PI indices of Pseudo Regular Graphs

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Abstract: The Padmakar-Ivan(PI) index of a graph G is the sum over all edges uv of G of the number of edges which are not equidistant from the vertices u ad v. The CO-PI index of G is defined as CO-PI$_v$(G) = $\sum_{e=uv\in E(G)}|n_u(e) - n_v(e)|$. In this paper, the PI index and CO-PI index of Pseudo-regular graphs are determined.

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1. Introduction

In theoretical chemistry Molecular structure descriptors, frequently called topological indices are used to design of chemical compounds with given physico-chemical properties or given pharmacologic and biological activities. The Wiener index [1] W is the most popular such index, see [2, 3] and references therein. The Szeged index is closed related to the Wiener index and is a vertex-multiplicative type index that takes into account how the vertices of a given molecular graph are distributed and in particular, the Wiener and the Szeged index coincide on trees.

The Padmakar-Ivan index is an additive index that would consider a corresponding distribution of edges. It is the unique topological index related to parallelism of edges. Many chemical applications of the PI index were presented and it was shown that the PI index correlates highly with Wiener and Szeged index as well as with the physico-chemical propertied and biological activities of a large number of diverse and complex compounds.Since on the otherhand it is usually easier to compute that the Wiener and Szeged index, PI is a topological index worth studying.

The Szeged index incorporates the distribution of vertices of a molecular graph, which the PI index does this job for the edges. Hence it seens that a combination of both could give good results in QSPR/QSAR studies. Indeed, the combination of the PI index and the Szeged index is the best for modeling polychlorinated biphyenyls(PCBs) in environment among the three possible pair of indices selected from the PI index, the Szeged index and the Wiener index [4]. For the Wiener and the Szeged index such studied were previously done . The PI index has been studied from many differernt point of views see[5,6]. In [7], SandiKlavzar computed the PI index for Cartesian product graphs.

Recently, Hassani et al. introduced a new topological index similar to the vertex version of PI index [8]. This index is called the Co-PI index of *G* and defined as:

$$\text{CO-PI}_v(G) = \sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|.$$

Here the summation goes over all edges of *G*. Fath-Tabar et al. proposed the Szegedmatrix and Laplacian Szeged matrix in [9]. Then Su et al. introduced the Co-PI matrix of agraph [10]. In this paper, we compute the PI index and CO-PI index for the different types of Pseudo-regular graphs.

2. Preliminaries

All graphs considered in this paper are simple, connected and finite. A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph G are also called vertices and edges of the graph and are denoted by V(G) & E(G) respectively. For u,v ϵ V(G), the distance between u & v in G, denoted by d(u,v), is the length of a shortest (u,v) – path in G.

Let e=uv an edge of G. $n_u(e)$ denotes the number of edges lying closer to the vertex u than the vertex v and $n_v(e)$ denotes the number of edges lying closer to the vertex v than the vertex u. The Padmakar-Ivan index (PI) of a graph G is defined as PI(G) = $\sum_{e=uv\in E(G)} |n_u(e) + n_v(e)|$.In this definition, edges equidistant from both ends of the edge e=uv are not counted.

Similar to the vertexversion of PI index,another important index Co-PI index of *G* which is defined as: CO-PI$_v$(G) = $\sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$. Here the summation goes over all edges of *G*.

Let G= (V, E) be a simple, connected undirected graph with n vertices and m edges. For any vertex $v_i \in$ V, the degree of v_i is the number of edges incident on v_i. It is denoted by d_i or d (v_i). A graph G is called regular if every vertex of G has equal degree. A bipartite graph is called semi regular if each vertex in the same part of a bipartition has the same degree. The 2-degree of v_i [11] is the sum of the degree of the vertices adjacent to v_i and denoted by t_i.[12]. The average degree of v_i is defined as t_i/d_i. For any vertex $v_i \in$ V, the average degree of v_i is also denoted by $m(v_i) = t_i/d_i$.

A graph G is called Pseudo-regular graph [11] if every vertex of G has equal average degree and $m(G) = \frac{1}{n}\sum_{v\in V(G)} m(u)$ is the average neighbor degree number of the graph G. A graph is said to be r-regular if all its vertices are of equal degree r. Every regular graph is a Pseudo-regular graph [13]. But the Pseudo-regular graph need not be a regular graph.

The relevance of pseudo-regular graph for the theory of nanomolecules and nanostructure should become evident from the following. There exist polyhedral (planar, 3-connected) graphs and infinite periodic planar graphs belonging to the family of the Pseudo-regular graphs. Among polyhedral, the deltoidalhexecontahedron possesses Pseudo-regular property[13]. The deltoidalhexecontahedron is a Catalan polyhedron with 60 deltoid faces, 120 edges and 62 vertices with degree 3, 4 and 5 and average degree of its vertices is 4.

The construction of Pseudo-regular graphs is shown in [14].

3. Pi Index And Copi Index Of Pseudo-Regular Graphs.

Theorem 3.1: For $p \geq 2$, the PI index of type I Pseudo-regular graph G_I is

$$PI(G_I) = p(p^2 - p + 1)\left|- p^3 + p^2 - p - 1\right|$$

Proof: Let $G = G_I$ be a type I Pseudo-regular graph.

Let $V(G) = \{ v_0, v_1, v_2, \ldots, v_m, u_1, u_2, \ldots\ldots, u_{m(p-1)}\}$ be the vertex set of G and v_0 as the central vertex of $K_{1,m}$ and $\{ v_1, v_2, \ldots, v_m\}$ are pendant vertices of $K_{1,m}$ where $m = p^2-p+1$ and the (p-1) pendant vertices $\{ u_1, u_2, \ldots, u_{m(p-1)}\}$ are attached with m pendant vertices $v_1, v_2, \ldots, v_m$.

Let $E(G) = (v_0v_i\,;\ 1 \leq i \leq m\} \cup \{v_1u_j;\ 1 \leq j \leq p-1\} \cup \{v_2u_j;\ p \leq j \leq 2p-2\} \cup \{v_3u_j;\ 2p-1 \leq j \leq 3p-3\} \cup \ldots\ldots\ldots\{v_mu_j\ ;(m-1)p-m+2 \leq j \leq mp-m\}$.The Pseudo-regular graph with p=3 is shown in Fig-1

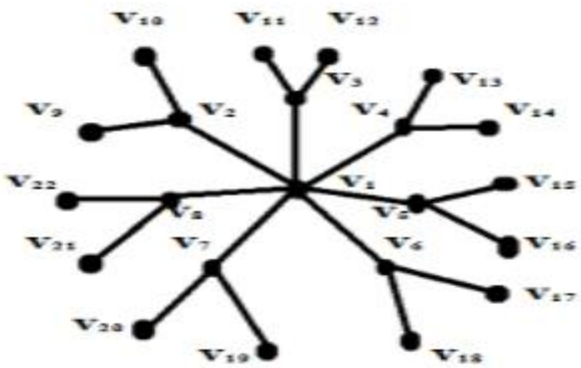

Fig-1

The PI index of G is given by PI(G) = $\sum_{e=uv\in E(G)} |n_u(e) + n_v(e)|$

Now

$$\begin{aligned} PI(G_I) &= \sum_{e=uv\in E(G)} |n_u(e) + n_v(e)| \\ &= \sum_{\text{pendant edge } e\in E(G)} |n_u(e) + n_v(e)| + \sum_{\text{non pendant edge } e\in E(G)} |n_u(e) + n_v(e)| \\ &= (p-1)(p^2-p+1)\left|1-(p(p^2-p+1)+1+1)\right| + (p^2-p+1)\left|p-(p(p^2-p+1)+1-p\right| \\ &= (p^2-p+1)\left[\left|-p^3+p^2-p-1\right|(p-1+1)\right] \\ &= p(p^2-p+1)\left|-p^3+p^2-p-1\right| \end{aligned}$$

Theorem 3. 2: For $p \geq 2$, the CO-PI index of type I Pseudo-regular graph G_I is

$$CO-PI(G_I) = (p^2-p+1)\left[(p-1)\left|-p^3+p^2-p+1\right| + \left|-p^3+p^2+p-1\right|\right]$$

Proof: Similar to theorem 1,

The CO-PI index of G is given by CO-PI(G) = $\sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$

Now

$$CO-PI(G_I) = \sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$$

$$= \sum_{\text{pendant edge } e\in E(G)} |n_u(e) - n_v(e)| + \sum_{\text{non pendant edge } e\in E(G)} |n_u(e) - n_v(e)|$$

$$= (p-1)(p^2-p+1)\left|1-(p(p^2-p+1)+1-1)\right| + (p^2-p+1)\left|p-(p(p^2-p+1)+1-p\right|$$

$$= (p-1)(p^2-p+1)\left|1-p^3+p^2-p\right| + (p^2-p+1)\left|p-p^3+p^2-1\right|$$

$$= (p^2-p+1)\left[(p-1)\left|-p^3+p^2-p+1\right| + \left|-p^3+p^2+p-1\right|\right]$$

Theorem 3.3: For $p \geq 3$, the PI index of type II Pseudo-regular graph G_{II} is $PI(G_{II})$ =

$$PI(G_{II}) = (p^2-3p+3)\left[6p^2-27p+31+(p-3)\left|-p^3+5p^2-9p+5\right|\right]$$

Proof: Let $G = G_{II}$ be a type II Pseudo-regular graph.

Let $V(G) = \{v_0, v_1, v_2, \ldots, v_m, u_1, u_2, \ldots, u_{m(p-3)}\}$ be the vertex set of G and v_0 as the central vertex of W_m and $\{v_1, v_2, \ldots, v_m\}$ are vertices of c_m in the clockwise direction and $\{u_1, u_2, \ldots, u_{m(p-3)}\}$ are the pendant vertices joined to every vertex in the cycle except the central vertex, where $m = p^2-3p+3$.

Let $E(G) = (v_0v_i;\ 1 \leq i \leq m\}\ U\{v_iv_{i+1}; 1\leq i\leq m-1\}U\{v_mv_1\}U\ \{v_1u_j;\ 1 \leq j \leq p-3\}\ U\{v_2u_j;\ p-2 \leq j \leq 2(p-3\}\ U\ldots\ldots\ldots.\{v_mu_j\ ;m\leq j \leq m(p-3)\}$.The construction of type II Pseudo-regular graph is shown in [14]. For p=5, we can get the following Pseudo-regular graph(Fig-2)

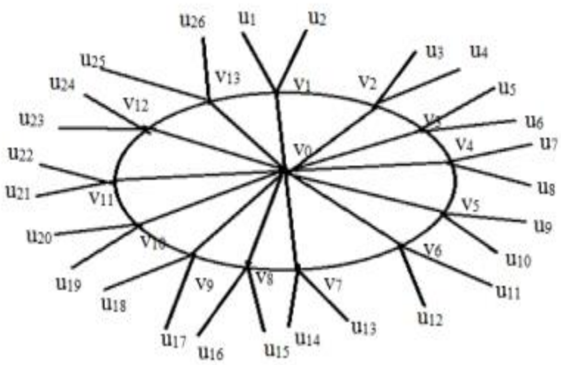

Fig-2

The PI index of G is given by PI(G) = $\sum_{e=uv\in E(G)} |n_u(e) + n_v(e)|$

Now

$$PI(G_{II}) = \sum_{e=uv\in E(G)} |n_u(e) + n_v(e)|$$

$$= \sum_{i=1}^{m} d(v_0, v_i) + \sum_{i=1}^{m}\sum_{j=i+1}^{m} d(v_i, v_j) + \sum_{i=1}^{m}\sum_{j=1}^{m(p-3)} d(v_i, u_j)$$

$$= (p^2-3p+3)\left[(2p-5)^2+(p-2)\right] + (p^2-3p+3)\left[(p-2)^2+(p-2)^2\right] + (p^2-3p+3)(p-3)\left|1-\{(p-2)(p^2-3p+3)+1+1\}\right|$$

$$= (p^2-3p+3)\left[6p^2-27p+31+(p-3)\left|-p^3+5p^2-9p+5\right|\right]$$

Theorem 3.4: For $p \geq 3$, the CO-PI index of type II Pseudo-regular graph G_{II} is $PI(G_{II})$ =
$$CO-PI(G_{II}) = (p^2-3p+3)\left[4p^2-21p+27+(p-3)\left|-p^3+5p^2-9p+7\right|\right]$$

Proof: Let G = G_{II} be a type II Pseudo-regular graph.

The CO-PI index of G is given by CO-PI(G) = $\sum_{e=uv\in E(G)} |n_u(e)-n_v(e)|$

Now

$$CO-PI(G_{II}) = \sum_{e=uv\in E(G)} |n_u(e)-n_v(e)|$$
$$= \sum_{i=1}^{m} d(v_0,v_i) + \sum_{i=1}^{m}\sum_{j=i+1}^{m} d(v_i,v_j) + \sum_{i=1}^{m}\sum_{j=1}^{m(p-3)} d(v_i,u_j)$$
$$= (p^2-3p+3)\left[(2p-5)^2-(p-2)\right] + (p^2-3p+3)\left[(p-2)^2-(p-2)^2\right] +$$
$$(p^2-3p+3)(p-3)\left|1-\{(p-2)(p^2-3p+3)+1-1\}\right|$$
$$= (p^2-3p+3)\left[4p^2-21p+27+(p-3)\left|-p^3+5p^2-9p+7\right|\right]$$

Theorem 3.5: For $p \geq 5$, the PI index of type III Pseudo-regular graph G_{III} is
$$PI(G_{III}) = (p^2-3p+1)\left[8p^4-142p^3+980p^2-3065p+3640\right]$$

Proof: Let G = G_{III} be a type III Pseudo-regular graph.
Let V(G) = $\{v_0,v_1,v_2,\ldots,v_m,u_1,u_2,\ldots\ldots,u_{m(p-5)},w_1,w_2,\ldots\ldots,w_m\}$ be the vertex set of G and v_0 as the central vertex of w_m where m = p^2-3p+1and $\{u_1,u_2,\ldots,u_{m(p-5)}\}$ are the pendant vertices and $\{w_1,w_2,\ldots,w_m\}$ are the vertices joined to the end vertices of each edge of a wheel graph except the central vertex.
Let E(G) = $(v_0v_i\,;\ 1 \leq i \leq m\}$ U$\{v_iv_{i+1};1\leq i\leq m-1\}U\{v_mv_1;1\leq j\leq m(p-5)\}$U $\{u_1v_i;\ 1 \leq i \leq 2\}$ U$\{u_2v_i;\ 2 \leq i \leq 32\}$……….$\{u_mv_i\ ;m-1\leq i \leq m\}U\{v_iw_j;1\leq j\leq p-5\}U\{v_2w_j;p-4\leq j\leq 2(p-5)\}U\{v_mw_j;m\leq j\leq m(p-5)\}$. The construction of type III Pseudo-regular graph is shown in [14]. For p=6, we can get the following Pseudo-regular graph(Fig-3)

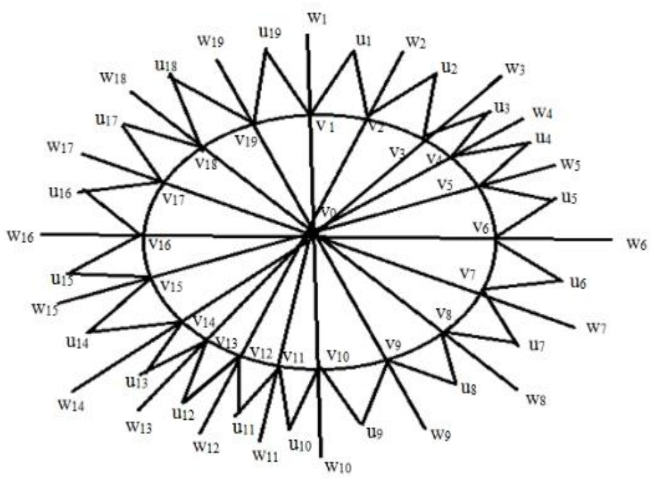

Fig-3

The PI index of G is given by PI(G) = $\sum_{e=uv\in E(G)} |n_u(e)+n_v(e)|$

Now

$$PI(G_{III}) = \sum_{e=uv\in E(G)} |n_u(e) + n_v(e)|$$

$$= \sum_{i=1}^{m} d(v_0, v_i) + \sum_{i=1}^{m}\sum_{j=i+1}^{m} d(v_i, v_j) + \sum_{i=1}^{m}\sum_{j=1}^{m} d(v_i, u_j) + \sum_{i=1}^{m}\sum_{j=1}^{m(p-5)} d(v_i, w_j)$$

$$= (p^2-3p+1)([8(p-4)(p-3)+(p-5)]+(p-2)]) + (p^2-3p+1)[(p-1)+(p-1)] + 2(p^2-3p+1)[(p-3)(p^2-3p-1)+(p-4)] + (p^2-3p+1)[((p-5)(p-1)+1)^2+(p-4)]$$

$$= (p^2-3p+1)[8p^4-142p^3+980p^2-3065p+3640]$$

Theorem 3.6: For p ≥ 5, the CO-PI index of type III Pseudo-regular graph G_{III} is

$$CO-PI(G_{III}) = (p^2-3p+1)[8p^4-142p^3+980p^2-3075p+3672]$$

Proof: Let G = G_{III} be a type III Pseudo-regular graph.

The CO-PI index of G is given by CO-PI(G) = $\sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$

Now

$$CO-PI(G_{III}) = \sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$$

$$= \sum_{i=1}^{m} d(v_0, v_i) + \sum_{i=1}^{m}\sum_{j=i+1}^{m} d(v_i, v_j) + \sum_{i=1}^{m}\sum_{j=1}^{m} d(v_i, u_j) + \sum_{i=1}^{m}\sum_{j=1}^{m(p-5)} d(v_i, w_j)$$

$$= (p^2-3p+1)([8(p-4)(p-3)+(p-5)]-(p-2)]) + (p^2-3p+1)[(p-1)-(p-1)] + 2(p^2-3p+1)[(p-3)(p^2-3p-1)-(p-4)] + (p^2-3p+1)[((p-5)(p-1)+1)^2-(p-4)]$$

$$= (p^2-3p+1)[8p^4-142p^3+980p^2-3075p+3672]$$

Theorem 3.7: For p = 3 only, the CO-PI index of type IV Pseudo-regular graph G_{IV} is

$$CO-PI(G_{IV}) = \frac{2x(x-3)}{3}, \text{where } x \geq 3n$$

Proof: Let G = G_{IV} be a type IV Pseudo-regular graph.

Let V(G) = { $v_0,v_1,v_2,\ldots,v_n,u_1,u_2,\ldots,u_{pn}$} be the vertex set of G and $v_0,v_1,v_2,\ldots,v_m$ be the central vertices form a cycle C_n. Adding P_4 on every vertex of C_n . i.e the end vertices of P_4 is joined with every vertex of C_n . Then the average degree of every vertex are equal. We obtained a Pseudoregular graph as below.

The construction of type III Pseudo-regular graph is shown in [14]. For p=3, we can get the following Pseudo-regular graph(Fig-4 and 5)

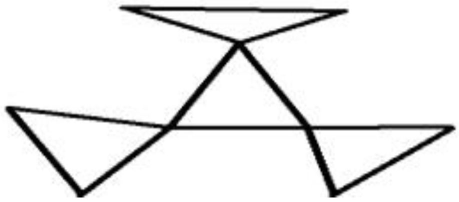

Fig-4

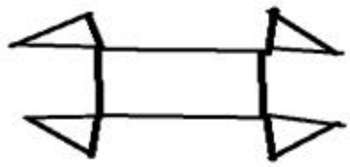

Fig-5

The CO-PI index of G is given by CO-PI(G) = $\sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$

Now

$$CO-PI(G_{III}) = \sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$$

$$= \sum_{i=1}^{n}\sum_{j=i+1}^{n} d(v_i, v_j) + \sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i, u_j) + \sum_{i=1}^{3n}\sum_{j=i+1}^{3n} d(u_i, u_j)$$

$$= \frac{2x(x-3)}{3}$$

Theorem 3.8: For p = 3 only, the CO-PI index of type V Pseudo-regular graph G_V is

$$CO-PI(G_V) = \frac{2x^2 - 8x}{3}, \text{ where } x \geq 3n$$

Proof: Let G = G_{IV} be a type V Pseudo-regular graph.

Let V(G) = { $v_0,v_1,v_2,\ldots,v_n,u_1,u_2,\ldots\ldots,u_{pn}$} be the vertex set of G and $v_0,v_1,v_2,\ldots,v_m$ be the central vertices form a cycle C_n. The n-copies of vertex – disjoint cycle C_4 are joined with C_n in such way that each C_4 and the cycle C_n have exactly one edge v_i v_j in common. It is denoted by G' $(C_{n,4})$.

The resulting graph is a Pseudo-regular graph is shown

The CO-PI index of G is given by CO-PI(G) = $\sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$

Now

$$CO-PI(G_V) = \sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$$

$$= \sum_{i=1}^{n}\sum_{j=i+1}^{n} d(v_i, v_j) + \sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i, u_j) + \sum_{i=1}^{3n}\sum_{j=i+1}^{3n} d(u_i, u_j)$$

$$= \frac{2x^2 - 8x}{3}$$

Theorem 3.9: For p = 3 only, the PI index of type V Pseudo-regular graph G_V is

$$PI(G_V) = \frac{-2x^3 + 60x^2 - 288x}{9}, \text{ where } x \geq 3n$$

Proof: Let G = G_{IV} be a type V Pseudo-regular graph.

Let V(G) = { $v_0,v_1,v_2,\ldots,v_n,u_1,u_2,\ldots\ldots,u_{pn}$} be the vertex set of G and $v_0,v_1,v_2,\ldots,v_m$ be the central vertices form a cycle C_n. The n-copies of vertex – disjoint cycle C_4 are joined with C_n in such way that each C_4 and the cycle C_n have exactly one edge v_i v_j in common. It is denoted by G' $(C_{n,4})$.

The resulting graph is a Pseudo-regular graph is shown

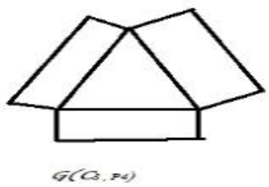

Fig-6

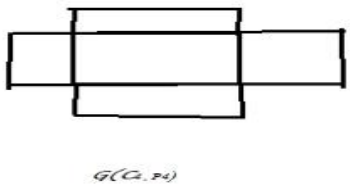

Fig-7

The CO-PI index of G is given by CO-PI(G) = $\sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$

Now

$$CO - PI(G_V) = \sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$$

$$= \sum_{i=1}^{n}\sum_{j=i+1}^{n} d(v_i, v_j) + \sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i, u_j) + \sum_{i=1}^{3n}\sum_{j=i+1}^{3n} d(u_i, u_j)$$

$$= \frac{-2x^3 + 60x^2 - 288x}{9}$$

Conclusion

In this paper. PI and Copi index of Pseudoregular graphs are computed.

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