Computation of Weighted PI Index of Lexicographic product graphs and for Silicates Networks

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Abstract

The study of chemical compounds' molecular structures is one of the most cutting-edge uses of graph theory, along with computer science, nanochemistry, network design in electrical and electronic engineering, and the depiction of graphs in Google Maps. The degree and distance between vertices of a graph are the basis for examining topological indices. The formula for computing the Weighted Padmakar Ivan index (WPI) of a graph G is

$$PI_w(G) = \sum_{e \in E(G)} [(d_G(u) + d_G(v)][|V(G)| - N_G(e)].$$

Graph operations have become widely used in many engineering disciplines to create the intricate structure of networks. In this manuscript, we determained the Weighted PI index (WPI index) of the lexicographic product of a few classes of graphs and computation of WPI index of various silicate networks has done.

Keywords: Path; Cycle; Complete graph; Weighted PI Index; Lexicographic Product; Silicate network

1 Introduction

Graph theory has been significantly applied in the field of chemistry, especially for modelling chemical structures. Molecular structures in chemistry can be represented as graphs. This application has furnished chemists with a range of valuable tools, including topological indices. A real number connected to a graph called a topological index acts as a structural invariant that doesn't change under any graph automorphism. A variety of topological indices have been established, many of which are applied in the modelling of pharmaceutical, chemical and other molecular properties.

The Wiener index and PI index are two examples of topological indices that are essential in mathematical chemistry. Topological indices have been deployed in chemistry since Harold Wiener presented the Wiener index in 1947. This well-known descriptor is used to determine the physical properties of alkenes. The Wiener index measures graph distances in chemical structures. On the other hand, the PI index, introduced by Khadikar in 2000,[2] focuses on equidistant vertices or parallelism of edges, offering simplicity in calculation and discrimination in certain molecular graphs. These topological indices find diverse applications in assessing chemical characteristics, particularly in the context of Chemical Graph Theory, where weighted PI indices are employed for measuring the features of chemical compounds. Khadikar et al.[3] studied a Novel Padmakar Ivan Index and its Applications to QSPR/QSAR.

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Graph indices, such as the Padmakar Ivan, Weighted Padmakar Ivan index, play a crucial role as molecular parameters. Modern toxicology research involves predicting chemical toxicity based on molecular structures, where the PI index is employed to study the toxicity of nitrobenzene derivatives, contributing to quantitative structure-toxicity relationships. For zig-zag polyhex nanotubes Ashrafi et al. in[4–6] invetigated PI index , armchair polyhex nanotubes, polyhex nanotori. Deng et al. in[7] studied about the PI index of phenylenes. Vertex and edge Padmakar Ivan indices were calculated by Khalifeh et al. in[8] for Cartesian product graphs. You et al. in[10] read about the Weighted vertex Padmakar Ivan of Unicyclic Graphs, while the same for bicyclic graphs was focused on by Ma et al. in.[15] For Some Special Graphs Yan et al. in[13] investigated about the Weighted Vertex Padmakar Ivan Index.

In constructing large graphs from smaller graphs, product of graphs, particularly the cartesian product, direct product, strong product, lexicographic product and corona product are the significant standard products of graphs have proven valuable in designing interconnection networks. Weighted PI index is determined by Gopika et al. in[16] for tensor product and strong product of graphs whereas Weighted Padmakar Ivan index of corona product of graphs is explored by Pattabiraman et al. in.[12,14] Researchers have explored the minimum degree, maximum degree, equidistant vertices, vertex-connectivity and edge-connectivity of these product graphs.

Extensive research has been conducted on the lexicographic product. For certain classes of lexicographic product graphs the total chromatic number was studied in,[18] another noteworthy graph product in[17] Hemalatha et al. computed the Somber index of edge corona product of some classes of graphs. Many studies have been extensively done in[19–21] about graph theoretic approaches to fuzzy differential equations and deep learning-based techniques. It's important to observe that when considering isomorphism, the direct product adheres to the commutative law, whereas the lexicographic product of graphs do not exhibit the same.

2 Lexicographic Product

Let the two simple graphs be G and H. The lexicographic product of $G \circ H$ is constructed by the set of vertices $V(G)V(H)$ and an edge is represented as $[(g,h),(g',h')]$ precisely if $(g,g') \in E(G)$, in otherwords $g = g'$ and $(h,h') \in E(H)$. The lexicographic product is also termed as Graph substitution in[18] from G by the replacement of a copy H_g of H for every vertex g of G and connecting every vertex of H_g with all vertices of H'_g if $(g,g') \in E(G)$. As we discussed earlier eventhough the lexicographic product is not commutative, it is associative.

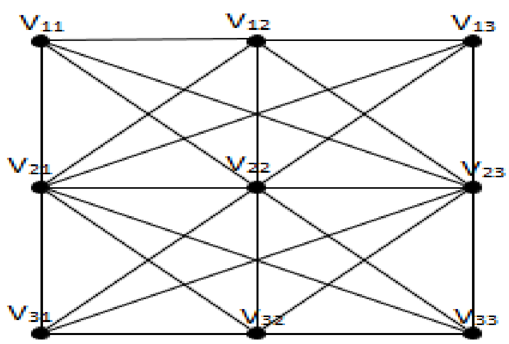

Figure 1: Lexicographic product $P_3 \circ P_3$

The *Weighted PI index(WPI)*, represented by PI_w, which is applied widely in the molecular chemistry is given by,

$$PI_w(G) = \sum_{e \in E(G)} [(d_G(u) + d_G(v)][|V(G)| - N_G(e)] \,,$$

where $N_G(e)$ represents the number of equidistant vertices for the edges of the graph G.

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Theorem 2.1. *The Weighted Padmakar Ivan index(WPI) of lexicographic product of a complete graph K_m with a path P_n is*

$$\begin{aligned} PI_w(K_m \circ P_n) &= 36m^2n + 8m^3n^2 - 40m^2n^2 - 16m^2 - 8m^3n - 72mn + 40mn^2 \\ &+52m - 4m^3n^3 - 2mn^3 + 32m^2n^3 + 2m^3n^4 - 4m^2n^4 + 2mn^4. \end{aligned}$$

Proof. Consider two simple graphs a complete graph K_m and a path P_n. Weighted Padmakar Ivan index for lexicographic product of a complete graph with a path is computed as follows:

Number of vertices and edges of K_m and P_n are m,n and $\frac{m(m-1)}{2}$, $n-1$ respectively. Also number of vertices in lexicographic product of a K_m with P_n is mn and edges is $m(n-1) + \frac{m(m-1)n^2}{2}$. Degree of the pendent vertices and non pendent vertices of path in lexicographic product graph is $1 + (m-1)n, 2 + (m-1)n$ respectively. Total number of edges are subdivided into three sets as E_1, E_2, E_3 based on their incidence with pendent vertices to pendent vertices, pendent vertices to Non-pendent vertices, Non-pendent vertices to Non-pendent vertices of P_n respectively. The sets E_1, E_2, E_3 have $2m(m-1)$, $2m(m-1)(n-2) + 2m$, $2m$, $\frac{m(m-1)(n-2)^2}{2} + m(n-3)$ number of edges respectively. Hence the overall edges of the graph is $\frac{m(m-1)n^2}{2} + m(n-1)$. Weighted PI index is one of the distance based topological indices which requires number of equidistant vertices$N_G(e)$. For each edge of the graph $N_G(e)$ is different depends on E_1, E_2, E_3. For the edges of E_1, $N_G(e)$ is $(m-2)n + 2$.Correspondingly for sets E_2, E_3 are $(m-2)n + 2$, $(m-2)n + 4$.

Weighted PI index is given by

$$\begin{aligned} PI_w(K_m \circ P_n) &= \sum_{e \in K_m \circ P_n} [d_{K_m \circ P_n}(u) + d_{K_m \circ P_n}(v)][|V(K_m \circ P_n| - N_{K_m \circ P_n}(e)] \\ PI_w(K_m \circ P_n) &= \sum_{uv \in E_1} [d_{K_m \circ P_n}(u) + d_{K_m \circ P_n}(v)][|V(K_m \circ P_n| - N_{K_m \circ P_n}(e)] \\ &+ \sum_{uv \in E_2} [d_{K_m \circ P_n}(u) + d_{K_m \circ P_n}(v)][|V(K_m \circ P_n| - N_{K_m \circ P_n} e)] \\ &+ \sum_{uv \in E_3} [d_{K_m \circ P_n}(u) + d_{K_m \circ P_n}(v)][|V(K_m \circ P_n| - N_{K_m \circ P_n}(e)]. \\ &= 2m(m-1)[2(1 + (m-1)n)][mn - (m-2)n - 2] \\ &+[2m(m-1)(n-2) + 2m][3 + 2(m-1)n][mn - (m-2)n - 2] \\ &+[\frac{m(m-1)(n-2)^2}{2} + m(n-3)][2(2 + (m-1)n)][mn - (m-2)n - 4]. \\ &= -52m^2n - 16m^3n^2 + 52m^2n^2 + 16m^2 + 8m^3n + 56mn \\ &-36mn^2 - 28m + 8m^3n^3 - 16m^2n^3 + 8mn^3 \\ &+(6mn - 10m + m^2n^2 - 4m^2n + 4m^2 - mn^2)(2 + (m-1)n)(2n-4). \end{aligned}$$

Therefore

$$\begin{aligned} PI_w(K_m \circ P_n) &= 36m^2n + 8m^3n^2 - 40m^2n^2 - 16m^2 - 8m^3n - 72mn + 40mn^2 \\ &+52m - 4m^3n^3 - 12mn^3 + 32m^2n^3 + 2m^3n^4 - 4m^2n^4 + 2mn^4. \end{aligned}$$

□

Theorem 2.2. *Let a path be P_m and a complete graph be K_n, then the Weighted Padmakar Ivan index of their lexicographic product is*
$PI_w(P_m \circ K_n) = -31n^4m + 26n^4 - 34n^3 + 35n^3m + 8n^2 + nm - 11n^2m + n^2m^2 + 9n^4m^2 - 6n^3m^2.$

Proof. As discussed in the previous theorems, to compute the WPI product of $PI_w(P_m \circ K_n)$ we require the following information. Edge set of $P_m \circ K_n$ is split up into four subsets depends on the connectivity with pendent and non-pendent copies of K_n the edges. In the lexicographic product graph, in place of all vertices

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of the path P_m a copy of K_n is replaced and all the vertices of one copy of K_n will be connected to all other vertices of the copies which follow the connectivity of the path P_m.

Hence we have number of edges and $N_G(e)$ belonging to pendent copies($uv \in K_n$ in pendent place) are $[n(n-1), (n-1)+n]$, non-pendent copies($uv \in K_n$ in pendent place) are $[\frac{(m-2)n(n-1)}{2}, (n-1)+2n]$ edges formed by connecting vertices of pendent copies to non-pendent copies are $[2n^2, 2(n-1)]$, edges of product between non-pendent to non-pendent copies are $[(m-3)n^2, 2(n-1)]$. Degree of the vertices in pendent copies is $2n-1$ and for non pendent copies is $3n-1$.

$$\begin{aligned} PI_w(P_m \circ K_n) &= \sum_{e \in P_m \circ K_n} [d_{P_m \circ K_n}(u) + d_{P_m \circ K_n}(v)][|V(P_m \circ K_n| - N_{P_m \circ K_n}(e)] \\ &= [n(n-1)][4n-2][mn-2n+1] + \frac{(m-2)n(n-1)}{2} \\ &\quad [6n-2][mn-3n+1] + [2n^2][5n-2][mn-2(n-1)] \\ &\quad +[(m-3)n^2][6n-2][mn-2(n-1)] \\ &= -31n^4m + 26n^4 - 34n^3 + 35n^3m + 8n^2 \\ &\quad +nm - 11n^2m + n^2m^2 + 9n^4m^2 - 6n^3m^2. \end{aligned}$$

□

Theorem 2.3. *Let P_m, C_n be a path and a cycle of m,n-vertices respectively. Then the WPI of lexicographic product of P_m with C_n is given by*

$$PI_w(P_m \circ C_n) = \begin{cases} -24n^2m + 24n^2 - 32n^3m + 36n^3 + 4n^2m^2 + 8n^3m^2 - 6n^4m + \\ \qquad 4n^4m^2; \text{n is even} \\ -28n^2m + 28n^2 - 32n^3m + 36n^3 + 4n^2m^2 - 4nm + 8n^3m^2 - \\ \qquad 6n^4m + 4n^4m^2; \text{n is odd.} \end{cases}$$

Proof. In the structure of the graph of lexicographic product of P_m with C_n contains mn number of vertices, $mn + (m-1)n^2$ number of edges. Considering the degrees of vertices we split the copies of cycle into two. One set lie in the place of pendent vertices and the other in the place of non-pendent vertices of P_m. Degree of the vertices of the copies in place of pendent vertices is $2+n$ and for copies in place of non-pendent vertices is $2+2n$.Number of equidistant vertices for edges of even cycle is n and for odd cycle is $n+1$. There are $2n+2n^2$ number of edges in copies lie on pendent places and $(m-2)n + (m-3)n^2$ edges in copies of non-pendent copies. Also the number of edges in pendent copies, non-pendent copies, pendent to non-pendent product edges, non-pendent to non-pendent product edges are $2n$, $(m-2)n$, $2n^2$, $(m-3)n^2$ respectively.

$$PI_w(P_m \circ C_n) = \sum_{e \in P_m \circ C_n} [d_{P_m \circ C_n}(u) + d_{P_m \circ C_n}(v)][|V(P_m \circ C_n| - N_{P_m \circ C_n}(e)].$$

Case (i). For n=even

$$\begin{aligned} PI_w(P_m \circ C_n) &= [2n][4+2n][mn-n] + [(m-2)n][4+4n][mn-2n] + [2n^2][4+3n][mn-4] \\ &+ [(m-3)n^2][4+4n][mn-4] \\ &= -24n^2m + 24n^2 - 32n^3m + 36n^3 + 4n^2m^2 + 8n^3m^2 - 6n^4m + 4n^4m^2. \end{aligned}$$

Case (ii). For n=odd

$$\begin{aligned} PI_w(P_m \circ C_n) &= [2n][4+2n][mn-n-1] + [(m-2)n][4+4n][mn-2n-1] \\ &+ [2n^2][4+3n][mn-4] + [(m-3)n^2][4+4n][mn-4] \\ &= -28n^2m + 28n^2 - 32n^3m + 36n^3 + 4n^2m^2 - 4nm + 8n^3m^2 - 6n^4m + 4n^4m^2. \end{aligned}$$

□

Theorem 2.4. *The WPI of lexicograpic product of C_m with P_n is computed as*

$$PI_w(C_m \circ P_n) = \begin{cases} -4m^2n^2 + 24mn - 6m^2n + 4m + 8m^2n^3 + 4m^2n^4 - 16mn^3; n = even \\ -4m^2n^2 + 4mn^2 + 30mn - 6m^2n + 4m + 8m^2n^3 - 24mn^3 \\ \qquad +4m^2n^4 - 4mn^4; n = odd. \end{cases} .$$

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Proof. In evaluation of WPI of lexicograpic product of C_m with P_n we require the following information. In C_m, P_n there are m, n and $m, n-1$ vertices and edges. In $C_m \circ P_n$ there are mn number of vertices and $m(n-1)+mn^2$ edges . Degree of pendent and non-pendent vertices of lexicograpic product graph is $2n+1$, $2n+2$ respectively, whereas $N_G(e)$ for every edge of the product graph is given by $2m + m[4(n-2)]$.
On the basis of valency the edge partition is E_1, E_2, E_3 where E_1 have edges connecting pendent vertices to pendent vertices, E_2 containing edges joining pendent vertices with non-pendent vertices whereas E_3 has edges associating non-pendent vertices with non-pendent vertices.The cardinality of E_1 is $4m$, for E_2 is $2m + 4m(n-2)$and for E_3 is $m(n-3) + m(n-2)^2$.
Hence

$$PI_w(C_m \circ P_n) = \sum_{e \in C_m \circ P_n} [d_{C_m \circ P_n}(u) + d_{C_m \circ P_n}(v)][|V(C_m \circ P_n)| - N_{C_m \circ P_n}(e)].$$

Case (i). For n is even

$$\begin{aligned} PI_w(C_m \circ P_n) &= 4m[4n+2][mn-2] + [2m+4m(n-2)][4n+3][mn-2] \\ &\quad +[m(n-3)+m(n-2)^2][4n+4][mn-4] \\ &= -4m^2n^2 + 24mn - 6m^2n + 4m + 8m^2n^3 + 4m^2n^4 - 16mn^3. \end{aligned}$$

Case (ii). For n is odd

$$\begin{aligned} PI_w(C_m \circ P_n) &= 4m[4n+2][mn-n-2] + [2m+4m(n-2)][4n+3][mn-2-n] \\ &\quad +[m(n-3)+m(n-2)^2][4n+4][mn-n-4] \\ &= -4m^2n^2 + 4mn^2 + 30mn - 6m^2n + 4m \\ &\quad +8m^2n^3 - 24mn^3 + 4m^2n^4 - 4mn^4. \end{aligned}$$

□

3 Chain and Cyclic Silicate Networks

The Earth's surface comprises silicon, oxygen, and aluminium as primary substances. Mostly in the form of silicates, silicon or oxygen accommodate in excess of 80 percent of the atoms in the solid crust. Tetrahedral units denoted by SiO_4, which are linked together in multiple designs, are the structural blocks of silicate minerals, which are composed of silicon and oxygen.[22,23] Approximately 95 percent of the earth's crust is made up of silicate minerals, such as silica.On the basis of the arrangement of tetrahedral units, the silicates are classified as orthosilicates, pyrosilicates, chain silicates, and cyclic silicates.Cyclic or ring silicates in which the SiO_4 tetrahedra are grouped in rings. Every tetrahedron forms closed loops or rings of varying diameters by sharing two of its oxygen atoms with two neighbouring tetrahedra. Rings in cyclic silicates can include varying numbers of tetrahedra; commonly, 3, 4, or 6 are termed three-membered rings, four-membered rings and six-membered rings respectively.

3.1 Applications of Silicates

Due to their multiple applications, silicates are vital for various industries. Their uses in construction, technology, agriculture, and healthcare are numerous and essential to contemporary living. Different silicates are employed in the building of materials, particularly glass and ceramics; silicates are also utilised in semiconductors and optoelectronics in the electronics industry, as well as for soil amendments in agriculture. Another silicate that has the perfect potential to vibrate at a high rhythmic frequency is quartz. Because of these qualities, quartz crystals are being used in watchmaking, pressure gauges, and radios. Silicates are used by industries to soften and purify waste water. In recognition of their smooth texture, absorbency, and shimmer effects, silicate minerals are widely used in cosmetics.

Theorem 3.1. *Let CS_p be a chain silicate network of length $p; p \geq 1$ then Weighted PI index is expressed as $PI_w(CS_p) = 144p^2 - 486p + 666$.*

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Proof. A chain silicate network is represented as CS_p of length p by arranging p number of tetrahedrons in linear manner. A CS_p has $3p + 1; p \geq 1$ number of vertices and $6p$ edges. Based on the valency of end vertices, the edge set is partioned into three subsets for which number of euidistant vertices are given in the following table. In the following figures of silicate networks the pink verteices represent silicon whereas blue vertices indicate oxygen.

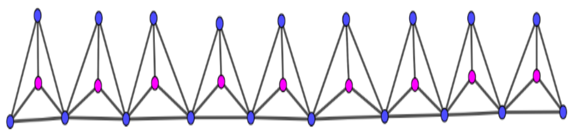

Figure 2: Chain silicate network

Cardinality of end vertices	Number of Edges	Number of the equidistant vertices
(3,3)	p+4	3p-1
(6,6)	p-2	2
(3,6)	(6, 4, 4p-16)	(2, 11, 8)

$$\begin{aligned}
PI_w(CS_p) &= \sum_{e \in CS_p} [d_{CS_p}(u) + d_{CS_p}(v)][|V(CS_p)| - N_{CS_p}(e)]. \\
&= (p-2)(6+6)[(3p+1)-2] + (p+2)(3+3)[(3p+1)-(3p-1)] \\
&\quad +6(3+6)[(3p+1)-2] + 4(3+6)[(3p+1)-11] \\
&\quad +(3+6)4(p-4)[(3p+1)-8] \\
&= 144p^2 - 486p + 642.
\end{aligned}$$

Thus, $PI_w(CS_p) = 144p^2 - 486p + 642$. □

Corollary 3.2. *If CS_p is a Orthosilicate which is discrete tetrahedral units, then the WPI of CS_p is $108p - 36$.*

Proof.

$$\begin{aligned}
PI_w(CS_p) &= \sum_{e \in CS_p} [d_{CS_p}(u) + d_{CS_p}(v)][|V(CS_p)| - N_{CS_p}(e)]. \\
&= 6(3+3)[3p-1] \\
&= 108p - 36.
\end{aligned}$$

□

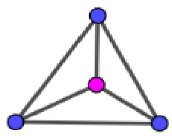

Figure 3: Orthosilicate

Corollary 3.3. *Let CS_p be a Pyrosilicate, then the WPI of CS_p is $270p - 252$.*

Proof. Pyrosilicates are two tetrahedral units where $p = 2$ are joined together at one of the vertices lie in the corner.

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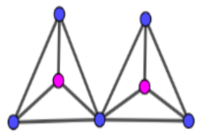

Figure 4: Pyrosilicate

$$\begin{aligned} PI_w(CS_p) &= \sum_{e \in CS_p} [d_{CS_p}(u) + d_{CS_p}(v)][|V(CS_p)| - N_{CS_p}(e)]. \\ &= 6(3+3)[3p-1] + 6(3+6)[3p-4] \\ &= 270p - 252. \end{aligned}$$

□

Theorem 3.4. *Weighted PI index of a cyclic silicate of 6-tetrahedral units SiO_4 is expressed as $PI_w(CS_p) = 114p^2 - 108p$.*

Proof. The graph of cyclic silicte of 6-tetrahedral units where $p = 6$ contains (3p,6p) edges and vertices respectively.
With the basis of the cardinality there are three subedgesets having the following data.

Cardinality of end vertices	Number of Edges	Number of the equidistant vertices
(3,3)	p	2p+4
(6,6)	p	4
(3,6)	4p	p+1

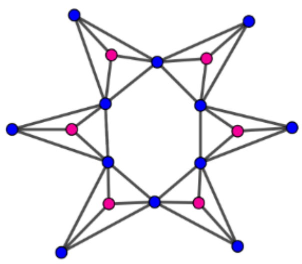

Figure 5: cyclic silicte of 6-tetrahedral units

$$\begin{aligned} PI_w(CS_p) &= \sum_{e \in CS_p} [d_{CS_p}(u) + d_{CS_p}(v)][|V(CS_p)| - N_{CS_p}(e)]. \\ &= p(3+3)[3p-(2p+4)] + p(6+6)[3p-4] + 4p(3+6)[3p-(p+1)] \\ &= 114p^2 - 108p. \end{aligned}$$

□

Corollary 3.5. *WPI of a cyclic silicate having 4-tetrahedral units is given by $PI_w(CS_p) = 114p^2 - 96p$.*

Proof. In evaluation of WPI of a cyclic silicate contains four tetrahedral units, the graph has 3p vertices and 6p edges.

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Cardinality of end vertices	Number of Edges	Number of the equidistant vertices
(3,3)	p	2p+2
(6,6)	p	4
(3,6)	4p	p+1

$$\begin{aligned} PI_w(CS_p) &= \sum_{e\in CS_p} [d_{CS_p}(u)+d_{CS_p}(v)][|V(CS_p)|-N_{CS_p}(e)]. \\ &= p(3+3)[3p-(2p+2)]+p(6+6)[3p-4]+4p(3+6)[3p-(p+1)] \\ &= 114p^2-96p. \end{aligned}$$

□

Corollary 3.6. *For a cyclic silicate linking 3-tetrahedral units, WPI index is given by* $PI_w(CS_p)=114p^2-78p$.

Proof. In this graph $p=3$ there are $3p$ and $6p$ number of vertices and edges.

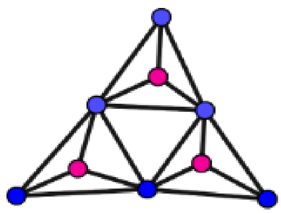

Figure 6: cyclic silicte of 6-tetrahedral units

Cardinality of end vertices	Number of Edges	Number of the equidistant vertices
(3,3)	p	2p+1
(6,6)	p	3
(3,6)	4p	p+1

$$\begin{aligned} PI_w(CS_p) &= \sum_{e\in CS_p} [d_{CS_p}(u)+d_{CS_p}(v)][|V(CS_p)|-N_{CS_p}(e)]. \\ &= p(3+3)[3p-(2p+1)]+p(6+6)[3p-3]+4p(3+6)[3p-(p+1)] \\ &= 114p^2-78p. \end{aligned}$$

□

4 Conclusion

Developing efficient algorithms for calculating the Weighted PI indices of lexicographic product is another area of research. This involves designing algorithms that can compute these indices for large graphs in a scalable and time-efficient manner. Efficient algorithms would be valuable for analyzing large chemical compounds and complex networks. The Weighted PI indices have applications in chemo informatics, where they are used to quantify the structural features and properties of chemical compounds. In this paper, Weighted PI index of some classes of simple graphs are studied for lexicographic product and also WPI index of various silicate networks has computed. Future research could focus on exploring the applications of WPI indices of lexicographic corona product in areas such as drug discovery, chemical similarity analysis, and property prediction.

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