4+2+3(1) + 3(2) = 15$
- Now, any vertex $ve_{i,j}, i = 1, 2, j=4, 5, 6$, (i) There are four vertices with distance 1 and one vertex with distance 2 within the set of vertices $\{ve_{i,k}, k=1, 2, 3, 4, 5, 6, k \neq j\}$, (ii) The vertices $ve_{2,l}, i \neq 2, l=1, 2, 3$, have the distances 1, (iii) The vertices $ve_{2,l}, i \neq 2, l=4, 5, 6$, have the distances 2, (iv) The vertices $ve_{1,l}, i \neq 1, l=1, 2, 3$, have the distances 3, (v) The vertices $ve_{1,l}, i \neq 1, l=4, 5, 6$, have the distances 2. Hence, $d_{L[CS(2)]}(ve_{1,j}) = 4+2+3(1) + 3(2) = 15$, $d_{L[CS(2)]}(ve_{2,j}) = 4+2+3(2) + 3(3) = 21$. Hence, the exponential Wiener index of $L[CS(n)]$ is $EW \{L[CS(2)]\} = \frac{1}{2} \sum_{u \in V\{L[CS(2)]\}} e^{d_{L[CS(2)]}(u)} = \frac{1}{2} (3e^{15} + 3e^{21} + 3e^{15} + 3e^{21}) = 3e^{15} (1 + e^6)$ and the multiplicative exponential Wiener index of $L[CS(n)]$ is $\prod EW \{L[CS(2)]\} = \frac{1}{2} \prod_{u \in V\{L[CS(2)]\}} e^{d_{L[CS(2)]}(u)} = \frac{1}{2} (e^{3(15)} e^{3(21)} e^{3(15)} e^{3(21)}) = \frac{1}{2} e^{216}$. □

Cyclic silicates

Cyclic linkage of three or more tetrahedral SiO_4^{4-} units results in the formation of $(SiO_3)_n^{2n-}$ ions, which are present in cyclic silicates. Here two oxygen atoms are shared by each unit with other units. The cyclic chain silicate's structure and its line graph is depicted below (Fig. 4 and 5).

Theorem 2.4 For the cyclic chain silicate networks $CS(n)$, the exponential Wiener index is $EW [CS(n)] = \frac{n}{2} \left[\begin{aligned} &e^{(\lfloor \frac{n-1}{2} \rfloor + 1)(2+3\lfloor \frac{n}{2} \rfloor)} \\ &+ 2e^{(\lfloor \frac{n}{2} \rfloor + 1)(2+3\lfloor \frac{n+1}{2} \rfloor) - 3} \end{aligned} \right]$ and the multiplicative exponential Wiener index is $\prod EW [CS(n)] = \frac{1}{2} e^{n[8\lfloor \frac{n+1}{2} \rfloor + 4\lfloor \frac{n}{2} \rfloor + 9\lfloor \frac{n+1}{2} \rfloor - 2]}$.

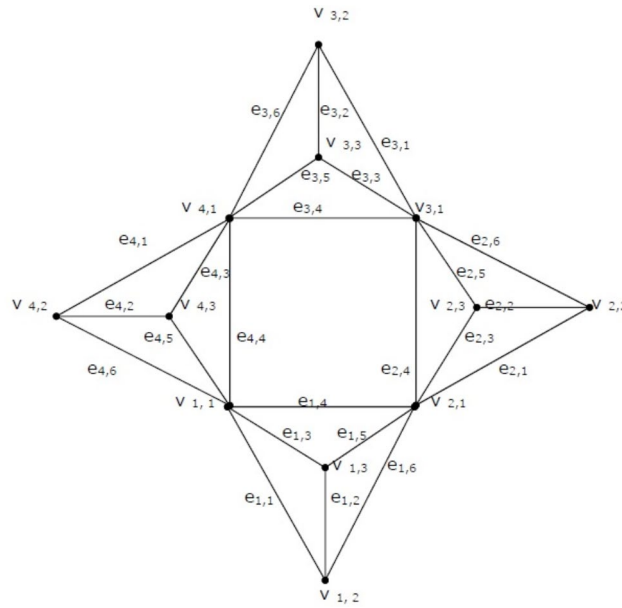


Figure 4. Cyclic chain silicate structure $CS(4)$.

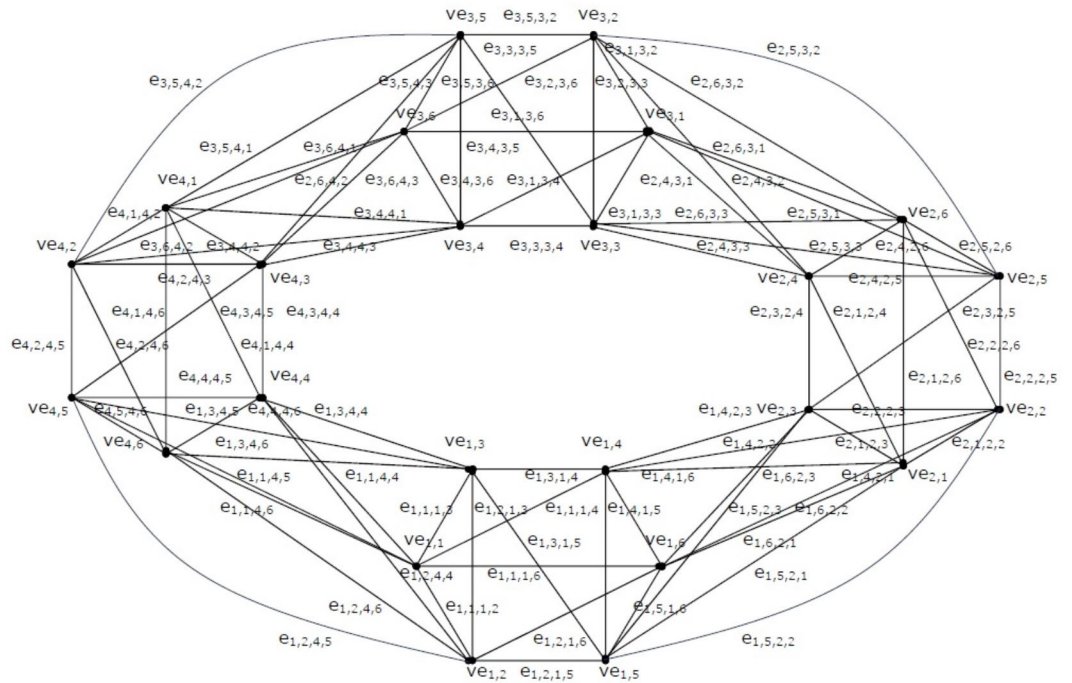


Figure 5. Line graph of cyclic chain silicate structure $L(CS(4))$.

Proof There are $3n$ vertices in the simple chain silicate network $CS(n)$. There are three groups created from these vertices.

- (a) The common oxygen atoms are represented by the vertices of the form $v_{i,1}$, $1 \leq i \leq n$. Corresponding to each $v_{i,1}$, the remaining $3n - 1$ vertices can be partitioned into $\lfloor \frac{n-1}{2} \rfloor + 1$ groups, each group contains 6 vertices except the last group which contains either 2 vertices or 5 vertices with the distances 1, 2, 3, ..., $\lfloor \frac{n-1}{2} \rfloor$, $\lfloor \frac{n-1}{2} \rfloor$. Hence, $d_{CS(n)}(v_{i,1}) = 6 \sum_{k=1}^{\lfloor \frac{n-1}{2} \rfloor} k + \{2 + 3[\lfloor \frac{n}{2} \rfloor - \lfloor \frac{n-1}{2} \rfloor]\} (\lfloor \frac{n-1}{2} \rfloor + 1) = 6 \left(\frac{\lfloor \frac{n-1}{2} \rfloor (\lfloor \frac{n-1}{2} \rfloor + 1)}{2} \right) + 2 (\lfloor \frac{n-1}{2} \rfloor + 1) + 3 \lfloor \frac{n}{2} \rfloor (\lfloor \frac{n-1}{2} \rfloor + 1) - 3 \lfloor \frac{n-1}{2} \rfloor (\lfloor \frac{n-1}{2} \rfloor + 1) = (\lfloor \frac{n-1}{2} \rfloor + 1) (2 + 3 \lfloor \frac{n}{2} \rfloor)$.

- (b) The nonshared oxygen atoms are represented by the vertices of the form $v_{i,2}, 1 \leq i \leq n$. Corresponding to each $v_{i,2}$, three vertices $v_{i,1}, v_{i,3}$ and $v_{i+1,1}$ or $v_{1,1}$ with the distance 1 and the remaining $3n - 4$ vertices can be partitioned into $\lfloor \frac{n-1}{2} \rfloor$ groups, each group contains 6 vertices except the last group which contains either 2 vertices or 5 vertices with the distances 2, 3, ..., $\lfloor \frac{n}{2} \rfloor, \lfloor \frac{n}{2} \rfloor$ and $n \geq 4$. For, $n = 3$, there is only one group with 5 vertices each with distance 2 other than the vertices $v_{i,1}, v_{i,3}$ and $v_{i+1,1}$ or $v_{1,1}$. Hence, $d_{CS(n)}(v_{i,2}) = 3(1) + 6 \sum_{k=2}^{\lfloor \frac{n}{2} \rfloor} k + \{2 + 3[\lfloor \frac{n+1}{2} \rfloor - \lfloor \frac{n}{2} \rfloor]\} (\lfloor \frac{n}{2} \rfloor + 1) = 3 + 6 \left(\frac{\lfloor \frac{n}{2} \rfloor (\lfloor \frac{n}{2} \rfloor + 1)}{2} \right) - 6 + 2(\lfloor \frac{n}{2} \rfloor + 1) + 3 \lfloor \frac{n+1}{2} \rfloor (\lfloor \frac{n}{2} \rfloor + 1) - 3 \lfloor \frac{n}{2} \rfloor (\lfloor \frac{n}{2} \rfloor + 1) = (\lfloor \frac{n}{2} \rfloor + 1) (2 + 3 \lfloor \frac{n+1}{2} \rfloor) - 3$.
- (c) The nonshared silicon atoms are represented by the vertices of the form $v_{i,3}, 1 \leq i \leq n$. It is similar with the previous case and hence $d_{CS(n)}(v_{i,3}) = (\lfloor \frac{n}{2} \rfloor + 1) (2 + 3 \lfloor \frac{n+1}{2} \rfloor) - 3$. Now, the exponential Wiener index of $CS(n)$ is

$$\begin{aligned} EW[CS(n)] &= \frac{1}{2} \sum_{u \in V[CS(n)]} e^{d_{CS(n)}(u)} \\ &= \frac{1}{2} \left[\sum_{i=1}^n e^{d_{CS(n)}(v_{i,1})} + \sum_{i=1}^n e^{d_{CS(n)}(v_{i,2})} + \sum_{i=1}^n e^{d_{CS(n)}(v_{i,3})} \right] \\ &= \frac{1}{2} \left[\sum_{i=1}^n e^{(\lfloor \frac{n-1}{2} \rfloor + 1)(2+3 \lfloor \frac{n}{2} \rfloor)} + \sum_{i=1}^n e^{(\lfloor \frac{n}{2} \rfloor + 1)(2+3 \lfloor \frac{n+1}{2} \rfloor) - 3} + \sum_{i=1}^n e^{(\lfloor \frac{n}{2} \rfloor + 1)(2+3 \lfloor \frac{n+1}{2} \rfloor) - 3} \right] \\ &= \frac{1}{2} \left[\sum_{i=1}^n e^{(\lfloor \frac{n-1}{2} \rfloor + 1)(2+3 \lfloor \frac{n}{2} \rfloor)} + 2 \sum_{i=1}^n e^{(\lfloor \frac{n}{2} \rfloor + 1)(2+3 \lfloor \frac{n+1}{2} \rfloor) - 3} \right] \\ &= \frac{n}{2} \left[e^{(\lfloor \frac{n-1}{2} \rfloor + 1)(2+3 \lfloor \frac{n}{2} \rfloor)} + 2e^{(\lfloor \frac{n}{2} \rfloor + 1)(2+3 \lfloor \frac{n+1}{2} \rfloor) - 3} \right]. \end{aligned}$$

The multiplicative exponential Wiener index of $CS(n)$ is

$$\begin{aligned} \prod EW[CS(n)] &= \frac{1}{2} \prod_{u \in V[CS(n)]} e^{d_{CS(n)}(u)} \\ &= \frac{1}{2} \left[\prod_{i=1}^n e^{d_{CS(n)}(v_{i,1})} \times \prod_{i=1}^n e^{d_{CS(n)}(v_{i,2})} \times \prod_{i=1}^n e^{d_{CS(n)}(v_{i,3})} \right] = \frac{1}{2} \left[\prod_{i=1}^n e^{(\lfloor \frac{n-1}{2} \rfloor + 1)(2+3 \lfloor \frac{n}{2} \rfloor)} \times \prod_{i=1}^n e^{(\lfloor \frac{n}{2} \rfloor + 1)(2+3 \lfloor \frac{n+1}{2} \rfloor) - 3} \times \prod_{i=1}^n e^{(\lfloor \frac{n}{2} \rfloor + 1)(2+3 \lfloor \frac{n+1}{2} \rfloor) - 3} \right] \\ &= \frac{1}{2} e^{\left[\sum_{i=1}^n (\lfloor \frac{n-1}{2} \rfloor + 1) (2 + 3 \lfloor \frac{n}{2} \rfloor) + 2 \sum_{i=1}^n (\lfloor \frac{n}{2} \rfloor + 1) (2 + 3 \lfloor \frac{n+1}{2} \rfloor) - 3 \right]} \\ &= \frac{1}{2} e^{n[8 \lfloor \frac{n+1}{2} \rfloor + 4 \lfloor \frac{n}{2} \rfloor + 9 \lfloor \frac{n}{2} \rfloor \lfloor \frac{n+1}{2} \rfloor - 2]}. \end{aligned}$$

□

Theorem 2.5 For the line graphs $L[CS(n)]$ of cyclic silicate networks $CS(n)$, the exponential Wiener index is $EW\{L[CS(n)]\} = 3ne^{3(n^2+1)}$ and the multiplicative exponential Wiener index is $\prod EW\{L[CS(n)]\} = \frac{1}{2}e^{18n(n^2+1)}$.

Proof There are $6n$ vertices in the line graphs $L[CS(n)]$ of cyclic silicate networks $CS(n)$. They are $ve_{i,1}, ve_{i,2}, ve_{i,3}, ve_{i,4}, ve_{i,5}, ve_{i,6}, i = 1, 2, \dots, n$. Now, any vertex $ve_{i,j}, i = 1$ to $n, j = 1, 2, 3, 4, 5, 6$ (i) There are four vertices with distance 1 and one vertex with distance 2 within the set of vertices $\{ve_{i,k}, k = 1, 2, 3, 4, 5, 6, k \neq j\}$, (ii) There are $n - 1$ sets containing 3 vertices such that all vertices in each group with the distances 1, 2, 3, ..., $n - 1$ in one side and (iii) There are $n - 1$ sets containing 3 vertices such that all vertices in each group with the distances 2, 3, ..., n in the other side. Hence, $d_{L[CS(n)]}(ve_{i,j}) = 3 \left(\sum_{k=1}^{n-1} k \right) + 3 \left(\sum_{k=2}^n k \right) + 4 + 2 = 3 \left[\frac{(n-1)n}{2} \right]$

$$+ 3 \left[\binom{n(n+1)}{2} - 1 \right] + 6 = 3(n^2 + 1). \text{ Hence, the exponential Wiener index of } L[CS(n)] \text{ is } EW\{L[CS(n)]\} = \frac{1}{2} \sum_{u \in V\{L[CS(n)]\}} e^{d_{L[CS(n)]}(u)} = \frac{1}{2} \left[\sum_{i=1}^n \sum_{j=1}^6 e^{d_{L[CS(n)]}(ve_{i,j})} \right] = \frac{1}{2} \left[\sum_{i=1}^n \sum_{j=1}^6 e^{3(n^2+1)} \right] = \frac{6n}{2} e^{3(n^2+1)} = 3ne^{3(n^2+1)}.$$

The multiplicative exponential Wiener index of $L[CS(n)]$ is $\prod EW\{L[CS(n)]\} = \frac{1}{2} \prod_{u \in V\{L[CS(n)]\}} e^{d_{L[CS(n)]}(u)} = \frac{1}{2} \left[\prod_{i=1}^n \prod_{j=1}^6 e^{d_{L[CS(n)]}(ve_{i,j})} \right] = \frac{1}{2} \left[\prod_{i=1}^n \prod_{j=1}^6 e^{3(n^2+1)} \right] = \frac{1}{2} e^{18n(n^2+1)}. \square$

Single chain silicate networks (or pyroxenes)

By sharing oxygen atoms on each tetrahedral's two corners, single chain silicates are created. Single chain silicate has the generic formula $(SiO_3)_n^{2n-}$. Spodumene $LiAl(SiO_3)_2$, Diopside- $CaMg(SiO_3)_2$ and Wollastonite $Ca_3(SiO_3)_3$ are three straightforward examples. Tetrahedra in single chain silicates exhibit a zigzag pattern. Figure 6 is a diagram of single chain silicate's structure and its line graph in generic form:

Theorem 2.6 For the single chain silicate networks $CS(n)$, the exponential Wiener index is $EW[CS(n)] =$

$$\frac{1}{2} e^{\frac{3}{2}n(n+1)} \left[2 + e^{3(n+1)} \sum_{i=2}^n e^{\frac{3}{2}[2i^2-2ni-4i]} + 2e^{3n} \sum_{i=1}^n e^{\frac{3}{2}[2i^2-2ni-2i]} \right] \text{ and the multiplicative exponential Wiener index is } \prod EW[CS(n)] = \frac{1}{2} e^{3n^2(n+1)}.$$

Proof There are $3n + 1$ vertices in the single chain silicate network $CS(n)$. There are four groups created from these vertices.

- (a) The first and last vertices $v_{1,1}$ and $v_{n+1,1}$ that correspond to the oxygen atoms that are not shared. Both of these two vertices have 3 vertices each with the distances 1, 2, 3, ..., n . Hence, $d_{CS(n)}(v_{1,1}) = d_{CS(n)}(v_{n+1,1}) = 3 \sum_{k=1}^n k = 3 \left[\frac{n(n+1)}{2} \right]$.
- (b) The common oxygen atoms are represented by the vertices of the form $v_{i,1}$, $2 \leq i \leq n$. The vertex $v_{i,1}$ is with the distance (i) 1 from the vertices $v_{i,2}$, $v_{i,3}$ and $v_{i+1,1}$, (ii) $i - k$ from the vertices $v_{k,1}$, $v_{k,2}$ and $v_{k,3}$ for $1 \leq k \leq i - 1$ and (iii) $k - i + 1$ from the vertices $v_{k,2}$, $v_{k,3}$ and $v_{k+1,1}$ for $i + 1 \leq k \leq n$. Hence,

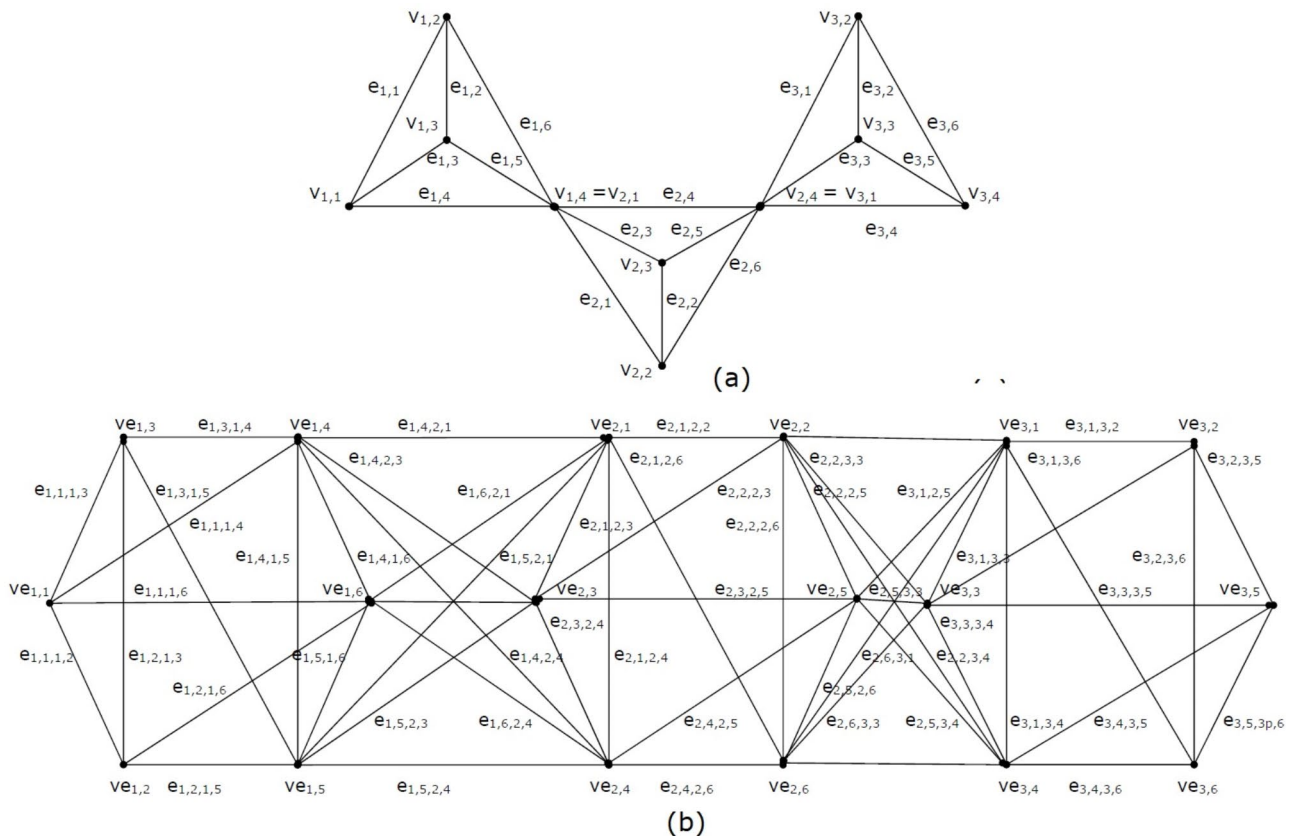


Figure 6. (a) Single chain silicate network $CS(3)$, (b) its line graph $L(CS(3))$.

- $d_{CS(n)}(v_{i,1}) = 3 \sum_{i=1}^{i-1} (i-k) + 3 + 3 \sum_{k=i+1}^n (k-i+1) = 3 \left[\frac{(i-1)i}{2} - \frac{(i-k-1)(i-k)}{2} \right] + 3 + 3 \left[\frac{(n-i+1)(n-i+2)}{2} - 1 \right]$
 $= \frac{3}{2} [n^2 - 2ni + 3n + 2i^2 - 4i + 2]$.
- (c) The non-shared oxygen atoms are represented by the vertices of the type $v_{i,2}$, $1 \leq i \leq n$. The vertex $v_{i,2}$ is with the distance (i) 1 from the vertices $v_{i,1}$, $v_{i,3}$ and $v_{i+1,1}$, (ii) $i-k+1$ from the vertices $v_{k,2}$, $v_{k,3}$ and $v_{k-1,1}$ for $1 \leq k \leq i-1$ and (iii) $k-i+1$ from the vertices $v_{k,2}$, $v_{k,3}$ and $v_{k+1,1}$ for $i+1 \leq k \leq n$. Hence, $d_{CS(n)}(v_{i,2}) = 3 \sum_{i=1}^{i-1} (i-k+1) + 3 + 3 \sum_{k=i+1}^n (k-i+1) = 3 \left[\frac{i(i+1)}{2} - 1 \right] + 3 + 3 \left[\frac{(n-i+1)(n-i+2)}{2} - 1 \right]$
 $= \frac{3}{2} [n^2 - 2ni + 3n + 2i^2 - 2i]$.
- (d) The silicate atoms are represented by the vertices of the type $v_{i,3}$, $1 \leq i \leq n$. The vertex $v_{i,3}$ is with the distance (i) 1 from the vertices $v_{i,1}$, $v_{i,2}$ and $v_{i+1,1}$, (ii) $i-k+1$ from the vertices $v_{k,2}$, $v_{k,3}$ and $v_{k-1,1}$ for $1 \leq k \leq i-1$ and (iii) $k-i+1$ from the vertices $v_{k,2}$, $v_{k,3}$ and $v_{k+1,1}$ for $i+1 \leq k \leq n$. Hence, $d_{CS(n)}(v_{i,3}) = 3 \sum_{k=1}^{i-1} (i-k+1) + 3 + 3 \sum_{k=i+1}^n (k-i+1) = 3 \left[\frac{i(i+1)}{2} - 1 \right] + 3 + 3 \left[\frac{(n-i+1)(n-i+2)}{2} - 1 \right]$
 $= \frac{3}{2} [n^2 - 2ni + 3n + 2i^2 - 2i]$. Now, the exponential Wiener index of $CS(n)$ is

$$EW [CS(n)] = \frac{1}{2} \sum_{u \in V[CS(n)]} e^{d_{CS(n)}(u)}$$

$$e^{d_{CS(n)}(u)} = \frac{1}{2} \left[e^{d_{CS(n)}(v_{1,1})} + e^{d_{CS(n)}(v_{n+1,1})} + \sum_{i=2}^n e^{d_{CS(n)}(v_{i,1})} \right]$$

$$+ \sum_{i=1}^n e^{d_{CS(n)}(v_{i,2})} + \sum_{i=1}^n e^{d_{CS(n)}(v_{i,3})}$$

$$= \frac{1}{2} \left[e^{3 \left[\frac{n(n+1)}{2} \right]} + e^{3 \left[\frac{n(n+1)}{2} \right]} + \sum_{i=2}^n e^{\frac{3}{2} [n^2 - 2ni + 3n + 2i^2 - 4i + 2]} \right]$$

$$+ \sum_{i=1}^n e^{\frac{3}{2} [n^2 - 2ni + 3n + 2i^2 - 2i]} + \sum_{i=1}^n e^{\frac{3}{2} [n^2 - 2ni + 3n + 2i^2 - 2i]}$$

$$= \frac{1}{2} e^{\frac{3}{2} n(n+1)} \left[2 + e^{3(n+1)} \sum_{i=2}^n e^{\frac{3}{2} [2i^2 - 2ni - 4i]} + 2e^{3n} \sum_{i=1}^n e^{\frac{3}{2} [2i^2 - 2ni - 2i]} \right].$$

The multiplicative exponential Wiener index of $CS(n)$ is

$$\prod EW [CS(n)] = \frac{1}{2} \prod_{u \in V[CS(n)]} e^{d_{CS(n)}(u)}$$

$$= \frac{1}{2} \left[e^{d_{CS(n)}(v_{1,1})} \times e^{d_{CS(n)}(v_{n+1,1})} \times \prod_{i=2}^n e^{d_{CS(n)}(v_{i,1})} \right]$$

$$\times \prod_{i=1}^n e^{d_{CS(n)}(v_{i,2})} \times \prod_{i=1}^n e^{d_{CS(n)}(v_{i,3})}$$

$$= \frac{1}{2} \left[e^{3 \left[\frac{n(n+1)}{2} \right]} \times e^{3 \left[\frac{n(n+1)}{2} \right]} \times \prod_{i=2}^n e^{\frac{3}{2} [n^2 - 2ni + 3n + 2i^2 - 4i + 2]} \right]$$

$$\times \prod_{i=1}^n e^{\frac{3}{2} [n^2 - 2ni + 3n + 2i^2 - 2i]} \times \prod_{i=1}^n e^{\frac{3}{2} [n^2 - 2ni + 3n + 2i^2 - 2i]}$$

$$= \frac{1}{2} e^{\left[3 \left[\frac{n(n+1)}{2} \right] + 3 \left[\frac{n(n+1)}{2} \right] \right.}$$

$$\left. + \frac{3}{2} \sum_{i=2}^n [n^2 - 2ni + 3n + 2i^2 - 4i + 2] \right.}$$

$$\left. + \frac{3}{2} \sum_{i=1}^n [n^2 - 2ni + 3n + 2i^2 - 2i] \right.}$$

$$\left. + \frac{3}{2} \sum_{i=1}^n [n^2 - 2ni + 3n + 2i^2 - 2i] \right]$$

$$= \frac{1}{2} e^{\left[3 [n(n+1)] + \frac{3}{2} (n-1) (n^2 + 3n + 2) - 3n \left[\frac{n(n+1)}{2} - 1 \right] \right.}$$

$$\left. + 3 \left[\frac{n(n+1)(2n+1)}{6} - 1 \right] - 6 \left[\frac{n(n+1)}{2} - 1 \right] + 3n (n^2 + 3n) \right.}$$

$$\left. - 6n \left[\frac{n(n+1)}{2} \right] + 6 \left[\frac{n(n+1)(2n+1)}{6} \right] - 6 \left[\frac{n(n+1)}{2} \right] \right]$$

$$= \frac{1}{2} e^{3n^2(n+3)}$$

□

Theorem 2.7 For the line graphs $L[CS(n)]$ of single chain silicate networks $CS(n)$, the exponential Wiener index is $EW \{L[CS(n)]\} = \frac{3}{2}e^{3(2n^2+n+1)} \left[e^{6(n+1)} \sum_{i=1}^n e^{3(4i^2-6i-4ni)} + \sum_{i=1}^n e^{3(4i^2-2i-4ni)} \right]$ and the multiplicative exponential Wiener index is $\prod EW \{L[CS(n)]\} = \frac{1}{2}e^{12n(2n^2+1)}$.

Proof There are $6n$ vertices in the line graphs $L[CS(n)]$ of single chain silicate networks $CS(n)$. There are two groups created from these vertices of which the first group contains $3n$ vertices, say $ve_{i,1}, ve_{i,2}, ve_{i,3}, i = 1, 2, \dots, n$ and the second group contains $3n$ vertices, say $ve_{i,4}, ve_{i,5}, ve_{i,6}, i = 1, 2, \dots, n$.

- (a) Now, any vertex $ve_{i,j}, i = 1$ to $n, j=1,2,3$, (i) There are four vertices with distance 1 and one vertex with distance 2 within the set of vertices $\{ve_{i,k}, k = 1, 2, 3, 4, 5, 6, k \neq j\}$, (ii) The vertices $ve_{k,l}, k = 1$ to $i - 1, l=1,2,3$, have the distances $2(k - i)$, (iii) The vertices $ve_{k,l}, k = 1$ to $i - 1, l=4,5,6$, have the distances $2(k - i) - 1$, (iv) The vertices $ve_{k,l}, k = i + 1$ to $n, l=1,2,3$, have the distances $2(k - i)$, (v) The vertices $ve_{k,l}, k = i + 1$ to $n, l=4,5,6$, have the distances $2(k - i) + 1$. Hence, $d_{L[CS(n)]}(ve_{i,j}) = 3 \sum_{k=1}^{i-1} [2(i - k)] + 3 \sum_{k=1}^{i-1} [2(i - k) - 1] + 4 + 2 + 3 \sum_{k=i+1}^n [2(k - i)] + 3 \sum_{k=i+1}^n [2(k - i) + 1] = 6 \left[\frac{(i-1)i}{2} \right] + 3(i - 1)^2 + 6 + 6 \left[\frac{(n-i)(n-i+1)}{2} \right] + 3[(n - i + 1)^2 - 1] = 3(4i^2 - 6i + 3 + 2n^2 - 4ni + 3n)$.
- (b) Now, any vertex $ve_{i,j}, i = 1$ to $n, j=4,5,6$, (i) There are four vertices with distance 1 and one vertex with distance 2 within the set of vertices $\{ve_{i,k}, k = 1, 2, 3, 4, 5, 6, k \neq j\}$, (ii) The vertices $ve_{k,l}, k = 1$ to $i - 1, l=1,2,3$, have the distances $2(i - k) + 1$, (iii) The vertices $ve_{k,l}, k = 1$ to $i - 1, l=4,5,6$, have the distances $2(i - k)$, (iv) The vertices $ve_{k,l}, k = i + 1$ to $n, l=1,2,3$, have the distances $2(k - i) - 1$, (v) The vertices $ve_{k,l}, k = i + 1$ to $n, l=4,5,6$, have the distances $2(k - i)$. Hence, $d_{L[CS(n)]}(ve_{i,j}) = 3 \sum_{k=1}^{i-1} [2(i - k) + 1] + 3 \sum_{k=1}^{i-1} [2(i - k)] + 4 + 2 + 3 \sum_{k=i+1}^n [2(k - i) - 1] + 3 \sum_{k=i+1}^n [2(k - i)] = 3(i^2 - 1) + 6 \left[\frac{(i-1)i}{2} \right] + 6 + 3(n - i)^2 + 6 \left[\frac{(n-i)(n-i+1)}{2} \right] = 3(4i^2 - 2i + 1 + 2n^2 - 4ni + n)$. Hence, the exponential Wiener index of $L[CS(n)]$ is

$$\begin{aligned} EW \{L[CS(n)]\} &= \frac{1}{2} \sum_{u \in V\{L[CS(n)]\}} e^{d_{L[CS(n)]}(u)} \\ &= \frac{1}{2} \left[3 \sum_{i=1}^n e^{d_{L[CS(n)]}(ve_{i,1})} + 3 \sum_{i=1}^n e^{d_{L[CS(n)]}(ve_{i,4})} \right] \\ &= \frac{3}{2} \left[\sum_{i=1}^n e^{3(4i^2-6i+3+2n^2-4ni+3n)} + \sum_{i=1}^n e^{3(4i^2-2i+1+2n^2-4ni+n)} \right] \\ &= \frac{3}{2} \left[e^{3(2n^2+3n+3)} \sum_{i=1}^n e^{3(4i^2-6i-4ni)} + e^{3(2n^2+n+1)} \sum_{i=1}^n e^{3(4i^2-2i-4ni)} \right] \\ &= \frac{3}{2} e^{3(2n^2+n+1)} \left[e^{6(n+1)} \sum_{i=1}^n e^{3(4i^2-6i-4ni)} + \sum_{i=1}^n e^{3(4i^2-2i-4ni)} \right]. \end{aligned}$$

The multiplicative exponential Wiener index of $L[CS(n)]$ is

Topological indices	Graphs with n vertices	n=3	n=4	n=5
Exponential Wiener Index	Cyclic Silicates	2.6691×10^7	1.0597×10^{11}	1.0733×10^{15}
	Line Graph of Cyclic Silicates	9.6178×10^{13}	1.6912×10^{23}	1.1248×10^{35}
	Single Chain Silicates	2.0384×10^8	3.2114×10^{13}	1.0481×10^{20}
	Line Graph of Single Chain Silicates	3.7732×10^{30}	2.7342×10^{38}	2.5690×10^{60}
Multiplicative Exponential Wiener Index	Cyclic Silicates	4.0066×10^{46}	2.8539×10^{100}	1.2666×10^{182}
	Line Graph of Cyclic Silicates	1.6519×10^{234}		
	Single Chain Silicates	1.1342×10^{70}	4.1871×10^{145}	1.8865×10^{260}
	Line Graph of Single Chain Silicates	5.7068×10^{296}		

Table 1. Numerical values of exponential Wiener index and multiplicative Wiener index for the molecular graphs of cyclic silicates, single chain silicates and their line graphs.

$$\begin{aligned}
\prod EW \{L[CS(n)]\} &= \frac{1}{2} \prod_{u \in V\{L[CS(n)]\}} e^{d_{L[CS(n)]}(u)} \\
&= \frac{1}{2} \left(\prod_{i=1}^n e^{d_{L[CS(n)]}(ve_{i,1})} \right)^3 \left(\prod_{i=1}^n e^{d_{L[CS(n)]}(ve_{i,4})} \right)^3 \\
&= \frac{1}{2} \left(\prod_{i=1}^n e^{3(4i^2-6i+3+2n^2-4ni+3n)} \right)^3 \left(\prod_{i=1}^n e^{3(4i^2-2i+1+2n^2-4ni+n)} \right)^3 \\
&= \frac{1}{2} \left(e^{9 \sum_{i=1}^n (4i^2-6i+3+2n^2-4ni+3n)} \right) \left(e^{9 \sum_{i=1}^n (4i^2-2i+1+2n^2-4ni+n)} \right) \\
&= \frac{1}{2} e^{12n(2n^2+1)}.
\end{aligned}$$

□

The numerical values of exponential Wiener index and multiplicative exponential Wiener index for the molecular graphs of cyclic silicates, single chain silicates and their line graphs are given in the Table 1.

Conclusion

Any graph that depicts a particular molecular structure can be given a topological graph index, also known as a molecular descriptor. This index can be used to examine numerical data and discover more about specific physical properties of molecules. In the current study, we have determined the new topological index for a few silicate structures, including cyclic, single chain, and Pyro silicates. This index is known as the exponential Wiener index. It is expanded to include their line graphs as well. Chemical graph theory could be expanded in the future to encompass graphs related to the double chain silicate molecular structure. Additionally, the physical characteristics and biological activity characteristics of various silicate structures can be analyzed (QSPR analysis and QAPR analysis). This study paved the way to the investigation of these topological indices with the entropy, acentric factor, enthalpy of vaporization, and standard enthalpy of vaporization of corresponding silicate structures.

Data availability

All data generated or analysed during this study are included in this published article.

Received: 21 August 2024; Accepted: 25 October 2024

Published online: 08 November 2024

References

- Gutman, I. & Trinajstić, N. Graph theory and molecular orbitals. Total ϕ -electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **17**, 535–538 (1972).
- Gutman, I. I., Rucić, B., Trinajstić, N. & Wilcox, C.F. Graph theory and molecular orbitals. XII. Acyclic polyenes. *J. Chem. Phys.* **62**, 3399–3405 (1975).
- Estrada, E., Torres, L., Rodriguez, L. & Gutman, I. An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes. *Indian J. Chem.* **37A**, 849–855 (1998).
- Randic, M. Characterization of molecular branching. *J. Am. Chem. Soc.* **97**, 6609–6615 (1975).
- Todeschini, R. & Consonni, V. New local vertex invariants and molecular descriptors based on functions of the vertex degrees. *MATCH Commun. Math. Comput. Chem.* **64**, 359–372 (2010).
- Gutman, I. Multiplicative Zagreb indices of trees. *Bull. Soc. Math. Banja Luka* **18**, 17–23 (2011).
- Das, K.C., Yurttas, A., Togan, M., Cevik, A.S. & Cangul, I.N. The multiplicative Zagreb indices of graph operations. *J. Ineq. Appl.* **90** (2013).
- Wiener, H. Structural determination of paraffin boiling points. *J. Am. Chem. Soc.* **69**, 17–20 (1947).
- Dankelmann, P., Gutman, I., Mukwembi, S. & Swart, H. C. The edge-Wiener index of a graph. *Discrete Math.* **309**, 3452–3457 (2009).
- Karbasious, A. The Wiener index of a new class of carbon nanojunctions. *Sci. Iran.* **18**, 1623–1626 (2011).
- Klavzar, S. & Nadjafi-Arani, M.J. Wiener index in weighted graphs via unification of Θ^* -classes. *Eur. J. Comb.* **36**, 71–76 (2014).
- Liu, R., Du, X. U. E. & Jia, H. Wiener index on traceable and Hamiltonian graphs. *Bull. Aust. Math. Soc.* **94**, 362–372 (2016).
- Yang, L. Wiener index and traceable graphs. *Bull. Aust. Math. Soc.* **88**, 380–383 (2013).
- Kuang, M., Huang, G. & Deng, H. Some sufficient conditions for Hamiltonian property in terms of Wiener-type invariants. *Proc. Math. Sci.* **126**, 1–9 (2016).
- Jagadeesh, R., Rajesh Kanna, M.R. & Indumathi, R.S. Some results on topological indices of graphene. *Nanomater. Nanotechnol.* **6**, 1–6 (2016).
- Cai, G., M. Ye, G.D. & Yu, L.R. Hyper-Wiener index and Hamiltonicity of graphs. *Ars Comb.* **139**, 175–184 (2018).
- Jia, H., Liu, R. & Du, X. Wiener index and Harary index on Hamilton-connected and traceable graphs. *Ars Comb.* **141**, 53–62 (2018).
- Qiannan, Z., Ligong, W. & Yong, L. Wiener-type invariants and Hamiltonian properties of graphs. *Filomat* **33**, 4045–4058 (2019).
- Yu, G.D., Ren, L.F., Li, X.X. Wiener index, hyper-Wiener index, Harary index and Hamiltonicity properties of graphs. *Appl. Math.-A J. Chin. Univ.* **34**, 162–172 (2019).
- Cruz, R. & Rada, J. The path and the star as extremal values of vertex-degree-based topological indices among trees. *MATCH Commun. Math. Comput. Chem.* **82**, 715–732 (2019).
- Akgunes, N. & Aydin, B. Introducing new exponential Zagreb indices for graphs. *J. Math.* **2021**, 6675321 (2021).
- Ma, Y., Dehmer, M., Künzi, U.M., Tripathi, S., Ghorbani, M., Tao, J. & Emmert-Streib, F. The usefulness of topological indices. *Inf. Sci.* **606**, 143–151 (2022).

23. Spiro, S. The Wiener index of signed graphs. *Appl. Math. Comput.* **416**, 126755 (2022).
24. Gurgel, M.A. & Wakabayashi, Y. On k -leaf-connected graphs, *J. Comb. Theo., Series B*, **41**, 1–16 (1986).
25. Ao, G., Liu, R., Yuan, J. & Yu, G. Wiener-type invariants and k -leaf-connected graphs. *Bull. Malay. Math. Sci. Soc.* **46**, 10 (2023).
26. Akhmedjanova, M. et al. Wiener index and graphs, almost half of whose vertices satisfy soltés property. *Discrete Appl. Math.* **325**, 37–42 (2023).
27. Öztürk, E., Eryaar, E. & Abdiolu, C. Forgotten topological and Wiener indices of prime ideal sum graph of $Z(n)$. *Curr. Organ. Synth.* (2023). <https://doi.org/10.2174/1570179420666230606140448>.
28. Klavžar, S. & Romih, G.D. The cut method on hypergraphs for the Wiener index *J. Math. Chem.* **61**, 1592–1603 (2023).
29. Sheikh, U., Tahir, Q.U., Anjam, Y. N. & Pincak, R. Analysis of a productive topological index correlated to fullerenes' physical properties. *Symmetry* **15**(1), 58 (2023).
30. Jahanbani, A., Sheikholeslami, S. M. & Filipovski, S. Relations between the energy and topological indices of a graph. *Medit. J. Math.* **20**, 264 (2023).
31. Fernando, T. & Cao, T. Quantized interband topological index in two-dimensional systems. *Phys. Rev. B* **108**, L081111 (2023).
32. Zaman, S., Ahmed, W., Sakeena, A., Bahri Rasool, K. & Abebe Ashebo, M. Mathematical modeling and topological graph description of dominating David derived networks based on edge partitions. *Sci. Rep.* **13**, 15159 (2023).
33. Javid, M., Rehman, M. U. & Cao, J. Topological indices of rhombus type silicate and oxide networks. *Can. J. Chem.* **95**(2), 134–143 (2017).
34. Arockiaraj, M., Kavitha, S. R. J. & Balasubramanian, K. Vertex cut method for degree and distance-based topological indices and its applications to silicate networks. *J. Math. Chem.* **54**, 1728–1747 (2016).
35. Sarkar, P., De, N. & Pal, A. The (a, b) -Zagreb index of line graphs of subdivision graphs of some molecular structures. *Int. J. Math. Indus.* **12**(1), 2050006–9 (2020).
36. Sarkar, P. & Pal, A. General fifth M-Zagreb polynomials of benzene ring implanted in the P-type-surface in 2D network. *Biointerface Res. Appl. Chem.* **10**(6), 6881–6892 (2020).
37. Sarkar, P., De, N. & Pal, A. On some topological indices and their importance in chemical sciences: A comparative study. *Eur. Phys. J. Plus* **137**(195), 1–12 (2022).
38. Sarkar, P., De, N. & Pal, A. On some neighbourhood degree-based multiplicative topological indices and their applications. *Polycycl. Aromatic Compds.* **42**(10), 7738–7753 (2022).
39. Sarkar, P., De, N., Pal, A. & Cangul, I. N. Generalized Zagreb indices for some silicate networks. *J. Discrete Math. Sci. Cryptogr.* **27**(3), 929–944 (2024).
40. Dobrynin, Andrey A., Mel'nikov, Leonid S. & Index, Wiener. Line graphs and the cyclomatic number. *MATCH Commun. Math. Comput. Chem.* **53**, 209–214 (2005).
41. Bertz, S. H. Branching in graphs and molecules. *Discrete Appl. Math.* **19**, 65–83 (1988).
42. Bertz, S. H. & Wright, W. F. The graph theory approach to synthetic analysis: definition and application of molecular complexity and synthetic complexity. *Graph Theory Notes Newyork* **35**, 32–48 (1998).
43. Estrada, E., Guevara, N. & Gutman, I. Extension of edge connectivity index, relationships to line graph indices and QSPR applications. *J. Chem. Inf. Comput. Sci.* **38**, 428–431 (1998).
44. Gutman, I. & Estrada, E. Topological indices based on the line graph of the molecular graph. *J. Chem. Inf. Comput. Sci.* **36**, 541–543 (1996).
45. Gutman, I., Popovic, L., Mishra, B.K., Kaunar, M., Estrada, E. & Guevara, N. Application of line graphs in physical chemistry. Predicting surface tension of alkanes. *J. Serb. Chem. Soc.* **62**, 1025–1029 (1997).

Acknowledgements

We thank the anonymous reviewers for their careful reading of our manuscript and their many insightful comments and suggestions, which helped us in improving the quality of the manuscript. We thank SASTRA Deemed to be University for their financial and continuous support for our research work.

Author contributions

All authors equally contributed towards this work.

Declarations

Competing interests

The authors declare no competing interests. Acknowledgements: We thank the anonymous reviewers for their careful reading of our manuscript and their many insightful comments and suggestions, which helped us in improving the quality of the manuscript. We thank SASTRA Deemed to be University for their financial and continuous support for our research work.

Additional information

Correspondence and requests for materials should be addressed to K.K.

Reprints and permissions information is available at www.nature.com/reprints.

Publisher's note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Open Access This article is licensed under a Creative Commons Attribution-NonCommercial-NoDerivatives 4.0 International License, which permits any non-commercial use, sharing, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if you modified the licensed material. You do not have permission under this licence to share adapted material derived from this article or parts of it. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by-nc-nd/4.0/>.

© The Author(s) 2024