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Wiener, Szeged and vertex PI indices of regular tessellations

PAUL MANUEL[1], INDRA RAJASINGH[2] AND MICHEAL AROCKIARAJ[2,•]

[1]*Department of Information Science, Kuwait University, Safat, Kuwait*

[2]*Department of Mathematics, Loyola College, Chennai 600 034, India*

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ABSTRACT

A lot of research and various techniques have been devoted for finding the topological descriptor Wiener index, but most of them deal with only particular cases. There exist three regular plane tessellations, composed of the same kind of regular polygons namely triangular, square, and hexagonal. Using edge congestion-sum problem, we devise a method to compute the Wiener index and demonstrate this method to all classes of regular tessellations. In addition, we obtain the vertex Szeged and vertex PI indices of regular tessellations.

Keywords: Wiener index; Szeged index; PI index; embedding; congestion; regular plane tessellations.

1. INTRODUCTION

A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. A graph G is connected if any two vertices are joined by a path. A maximal connected subgraph of G is called a component of G. A molecular graph is a collection of vertices representing the atoms in the molecule and a set of edges representing the covalent bonds. Graph representation of molecular structures is widely used in computational chemistry. Trinajstić noted that the roots of chemical graph theory may be found in the works by chemists of 18-19th centuries such as Higgins, Kopp and Crum Brown [34].

Quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR) represent attempts to correlate activities or properties with structural descriptors of compounds. To correlate and predict physical, chemical and biological activity/property from molecular structure is a very important and an unsolved

• Corresponding author (Email: marockiaraj@gmail.com)

problem in theoretical and computational chemistry [33]. The most important step in QSAR/QSPR is to numerically code the chemical structures of various molecules so as to build a correlation model between the chemical structures of various chemical compounds and the corresponding chemical and biological activities/properties. Thus, how to exactly transfer the chemical formula (or molecular graph) into numerical format has been a major task in QSAR/QSPR researches. There are many methods to quantify the molecular structures, of which the topological index is the most popular since it can be obtained directly from molecular structures and rapidly computed for large number of molecules [1, 4, 27, 40].

Topological indices are designed basically by transforming a molecular graph into a number. The first use of a topological index was made in 1947 by the chemist Harold Wiener [36]. The Wiener index is used to study the relation between molecular structure and physical and chemical properties of certain hydrocarbon compounds. It is defined as the sum of the distances between every pair of vertices of G. In the initial applications, the Wiener index is employed to predict physical parameters such as boiling points, heats of vaporization, molar volumes and molar refractions of alkanes [5, 8]. The study of Wiener index is one of the current areas of research in mathematical chemistry [3]. Researchers made some attempts to devise techniques for finding the Wiener index of chemical compounds [3, 5, 8, 12, 13, 16, 19, 31, 32] and also used brute force method based on distance matrix to compute the same [28]. In theoretical computer science, Wiener index is considered as one of the basic descriptors of fixed interconnection networks because it provides the average distance between any two nodes of the network [9, 37].

The rest of the paper is organized as follows: In Section 2, we survey the techniques for computing the Wiener index. In Section 3 we develop a method to find the Wiener index using edge congestion-sum problem. The Wiener indexes of all classes of regular tessellations are given in Section 4. In Sections 5 and 6 respectively, we give the vertex Szeged index and the vertex PI index of regular tessellations. Finally, in Section 7, we conclude the paper with a remark.

2. THE EXISTING TECHNIQUES FOR WIENER INDEX

For a graph G, let $d_G(u,v)$ be the number of edges on any shortest path joining vertex u to vertex v. The Wiener index is defined as

$$W(G)=\frac{1}{2}\sum_{(u,v)\in V(G)\times V(G)} d_G(u,v)$$

where the sum runs over all ordered pairs of vertices. The factor $(1/2)$ is needed in order to count each pair exactly once. If the vertex set is linearly ordered, we can write

$$W(G)=\sum_{u<v,\ u,v\in V(G)} d_G(u,v)$$

In this section we present the methods that are available in the literature [25] to find the Wiener index.

The Cut Method: Given two connected graphs H and G, we say that H admits an isometric embedding into G if there exists a mapping $\iota : V(H)\to V(G)$ such that for all vertices $u,v\in V(H)$ we have $d_G(\iota(u),\iota(v))=d_H(u,v)$. Clearly, ι is injective and maps edges to edges, thus H can be considered as an induced subgraph of G. We can also say that H is an isometric subgraph of G [24].

The n-dimensional hypercube Q_n is the Cartesian product of n copies of the complete graph K_2 on two vertices. In other words, if we set $V(K_2)=\{0,1\}$, then the vertex set of Q_n consists of all strings of length n over $\{0,1\}$ and two such strings are adjacent if and only if they differ in exactly one position.

Graphs that can be isometrically embedded into a hypercube are called partial cubes. In other words, a graph G is a partial cube, if there is an isometric embedding $\iota : V(G)\to V(Q_n)$ for some n. The class of graphs that consists of all isometric subgraphs of hypercubes turns out to be very important in the field of chemical graph theory. It was observed that hypercubes, even cycles, trees, median graphs (in particular acyclic cubical complexes), benzenoid graphs, phenylenes, and Cartesian products of partial cubes are partial cubes [25].

Let G be a connected graph. Then the edges $e=(x,y)$ and $f=(u,v)$ are in the Djokovic-Winkler [11, 38] relation Θ if $d_G(x,u)+d_G(y,v)=d_G(x,v)+d_G(y,u)$. The relation is always reflexive and symmetric, and is transitive on partial cubes. Therefore, Θ partitions the edge set of a partial cube G into equivalence classes, called Θ-classes.

Theorem 1. [*22*] *Let G be a partial cube and let $F_1,F_2,...,F_k$ be its Θ-classes. Let $n_1(F_i)$ and $n_2(F_i)$ be the number of vertices in the two connected components of $G-F_i$. Then* $W(G)=\sum_{i=1}^{k} n_1(F_i)\cdot n_2(F_i)$.

Elementary Cut Method: The elementary cut method is based on the result of Theorem 1 and was first introduced for calculation of the Wiener index of benzenoid graphs [18]. Let B be a benzenoid graph. A straight line segment C in the plane with end points P_1 and P_2 is called a cut segment if C is orthogonal to one of the three edge directions, each P_1 and P_2 is the centre of an edge and the graph obtained from B by deleting all edges intersected by C has exactly two connected components. An elementary cut is the set of all edges intersected by a cut segment. Let $\mathbf{C}(B)$ be the set of all elementary cuts of B. In benzenoid graphs the Θ-classes are precisely their elementary (orthogonal) cuts. For $C \in \mathbf{C}(B)$, let $n_1(C)$ and $n_2(C)$ be the number of vertices in the connected components of $B - C$.

Lemma 1. [*18*] *For a benzenoid graph* B*, we have* $W(B) = \sum_{C \in \mathbf{C}(B)} n_1(C) \cdot n_2(C)$.

***L*₁–Graphs:** In 1997, Chepoi et al. [7] extended Theorem 1 from partial cubes to the class of all L_1-graphs that contains also many (chemical) non-bipartite graphs. A graph G is an L_1-graph if it admits a scale λ embeddable into a hypercube, where a scale λ embeddable of H into G is a mapping $\iota : V(H) \to V(G)$ such that $d_G(\iota(u), \iota(v)) = \lambda d_H(u,v)$ holds for some fixed integer λ and all vertices $u, v \in V(H)$. Hence a scale λ embeddable with $\lambda = 1$ is an isometric embedding.

A subset S of vertices of graph G is convex if for any vertices $u, v \in S$ all vertices on shortest (u,v)-paths belong to S. If G is an L_1-graph then for every cut $\{A, B\}$ occurring in the L_1-decomposition of d_G both sets A and B are convex (we call such cuts convex). As was established in [10] a graph G is scale λ embeddable into a hypercube if and only if there exists a collection $\mathbf{C}(G)$ of (not necessarily distinct) of convex cuts of G, such that every edge of G is cut by exactly λ cuts from $\mathbf{C}(G)$.

Theorem 2. [*7*] *Let* G *be a scale* λ *embeddable into a hypercube and let* $\mathbf{C}(G)$ *be the family of convex cuts defining this embedding. Then* $W(G) = \frac{1}{\lambda} \sum_{\{A,B\} \in C(G)} |A|.|B|$.

Generalized Elementary Cut Method: In 2002, Shiu et al. [32] introduced the generalized elementary cut method for computing the Wiener index of irregular convex triangular hexagons. Let G be an n-net and $s = \lfloor n/2 \rfloor$. Let e be an edge in a cell of G. The s^+-edge of e is the s^{th} edge e' in the same cell counting in anti-clockwise direction from e, whereas the s^--edge of e is the s^{th} edge e'' in the same cell counting in clockwise direction from e. Let ∂G denote the boundary of G. For any $e \in \partial G$, define two generalized elementary cuts $C^+(e)$ and $C^-(e)$. A cut line for $C^+(e)$ is obtained by joining a number of line segments. The first of such line segments, say L^+, links the mid-point M of e with the mid-point of e. If $e' \notin \partial G$, then e' belongs to another cell of G, say P. In P, draw a straight line segment L^- through the mid-point of e' and the mid-point of e. If

$e^{''} \in \partial G$, then stop. Otherwise, continue the process with alternate orientation until it reaches the boundary (say at the point *N*). The other generalized elementary cut, starting at the edge e with reverse orientation, that is, joining e to s^{-}-edge of e and continue with alternate orientation.

Finally, let C be a polygonal path joined by M and N followed by the line segments defined above. Then C is a straight line and C with endpoints M and N is called a generalized elementary cut pertaining to *e*. Identify the generalized elementary cut C with the set of edges of G which are crossed by C. The set of all generalized elementary cuts of G is denoted by $\mathbf{C}(G)$.

Let C be a generalized elementary cut of G. The $G-C$ consists of two components denoted by $G'(C)$ and $G''(C)$.

Lemma 2. [*32*] *Let* G *be an* n*-net, where n is odd. Further assume that* ∂G *is connected. Then* $W(G)=\frac{1}{2}\sum_{C\in\mathbf{C}(G)}\left|G^{'}(C)\right|\times\left|G^{''}(C)\right|$, *where* $|H|$ *denotes the order of* H

In this section, we use embedding as a tool to devise an elegant and simple method for computing the Wiener index of graphs. Indeed this method coincides the result of Theorem 2. We begin with certain definitions of the embedding problem.

Graph embedding has been known as a powerful tool for implementation of parallel algorithms or simulation of different interconnection networks. A graph *embedding* [2] of a guest graph G into a host graph H is defined by an injective function $f : V(G)\to V(H)$ together with a mapping P_f which assigns to each edge (u,v) of G a path $P_f((u,v))$ between $f(u)$ and $f(v)$ in H. If $e=(u,v)\in E(G)$, then the length of $P_f((u,v))$ in H is called the dilation of the edge e.

The dilation-sum [29] $\widetilde{D_f}(G,H)$ of an embedding f of G into H is defined as

$$\widetilde{D_f}(G,H) = \sum_{u,v\in E(G)} d_H(f(u),f(v))$$

where $d_H(f(u),f(v))$ is the length of the path $P_f((u,v))$ in H.

The minimum dilation-sum of G into H is defined as

$$\widetilde{D}(G,H) = \min_f \widetilde{D_f}(G,H)$$

where the minimum is taken over all embeddings f of G into H.

The *congestion* of an embedding f of G into H is the maximum number of edges of the guest graph that are embedded on any single edge of the host graph. Let $C_f(G,H(e))$ denote the number of edges (u,v) of G such that e is in the path $P_f((u,v))$. In other words,

$$C_f(G,H(e)) = |\{(u,v) \in E(G):\ e \in P_f((u,v))\}|.$$

For $S \subseteq E(H)$, the congestion on S is the sum of the congestions on the edges in S. That is, $C_f(G,H(S)) = \sum_{e\in S} C_f(G,H(e))$. The congestion-sum [29] $\widetilde{C_f}(G,H)$ of an embedding f of G into H is defined as

$$\widetilde{C_f}(G,H) = \sum_{e\in E(G)} C_f(G,H(e))$$

The minimum congestion-sum of G into H is defined as

$$\tilde{C}(G,H) = \min_f \widetilde{C_f}(G,H)$$

where the minimum is taken over all embeddings f of G into H. For any embedding, the congestion-sum and the dilation-sum are one and the same [29]. This motivates the following result.

Theorem 3. (k-Division Method) *Let G be a graph on n vertices. Let $E^k(G)$ denote a collection of edges of G with each edge in G repeated exactly k times. Let $\{S_1, S_2, ..., S_m\}$ be a partition of $E^k(G)$ such that each S_i is an edge cut of G and the removal of edges of S_i leaves G into 2 components G_i and G_i'. Also each S_i satisfies the following conditions:*

(i) For any two vertices $u, v \in G_i$, a shortest path between u and v has no edges in S_i.

(ii) For any two vertices $u, v \in G_i'$, a shortest path between u and v has no edges in S_i.

(iii) For any two vertices $u \in G_i$ and $v \in G_i'$, a shortest path between u and v has exactly one edge in S_i.

Then $W(G) = \frac{1}{k}\sum_{i=1}^{m} |V(G_i)|(n - |V(G_i)|)$.

Proof. Let K_n be a complete graph on n vertices with vertex set $V(K_n) = \{1, 2, \ldots, n\}$. Let $f : V(K_n) \to V(G)$ be an embedding given by $f(x) = x$ such that every edge (u,v) in K_n is mapped to a shortest path between u and v in G, for all $1 \le u \ne v \le n$. For each edge cut S_i, $1 \le i \le m$, clearly $f^{-1}(G_i)$ induces a complete graph on $|V(G_i)|$ vertices. By condition (i), no pair of vertices in G_i contributes to $C_f(K_n, G(S_i))$ and also by condition (ii), no pair of vertices in G_i' contributes to $C_f(K_n, G(S_i))$. By condition (iii), any pair of vertices $u \in G_i$ and $v \in G_i'$ increments $C_f(K_n, G(S_i))$ by *1*. Hence $C_f(K_n, G(S_i)) = |V(G_i)| \times |V(G_i')|$

for all i. The congestion-sum

$$\widetilde{C_f}(K_n,G) = \sum_{e\in E(G)} C_f(K_n,G(e))$$

$$= \frac{1}{k}\sum_{i=1}^{m} C_f(K_n,G(S_i))$$

$$= \frac{1}{k}\sum_{i=1}^{m} |V(G_i)|\times|V(G_i^{'})|$$

$$= \frac{1}{k}\sum_{i=1}^{m} |V(G_i)|(n-|V(G_i)|).$$

The dilation-sum

$$\widetilde{D_f}(K_n,G) = \sum_{(u,v)\in E(K_n)} d_G(u,v)$$

$$= \sum_{u<v,\ u,v\in V(K_n)} d_G(u,v)$$

$$= \sum_{u<v,\ u,v\in V(G)} d_G(u,v)\ .$$

Since congestion-sum is equal to dilation-sum, we get

$\sum_{u<v,\ u,v\in V(G)} d_G(u,v) = \frac{1}{k}\sum_{i=1}^{m} |V(G_i)|(n-|V(G_i)|)$. Hence $W(G) = \frac{1}{k}\sum_{i=1}^{m} |V(G_i)|(n-|V(G_i)|)$. □

Illustration for 1-Division Method: Consider the 3-dimensional hypercube Q_3. Let $\{S_1,S_2,S_3\}$ be a partition of $E(Q_3)$ such that the removal of edges of S_i leaves Q_3 into 2 components G_i and $G_i^{'}$ where $|V(G_i)|=4$ and $|V(G_i^{'})|=4$. See Figure 1. Hence $W(Q_3)=4\times4+4\times4+4\times4=48$.

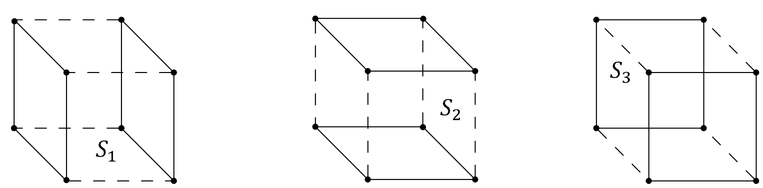

Figure 1. S_1,S_2,S_3 are Edge Cuts of Q_3.

Illustrations for 2-Division Method:

(a) Consider the triangular snake ΔS_5. Let $\{S_1,S_2,S_3, S_4,S_5,S_6\}$ be a partition of $E^2(\Delta S_5)$. For $i=1,2,3,6$, the removal of edges of S_i leaves ΔS_5 into 2 components G_i and G_i' where $|V(G_i)|=1$ and $|V(G_i')|=4$. For $i=4,5$, the removal of edges of S_i leaves ΔS_5 into 2 components G_i and G_i' where $|V(G_i)|=2$ and $|V(G_i')|=3$. See Figure 2. Hence $W(\Delta S_5)=\frac{1}{2}\{4(1\times 4)+2(2\times 3)\}=14$.

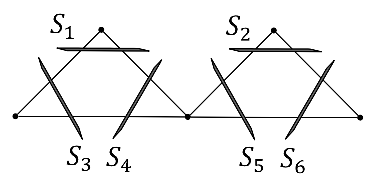

Figure 2. $S_1, S_2, S_3, S_4, S_5, S_6$ are Edge Cuts of ΔS_5.

(b) Consider the irregular triangular snake ΔS_6. Let $\{S_i : 1 \le i \le 9\}$ be a partition of $E^2(\Delta S_6)$. For $i=1,2,3,8,9$, the removal of edges of S_i leaves ΔS_6 into 2 G_i and G_i' where $|V(G_i)|=1$ and $|V(G_i')|=5$. For $i=4,6,7$, the removal of edges of S_i leaves ΔS_6 into 2 components G_i and G_i' where $|V(G_i)|=2$ and $|V(G_i')|=4$. For $i=5$, the removal of edges of S_i leaves ΔS_6 into 2 components G_i and G_i' where $|V(G_i)|=3$ and $|V(G_i')|=3$. See Figure 3. Hence $W(\Delta S_6)=\frac{1}{2}\{5(1\times 5)+3(2\times 4)+3\times 3\}=29$.

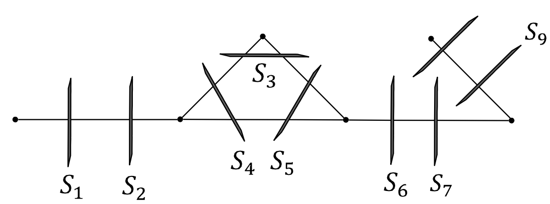

Figure 3. S_i: $1 \le i \le 9$ is an Edge Cut of ΔS_6.

3. REGULAR TESSELLATIONS

Patterns covering the plane by fitting together replicas of the same basic shape have been created by Nature and Man either by accident or by design. Examples range from the simple hexagonal pattern of the bees' honeycomb or a tiled floor to the intricate decorations. These patterns are called tessellations. A regular tessellation is a pattern made by repeating a regular polygon. There are only three regular tessellations, composed of the same kind of regular polygons namely equilateral triangles, squares and hexagons. See

Figure 4. These are the basis for the design of direct interconnection networks with highly competitive overall performance. Mesh connected computers and tori are based on regular square tessellations and are popular and well-known models for parallel processing. Hexagonal and honeycomb networks are based on regular triangular and hexagonal tessellations respectively. The inconsistency in the name selection (note that a hexagonal network is not based on a hexagon, but on a triangular tessellation) is due to the duality of the two tessellations (one can be obtained from the other by joining the centres of the neighbouring polygons).

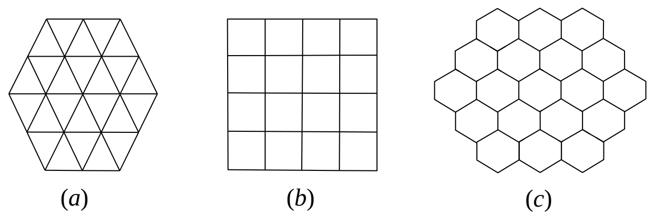

Figure 4. Three Regular Tessellations Composed of the Same Kind of Regular Polygons: (a) Equilateral Triangles (b) Squares and (c) Hexagons.

Honeycomb and hexagonal networks have been studied in a variety of contexts. They have been applied in chemistry to model benzenoid hydrocarbons in image processing [35], computer graphics [26] and cellular networks [14]. Honeycomb architecture was investigated in [30], where a suitable addressing scheme, routing and broadcasting algorithms were proposed. An addressing scheme for processors and corresponding routing and broadcasting algorithms for hexagonal network are studied in [6].

A two dimensional mesh $M(m,n)$ is defined as the Cartesian product $P_m \times P_n$ where P_m and P_n denote the path on m and n vertices respectively. The Wiener index of mesh $M(m,n)$ had incorrectly stated in [23], we here give the correct value.

Lemma 3. *The Wiener index of mesh is given by* $W(M(m,n)) = \frac{1}{6}mn(m+n)(mn-1)$.

Honeycomb networks can be built from hexagons in various ways. A hexagon is treated as a honeycomb of size one, denoted by $HC(1)$. The honeycomb $HC(2)$ of size two is obtained by adding six hexagons to the boundary edges of $HC(1)$. Inductively, honeycomb $HC(n)$ of size n is obtained from $HC(n-1)$ by adding a layer of hexagons around the boundary of $HC(n-1)$. Alternatively, the size n of $HC(n)$ is determined as the number of hexagons between the centre and boundary (inclusive) of $HC(n)$. The number of vertices and edges of $HC(n)$ are $6n^2$ and $9n^2-3n$, respectively [30]. In the literature honeycomb network is also known as circumcoronene series.

Lemma 4. *[18, 31] The Wiener index of Honeycomb network is*

$$W(HC(n)) = \frac{1}{5}(164n^5 - 30n^3 + n).$$

Hexagonal networks are based on the partition of a plane into equilateral triangles. Hexagonal network $HX(n)$ of dimension n has $3n^2 - 3n + 1$ vertices and $9n^2 - 15n + 6$ edges, where n is the number of vertices on one side of the hexagon [6]. The diameter is $2n - 2$. There are six vertices of degree three which we call as corner vertices. There is exactly one vertex v at distance $n-1$ from each of the corner vertices. This vertex is called the centre of $HX(n)$ and is represented by O. For convenience we shall introduce a coordinate system for the hexagonal network. In this system, three axes x, y and z are parallel to three edge directions and are at a mutual angle of 120 between any two of them at O. Any line parallel to x-axis in the clockwise (anti clockwise) direction at a distance i from the corner vertex of x-axis is denoted by x_i-line (x_{-i}-line). Similarly we define y_i-line, y_{-i}-line, z_i-line and z_{-i}-line. For convenience we denote the x, y and z axes by x_0-line, y_0-line and z_0-line respectively. See Figure 5.

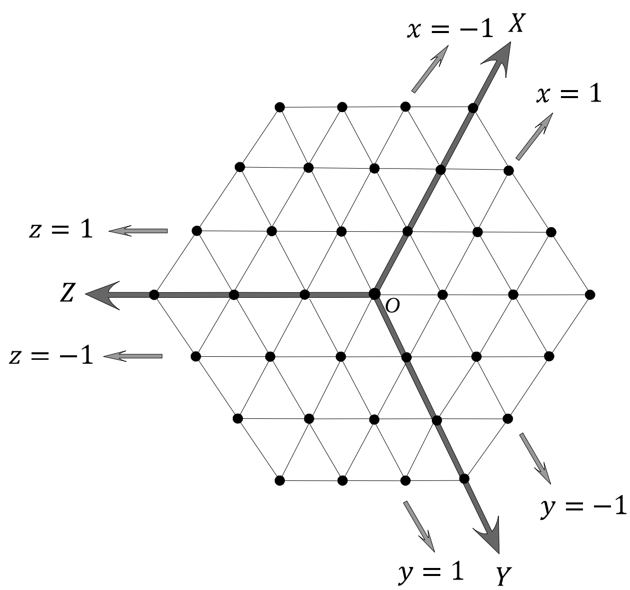

Figure 5. Coordinate System for Hexagonal Network.

The Wiener index of hexagonal networks have been obtained using the generalized elementary cut method [32], whereas the *k*-division method, introduced in the paper is successful in computing the same in simple and elegant way.

Theorem 4. *The Wiener index of hexagonal network is given by*

$$W(HX(n)) = (n/10)(41n^4 + 100n^2 + 9) - (n^2/4)(41n^2 + 19).$$

Proof. For $1 \le i \le n-1$, let A_i (resp. A_{-i}) be the set of edges in the hexagonal network such that each edge has one vertex in x_{i-1}-line (resp. $x_{-(i-1)}$-line) and the other vertex in x_i-line (resp. x_{-i}-line). For $1 \le i \le n-1$, let B_i (resp. B_{-i}) be the set of edges in the hexagonal network such that each edge has one vertex in y_{i-1}-line (resp. $y_{-(i-1)}$-line) and the other vertex in y_i-line (resp. y_{-i}-line). For $1 \le i \le n-1$, let C_i (resp. C_{-i}) be the set of edges in the hexagonal network such that each edge has one vertex in z_{i-1}-line (resp. $z_{-(i-1)}$-line) and the other vertex in z_i-line (resp. z_{-i}-line). See Figure 6.

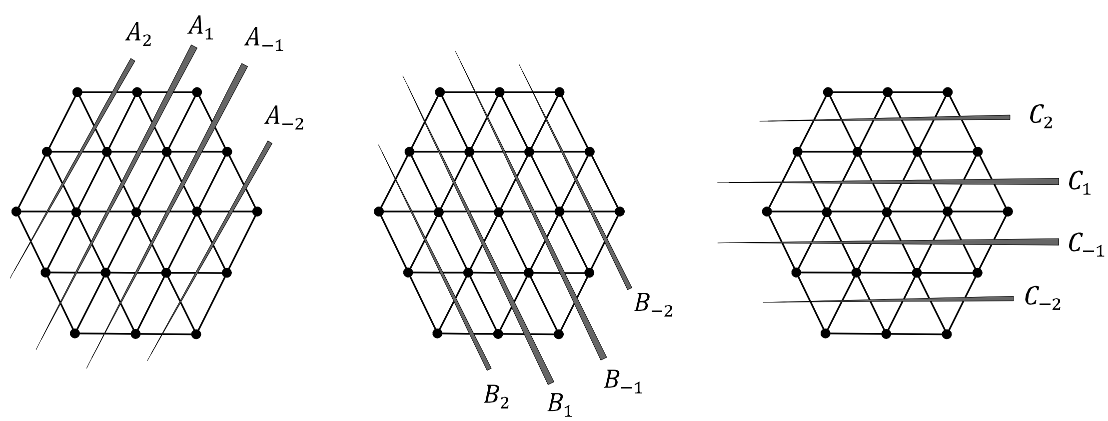

Figure 6. Edge Cuts of *HX*(3).

Thus $\{A_i, A_{-i}, B_i, B_{-i}, C_i, C_{-i} \ : 1 \le i \le n-1\}$ is a partition of $E^2(HX(n))$. For $1 \le i \le n-1$, the removal of A_i leaves $HX(n)$ into two components G_{A_i} and G'_{A_i} where $\left|V(G_{A_i})\right| = \frac{1}{2}(n-i)(3n-i-1)$ and $\left|V(G'_{A_i})\right| = (3n^2 - 3n + 1) - \frac{1}{2}(n-i)(3n-i-1)$. By the symmetry of hexagonal network, for $1 \le i \le n-1$, $HX(n) \setminus A_i, HX(n) \setminus A_{-i}$, $HX(n) \setminus B_i$, $HX(n) \setminus B_{-i}, HX(n) \setminus C_i$ and $HX(n) \setminus C_{-i}$ are all isomorphic. The edge cuts $A_i, A_{-i}, B_i, B_{-i}, C_i, C_{-i}$, $1 \le i \le n-1$, satisfy conditions (i)-(iii) of the 2-Division Method. Hence $W(HX(n)) = \frac{1}{2} \times 6 \times \sum_{i=1}^{n-1} \left(\frac{1}{2}(n-i)(3n-i-1)\right) \times \left((3n^2 - 3n + 1) - \frac{1}{2}(n-i)(3n-i-1)\right)$ $= (n/10)(41n^4 + 100n^2 + 9) - (n^2/4)(41n^2 + 19)$. See Figure 7 for the graph representation of $W(HX(n))$ drawn using MATLAB. □

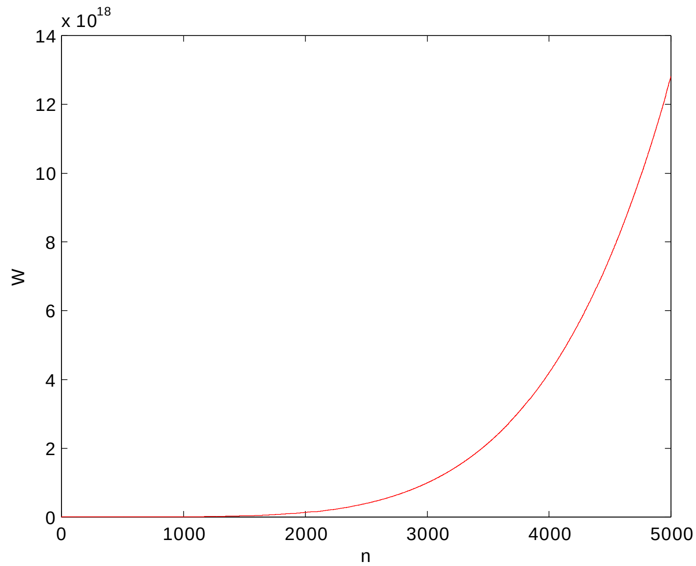

Figure 7. Graph Representation of $W(HX(n))$.

4. VERTEX SZEGED INDEX

The Wiener index is the first topological index introduced by the chemist Harold Wiener for investigating boiling points of alkanes [36]. Let $e=(u,v)$ be an edge of the graph G. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e)$. In other words, $n_u(e)=|\{w : w\in V(G), d_G(u,w)<d_G(v,w)\}|$. Analogously, $n_v(e)$ is the number of vertices of G whose distance to the vertex v is smaller than the distance to the vertex u. In other words, $n_v(e)=|\{w : w\in V(G), d_G(v,w)<d_G(u,w)\}|$. Note that the vertices equidistant to u and v are not counted. Wiener [36] defined his index for tree (acyclic graph) T as $W(T)=\sum_{e=(u,v)\in E(T)} n_u(e)\cdot n_v(e)$. It is natural to ask, what would happen if one would apply it to cyclic graphs? Research along these lines led to the concept of Szeged index [15]. The vertex Szeged index [15, 21] is a molecular structure descriptor and is defined as

$$S_{z_v}(G)=\sum_{e\in E(G)} S_{z_v}(e)=\sum_{e=(u,v)\in E(G)} n_u(e)\cdot n_v(e).$$

Let $e=(u,v)$ be an edge of a partial cube G and suppose that it belongs to the Θ-class F. Then it follows easily from definitions that $n_u(e)$ and $n_v(e)$ induce the connected components of $G-F$. Therefore, Theorem 1 has its variant for the vertex Szeged index.

Theorem 5. [25] *Let G be a partial cube and let $F_1, F_2, \ldots, F_k$ be its Θ-classes. Let $n_1(F_i)$*

and $n_2(F_i)$ *be the number of vertices in the two connected components of* $G-F_i$. *Then* $S_{z_v}(G)=\sum_{i=1}^{k}|F_i|\cdot n_1(F_i)\cdot n_2(F_i)$.

By elaborating Theorem 5, the vertex Szeged index of benzenoid system has been computed by considering its elementary cuts or orthogonal cuts [17]. An elementary cut is a line segment that starts at the center of a peripheral edge of a benzenoid system B, goes orthogonal to it and ends at the first next peripheral edge of B. We denote an elementary cut by C and the number of edges that it intersects by $|C|$.

Lemma 5. *The vertex Szeged index of the benzenoid system* B *is given by* $S_{z_v}(B)=\sum_{C\in \mathbf{C}(B)}|C|\times n_1(C)\times n_2(C)$ *where* $n_1(C)$ *and* $n_2(C)$ *are the numbers of vertices lying on the two sides of the elementary cut* C, *and where the summation goes over all elementary cuts of* B.

Note that $n_1(C)+n_2(C)=|V(B)|$ for all elementary cuts. This technique leads to computation of vertex Szeged index of mesh and honeycomb network, but fails to compute the vertex Szeged index of hexagonal network. We note that the vertex Szeged index of mesh $M(m,n)$ had wrongly stated in [23], we here give the correct value.

Lemma 6. *The vertex Szeged index of mesh is given by*

$$S_{z_v}(M(m,n))=\tfrac{1}{6}mn(2m^2n^2-m^2-n^2).$$

Lemma 7. [*17*] *The vertex Szeged index of Honeycomb network is*

$$S_{z_v}(HC(n))=\tfrac{3n^2}{2}(36n^4-n^2+1).$$

We compute the vertex Szeged index of hexagonal network using coordinate system.

Theorem 6. *The vertex Szeged index of hexagonal network is given by*

$$S_{z_v}(HX(n))=\tfrac{1}{24}\{101n^6-303n^5+383n^4-261n^3+92n^2-12n\}\ .$$

Proof. We partition the edge set of $HX(n)$ into 3 sets namely A, B and C where

$A=\{e\ :\ e$ lies in x_0-line or x_i-line or x_{-i}-line for $1\le i\le n-1\}$,

$B=\{e\ :\ e$ lies in y_0-line or y_i-line or y_{-i}-line for $1\le i\le n-1\}$ and

$C=\{e\ :\ e$ lies in z_0-line or z_i-line or z_{-i}-line for $1\le i\le n-1\}$.

By the symmetry of hexagonal network,

$$S_{z_v}(HX(n)) = \sum_{e\in A} S_{z_v}(e) + \sum_{e\in B} S_{z_v}(e) + \sum_{e\in C} S_{z_v}(e) = 3\sum_{e\in C} S_{z_v}(e)$$

For convenience we shall describe the set C as follows: The edges on the z_0-line will be represented by $e_{0,i}$, $1 \le i \le 2n-2$, from left to right. Similarly, when $1 \le j \le n-1$, the edges on the z_j-line (resp. z_{-j}-line) will be represented by $e_{j,i}$ (resp. $e_{-j,i}$), $1 \le i \le 2n-2-j$ from left to right.

Let $R_1 = \{e_{0,i} \ : \ 1 \le i \le n-1\} \cup \{e_{\pm j,i} \ : \ 1 \le j \le n-1, 1 \le i \le n-1-j\}$,

$R_2 = \{e_{j,i} : 1 \le j \le n-1, n-j \le i \le n-1\}$

$R_3 = \{e_{0,i} \ : \ n \le i \le 2n-2\} \cup \{e_{\pm j,i} \ : \ 1 \le j \le n-1, n \le i \le 2n-2-j\}$ and

$R_4 = \{e_{-j,i} \ : \ 1 \le j \le n-1, n-j \le i \le n-1\}$. See Figure 8.

Again by the symmetry of hexagonal network,

$$\sum_{e\in R_1} S_{z_v}(e) = \sum_{e\in R_3} S_{z_v}(e) \text{ and } \sum_{e\in R_2} S_{z_v}(e) = \sum_{e\in R_4} S_{z_v}(e) .$$

Therefore

$$S_{z_v}(HX(n)) = 3\{\sum_{e\in R_1} S_{z_v}(e) + \sum_{e\in R_2} S_{z_v}(e) + \sum_{e\in R_3} S_{z_v}(e) + \sum_{e\in R_4} S_{z_v}(e)\} = 6\{\sum_{e\in R_1} S_{z_v}(e) + \sum_{e\in R_2} S_{z_v}(e)\}.$$

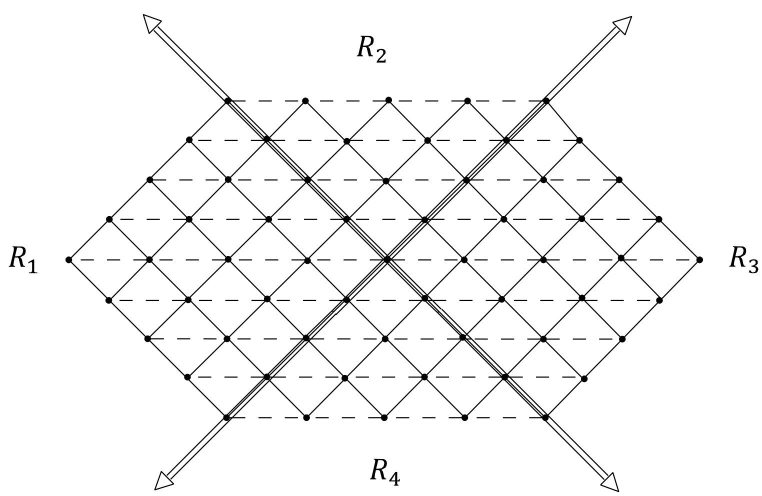

Figure 8. The Edges on C is Partitioned into Four Sets R_1, R_2, R_3 and R_4.

To compute $n_u(e)$ and $n_v(e)$ for each edge $e = (u,v)$ on z-line, we can find vertices a and b if exist) adjacent to u and v on above and below the z-line and the number of vertices between x-line and y-line intersecting at u and v are $n_u(e)$ and $n_v(e)$ respectively. See Figure 9.

For an edge $e_{j,i}$, $0 \le j \le n-1, 1 \le i \le n-1-j$,

$n_u(e_{j,i}) = i(j+1) + 2\{1+2+...+(i-1)\} = (i^2+ij)$ and

$n_v(e_{j,i}) = (2n-1-j-i)j + \{(2n-1-j-i)+(2n-2-j-i)+\cdots(n\,\text{terms})\}+$

$\{(2n-2-j-i)+(2n-3-j-i)+\cdots(n-1-j)\,\text{terms} =$

$\{3n^2-3n+1-(2n-1)j/2-j^2/2-(2n-1)i\}$.

For an edge $e_{j,i}$, $1 \le j \le n-1, n-j \le i \le n-1$,

$n_u(e_{j,i}) = ij + \{1+2+...+(i-1)\} + \{i+(i-1)+\cdots(n-j)\,\text{terms}\} =$

$\frac{1}{2}\{i^2+(i+j)(2n-1)-j^2-n^2+n\}$ and

$n_v(e_{j,i}) = (2n-1-i)(n-j) + \{(2n-2-i)+(2n-3-i)+\cdots(n-1-i)\,\text{terms}\} =$

$\frac{1}{2}\{7n^2-7n+2-(3i+2j)(2n-1)+i^2+2ij\}$.

Hence

$$\sum_{e\in R_1} S_{z_v}(e) = \sum_{i=1}^{n-1} i^2 \times \{3n^2-3n+1-i(2n-1)\} +$$
$$2\sum_{j=1}^{n-1}\sum_{i=1}^{n-1-j}(i^2+ij)\times\{3n^2-3n+1-(2n-1)j/2-j^2/2-(2n-1)i\}$$

and

$$\sum_{e\in R_2} S_{z_v}(e) = \sum_{j=1}^{n-1}\sum_{i=n-j}^{n-1} \tfrac{1}{2}\{i^2+(i+j)(2n-1)-j^2-n^2+n\}\times\tfrac{1}{2}\{7n^2-7n+2-(3i+2j)(2n-1)+i^2+2ij\}$$

implies that $S_{z_v}(HX(n)) = \frac{1}{24}\{101n^6-303n^5+383n^4-261n^3+92n^2-12n\}$. □

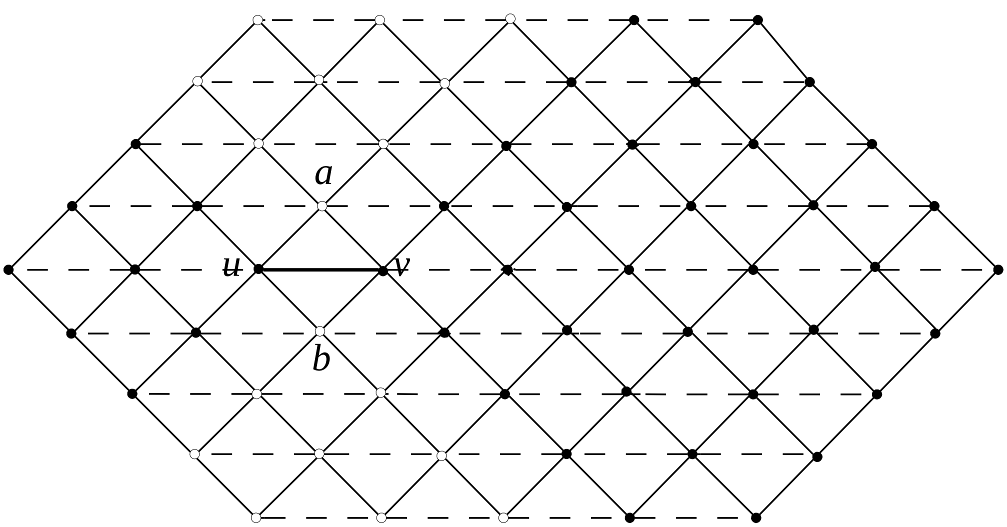

Figure 9. The Vertices Equidistant to *u* and *v* are Represented by Hollow Vertices.

5. VERTEX PI INDEX

The vertex PI index is a distance-based molecular structure descriptor, which recently found numerous chemical applications. The vertex PI index is defined as $PI_v(G) = \sum_{e\in E(G)} PI_v(e) = \sum_{e=(u,v)\in E(G)} n_u(e) + n_v(e)$. If G is a bipartite graph then $PI_v(G) = |V(G)||E(G)|$, because G is without odd cycles [39]. This implies the following results.

Lemma 8. *The vertex PI index of mesh is given by* $PI_v(M(m,n)) = mn(2mn - m - n)$.

Lemma 9. *The vertex PI index of Honeycomb network is given by*

$$PI_v(HC(n)) = 18n^3(3n-1).$$

Using the proof techniques of Theorem 6, we compute the vertex PI index of hexagonal network.

Theorem 7. *The vertex PI index of hexagonal network is given by*

$$PI_v(HX(n)) = 18n^4 - 50n^3 + 54n^2 - 28n + 6 .$$

Proof. As in the proof of Theorem 6,

$$PI_v(HX(n)) = \sum_{e\in A} PI_v(e) + \sum_{e\in B} PI_v(e) + \sum_{e\in C} PI_v(e) = 3\sum_{e\in C} PI_v(e)$$

and therefore $PI_v(HX(n)) = 6\{\sum_{e\in R_1} PI_v(e) + \sum_{e\in R_2} PI_v(e)\}$. But

$$\sum_{e\in R_1} PI_v(e) = \sum_{i=1}^{n-1} i^2 + \{3n^2 - 3n + 1 - i(2n-1)\} +$$
$$2\sum_{j=1}^{n-1}\sum_{i=1}^{n-1-j} (i^2 + ij) + \{3n^2 - 3n + 1 - (2n-1)j/2 - j^2/2 - (2n-1)i\}$$

and

$$\sum_{e\in R_2} PI_v(e) = \sum_{j=1}^{n-1}\sum_{i=n-j}^{n-1} \tfrac{1}{2}\{i^2 + (i+j)(2n-1) - j^2 - n^2 + n\} +$$
$$\tfrac{1}{2}\{7n^2 - 7n + 2 - (3i + 2j)(2n-1) + i^2 + 2ij\}$$

implies that $PI_v(HX(n)) = 18n^4 - 50n^3 + 54n^2 - 28n + 6$. □

6. CONCLUDING REMARK

In this paper we have devised an elegant method to compute the Wiener index of graphs. We have good reasons to believe that many more chemical graphs remain to be explored whose Wiener index can be computed applying our technique.

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