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Research article

Computing Edge-PI index and Vertex-PI index of Circumcoronene Series of Benzenoid H_k by use of Cut Method

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Abstract

For a simple finite connected molecular graph *G=(V,E)*, we have many topological indices in graph theory. In molecular graph *G*, vertices are corresponding to the atoms and edges corresponding to the bonds. The number of atoms (vertices), and bonds (edges), are equal to $n=|V|$ and $m=|E(G)|$, respectively.

A simple topological index of *G* is the distance between vertices *u* and *v* of *G* (denoted by *d(u,v))*, and defined as the number of edges in a shortest path connecting them. One of oldest topological index of graph is Wiener index $W(G)=\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}d(u,v)$. Recently, we know *Padmakar-Ivan index* and *Szeged index* that are related to Wiener index and defined as $PI_e(G)=\sum_{e\in E(G)}\left(m_u(e|G)+m_v(e|G)\right)$ and $Sz_v(G)=\sum_{e\in E(G)}(n_u(e|G)n_v(e|G))$. The new version of *Padmakar-Ivan* index (Vertex Version of *PI* index, is $PI_v(G)=\sum_{e\in E(G)}(n_u(e|G)+n_v(e|G))$. In this paper, we focus on the structure of the circumcoronene series of benzenoid H_k and Computing a closed formula for $PI_e(H_k)$ and $PI_v(H_k)$ by use of *Cut Method*.

Keywords: Circumcoronene series of benzenoid; Wiener index; Padmakar-Ivan index; Szeged index; Cut Method.

Introduction

Let $G=(V,E)$, be a simple connected molecular graph of finite order $n=|V|$, such that it has vertex set $V=V(G)$, and edge set $E=E(G)$. In molecular graph G, vertices are corresponding to the atoms and edges corresponding to the bonds. An edge $e=uv$ of graph G is joined between two vertices u and v. The number of vertices and edges of G are denoted by n and $m=|E(G)|$, respectively.

In graph theory, an important terminology of graph is degree d_v of a vertex $v\in V(G)$ that it is the number of adjacent vertices with v or the size of first neighbourhood of vertex v. A general reference for the notation in graph theory is [1]. In mathematics chemistry, we have many topological indices for any molecular graph, that they are invariant on the graph automorphism. A simple topological index of G is the distance between vertices u and v of G. The distance between vertices u and v of G, denoted by $d(u,v)$, is the number of edges in a shortest path connecting them. Obviously, for edge $e=uv$, $d(u,v)=1$.

Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor. The Wiener index $W(G)$, is the oldest topological indices (based structure descriptors) [2-5], which have very chemical applications and mathematical properties. This defined as follow:

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

The other topological indices of graph (based structure descriptor), that was conceived somewhat later [5, 6], is the *hyper-Wiener index*

$$WW(G)=\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}\left(d(u,v)+d(u,v)^2\right).$$

$$=\frac{1}{2}W(G)+\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}d(u,v)^2.$$

Recently, Khadikar and co-authors [7-10] defined a new topological index and named it the Padmakar-Ivan index. Here Padmakar comes from *Padmakar Khadikar*, and Ivan from *Ivan Gutman*. They abbreviated this new topological index as $PI(G)$, (Of course, more precisely, we abbreviate it as $PI_e(G)$, because there exists also a vertex version of PI index). On the other hands, the Szeged index is another topological index which was introduced by Ivan Gutman (in 1994), and denoted by $Sz(G)$, (or, more precisely, $Sz_v(G)$) [11-13].

Suppose $e=uv\in E(G)$ is an edge connecting the vertices u and v, thus edge version of Padmakar-Ivan index and Szeged index of graph G are defined as

$$PI_e=\sum_{e\in E(G)}\left(m_u(e|G)+m_v(e|G)\right)$$

$$Sz_v=\sum_{e\in E(G)}\left(n_u(e|G)n_v(e|G)\right),$$

respectively. Also, $m_u(e|G)$ is the number of edges of G lying closer to u than to v and $m_v(e|G)$ is the number of edges of G lying closer to v than to u. $n_u(e|G)$ is the number of vertices of G lying closer to u and $n_v(e|G)$ is the number of vertices of G lying closer to v. Vertices and edges equidistance from u and v are not taken into accounts. In other words,

$$m_u(e|G)=\{x|x\in E(G),d(u,x)<d(x,v)\},$$

$$m_v(e|G)=\{x|x\in E(G),d(v,x)<d(x,u)\},$$

$$n_u(e|G)=\{y|y\in V(G),d(u,y)<d(y,v)\},$$

$$n_v(e|G)=\{y|y\in V(G),d(v,y)<d(y,u)\},$$

In 2007, A.R. Ashrafi and co-author introduced the vertex PI index of G, $PI_v(G)$, as the sum of $[n_u(e|G)+n_v(e|G)]$ over all edges of G. see [14]. We know an alternative formula for calculating the vertex PI index and edge PI index from [15] are equal to

$$PI_v=|V|.|E|-\sum_{e\in E(G)} n(e),$$

$$PI_e=\sum_{e\in E(G)}\left(m_u(e|G)+m_v(e|G)\right)=|E|^2-\sum_{e\in E(G)} m(e),$$

respectively. Where $n(e)$ and $m(e)$, denotes the number of vertices and edges equidistant from u,v respectively. Some applications of Padmakar-Ivan Index in Nanotechnology can be see in the review paper [16].

In this paper, we focus on the structure of the circumcoronene series of benzenoid H_k and obtain a closed formula for $PI_e(H_k)$ and $PI_v(H_k)$ by use of *Cut Method*. By these terminologies, we have following theorems. The following theorems are remake report and main result in this paper.

Theorem 1. *([17-19]), For the graphs from the circumcoronene series of benzenoid H_k ($k\geq 1$)*

$$W(H_k)=\tfrac{1}{5}(164k^5-30k^3+k)$$

***Theorem* 2.** *([6, 17]), The Hyper-Wiener index of the circumcoronene series of benzenoid H_k ($k\geq 1$) is equal to*

$$WW(H_k)=\frac{548}{15}k^6+\frac{82}{5}k^5-\frac{55}{6}k^4-3k3+\frac{17}{15}k^2+\frac{1}{10}k.$$

Theorem 3. *([17]), Let G be the the circumcoronene series of benzenoid H_k ($k\geq 1$). Then*

$$SZ_v(H_k)=\tfrac{3}{2}k^2(36k^4-k^2+1)$$

Theorem 4. *Consider the graph $G=H_k$ ($k\geq 1$) is circumcoronene series of benzenoid. Then edge version of PI index of G is equal to*

$$PI_e(H_k)=81k^4-68k^3+12k^2-k$$

Theorem 5. *The vertex-PI index of circumcoronene series H_k ($k\geq 1$) is $PI_v(H_k)=54k^4-18k^2$*

In next section, we introduce the modify form of cut method and rewrite the definition of it for circumcoronene series of benzenoid H_k $(k\geq 1)$. Finally, we proof the theorems 4 and 5 by use of Orthogonal Cuts of H_k.

Main Results and Discussions

The benzene molecule is a usual chemical structure in chemistry, physics and nano sciences. This molecule is very useful to synthesize aromatic compounds. The circumcoronene series of benzenoid H_k is one family that generate from benzene molecule. A famous member of this family is coronene H_2 (or $Ca(C_6)$ that it is first term of Capra-designed planar benzenoid series $Ca_n(C_6)$, see [20-30]).

The first terms of this series are H_1=*Benzene*, H_2=*Coronene*, H_3=Circumcoronene H_4=Circumcircumcoronene see Figure 1, where they are shown. The general representation of circumcoronene series of benzenoid is shown in Figure 2. For more study of these molecular graphs see the paper series [6, 17, 18, 20, 21, 31-62].

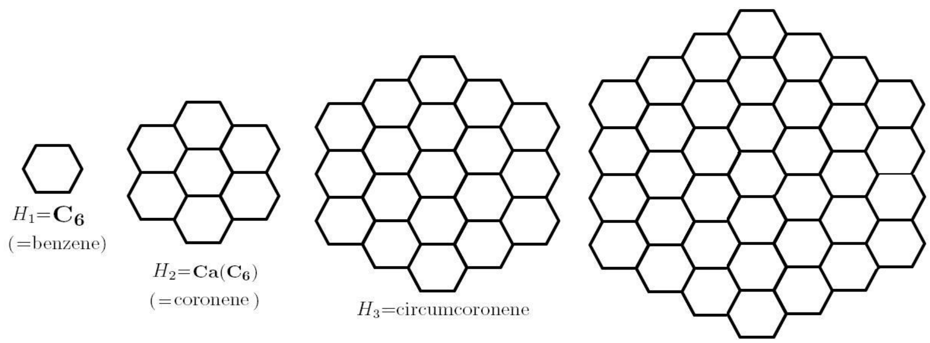

Figure 1: The first three graphs H_1, H_2, H_3 and H_4 from the circumcoronene series, such that H_1, H_2 are graphs C_6 and the Capra of planer benzenoid $Ca(C_6)$, respectively.

On the other hands, since the circumcoronene series of benzenoid has a very remarkable structure, we lionize it and present a closed formula for the vertex-PI index and edge-PI index of general case of circumcoronene series of H_k $(k\geq 1)$ For computing the vertex-PI index and edge-PI index and achieve our aims, we using the *Cut Method* and find *Orthogonal Cuts* of H_k. For a molecular graph G, *Sandi Klavžar* described and studied the general form of cut method in the paper [17] and we introduce the following definition from [17].

Definition 1. *Let G=(V,E), be molecular graph. Then, the cut method, dividing edge set and vertex set of G into several partitions as follow:*

1- Partition the edge set of G into classes $C_1,...,C_h$ *call them cuts, such that each of the sub-graphs G-*C_i *i=1,...,h, consists of two (or more, connected components.*

2- Use properties (of the components), of the graphs G-C_i *to derive a required property of G.*

The cut method can hardly be studied in the above generality and isn't useful for our aims. The cut method turned out to be especially useful when if comes to metric properties of graphs.

So, we are using an especial form of the cut method. These interesting cuts, which called Orthogonal Cuts. An orthogonal cut $C(e)$, with respect to edge e is the set of all edges $e\in E(G)$ which are strongly co-distant to e [62].

$$C(e):=\{e' \in E(G) | e' \text{ is co-distant with } e\}$$

Reader can see these cut of circumcoronene series of benzenoid H_4 in Figure 3. Also, for further research and study of the cut method and orthogonal cuts in some classes of chemical graphs, see [17, 62]. Some applications of the cut method include the Wiener index, hyper-Wiener index, weighted Wiener index, Wiener-type, edge Szeged index and classes of chemical graphs such as trees, benzenoid graphs and phenylenes.

Now, we start the proof of theorems, which exhibited in above section.

Proof of Theorem 4. Let $G=H_k$ be the circumcoronene series of benzenoid. We know that the general case of this family have $6k^2=n_k$ vertices and $9k^2-3k=m_k$ edges. By according to Figure 3, we see that the number of cutting edges by orthogonal cut C_i, $i=1,...,k$ (a particular case of Definition 1 is $h=k$, is equal to $k+i$ and $|C_i|=k+i$. Obviously, there exist five other cuts similar to cut C_i $(i=1,\ldots,k-1)$ and are two cuts similar to C_k. In other words,

$$m_k = 3|C_k| + 6|C_{k-1}| + \ldots + 6|C_1| = 6\sum_{i=1}^{k}[k+i] - 6k.$$

Now, by refer to definition of edge-PI index, we need to compute $m_u(e|H_k)$ and $m_v(e|H_k)$ for every edge $e \in E(G)$. So, we denote all edge $e=uv$ belong to cut C_i by $e(i)$ and rewrite $m_v(e(i)|H_k)=mv_i$ as the number of edges from small half of sub-graph G-C_i and $m_u(e(i)|H_k)=mu_i$ as the number of edges from large half of sub-graph G-C_i, see Fig. 3.

Thus $$PI_e = \sum_{e \in E(G)} \left(m_u(e|G) + m_v(e|G)\right) = \sum_{e(i) \in C_i, i=1}^{k} \left(mu_i + mv_i\right)$$

On the other hands, an important property of orthogonal cut is determining the co-distance edges of G ($\forall\, e=uv$, $f=xy \in C_i$ $d(e,x)=d(e,y)$ and $d(f,u)=d(f,v)$), see Figure 3. Thus, $mu_i+mv_i = \underbrace{|E(G)| - |C_i|}_{m(e(i))}$. We denote the distance between mv_i and mv_{i-1} by xm_i (or $xm_i=mv_i-mv_{i-1}=mu_{i-1}-mu_i$). It is clear that $xm_i = |C_{i-1}| + 2|C_{i-1}|$ such that $xm_1=2k=mv_1$, see Figure 3. So,

$$\begin{aligned}
mv_i &= xm_i + mv_{i-1} \\
&= xm_i + xm_{i-1} + mv_{i-2} \\
&= \vdots \\
&= \sum_{j=2}^{i} xm_j + mv_1 \\
&= 2k + 3\sum_{j=2}^{i}(k+j-1) \\
&= 2k + 3k(i-1) + 3\sum_{j=1}^{i-1} j
\end{aligned}$$

$$= 3ki - k + \frac{3i(i-1)}{2}$$

$$= \frac{3}{2}i^2 + i\left(3k - \frac{3}{2}\right) - k$$

It is obvious that $mv_k = \frac{9}{2}k^2 - \frac{5}{2}k$.

Now, in continue of equation 2.1,

$$PI_e = \sum_{i=1}^{k}[6|C_i|(mu_i + mv_i)] - 3|C_k|(mu_k + mv_k)$$

$$= 6\sum_{i=1}^{k}[(k+i)(m-|C_i|)] - 6k(9k^2 - 5k)$$

$$= 6\sum_{i=1}^{k}[9k^3 - 4k^2 + i(9k^2 - 5k) - i^2] - 54k^3 - 30k^2)$$

$$= 54k^3 - 24k^2 + \frac{6k(k+1)}{2}\left(9k^2 - 5k\right) - \frac{6k(k+1)(2k+1)}{6} - \left(54k^3 - 30k^2\right)$$

$$= 54k^4 - 24k^3 + 3k^2(k-1)(9k-5) - 2k^3 - 3k^2 - k$$

$$= 81k^4 - 68k^3 + 12k^2 - k$$

Hence, this completes the proof of Theorem 4.■

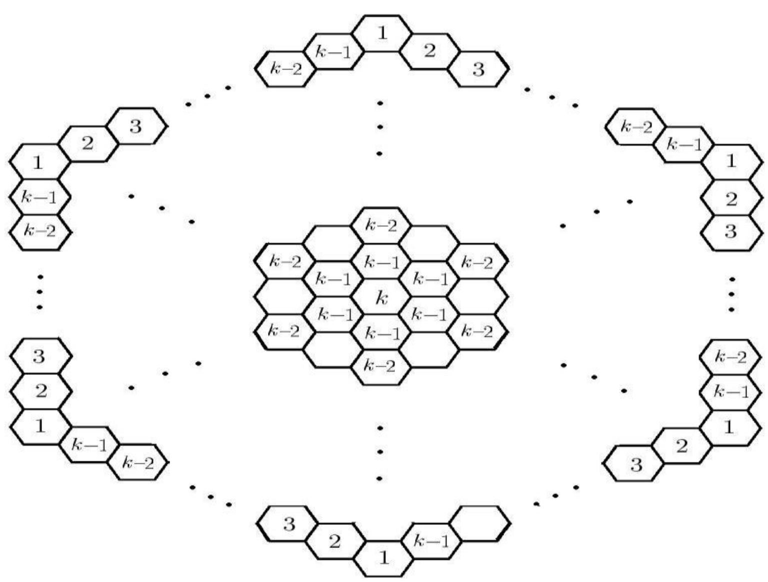

Figure 2: The circumcoronene series of benzenoid H_k $(k \geq 1)$.

Example 1. The edge-PI index of circumcoronene H_3 is $PI_e(H_3)=4938$. Since, there exist 3 orthogonal cuts and implies that $mu_1=6$, $mv_1=62$, $mu_2=18$, $mv_2=49$, $mu_3=33$ and $mv_3=33$, see Figure 3. The number of repetition of first and second orthogonal cuts are equal to six and the number of repetition of third orthogonal cut is equal to three. Thus,

$$PI_e(H_3) = \sum_{e \in E(H_3)} \left(m_u(e \mid H_3) + m_v(e \mid H_3) \right) = 6\times4(6+62)+6\times5(18+49)+3\times6(33+33)=4938$$

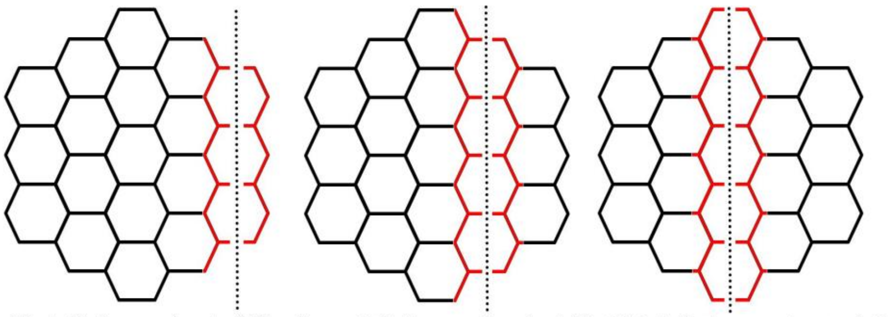

Figure 3: The presentation of cut method (orthogonal cut) on the circumcoronene $H_{3.}$

Proof of Theorem 5. Consider circumcoronene series of benzenoid H_k for every $k \geq 1$. We denote the number of vertices from small half of sub-graph G-C_i for all edge $e(i)$, belong of cut C_i ($\forall\ 1,\ldots,k$) by $nv_i = n_v(e(i)|H_k)$ and the number of edges from large half of sub-graph G-C_i by $nv_{i.}$ Now, let the distance between nv_i and nv_{i-1} be equal to nv_i (or $xn_i = nv_i - nv_{i-1} = nu_{i-1} - nu_i$ and $xn_1 = nv_1 = 2k+1$ By refer to Figure 3, it is obvious that $xn_i = 5k+2i-1(\forall\ 1,\ldots,k)$. So, by solve this recursive sequence, nv_i is equal to

$$\begin{aligned}
nv_i &= xn_i + nv_{i-1} \\
&= xn_i + xn_{i-1} + nv_{i-2} \\
&= \vdots \\
&= \sum_{j=2}^{i} xn_j + nv_1 \\
&= \sum_{j=1}^{i} (2k+2j-1) \\
&= i(2k-1) + 2\underbrace{\sum_{j=1}^{i} j}_{\frac{i(i+1)}{2}} \\
&= i^2 + ki
\end{aligned}$$

Obviously from equation 2.4, $nv_k = nu_k = k^2 + 2k^2 = n/2$ and $nu_i = n_k - nv_i = 6k^2 + 2ki - i^2$ (since $n(e(i))=0$). Now, by similar argument with above proof and using definition of vertex-PI index, we have

$$PI_v = \sum_{e \in E(G)} \left(n_u(e \mid G) + n_v(e \mid G) \right)$$

$$= \sum_{e(i)\in C_i, i=1}^{k} (nu_i + nv_i)$$

$$= \sum_{i=1}^{k-1} [6|C_i|(nu_i + nv_i)] + 3|C_k|(nu_k + nv_k)$$

$$= 6n_k \sum_{i=1}^{k-1} [k+i] + 3(2k)n_k$$

$$= 36k^2[k(k-1) + \frac{k(k-1)}{2}] + 36k^3$$

Thus, vertex-PI index of circumcoronene series of benzenoid H_k $(k\geq 1)$ is equal to $PI_v(H_k)=54k^4-18k^2$ and this completes the proof.■

Example 2. The vertex-PI index of circumcoronene H_3 is $PI_v(H_3)=3888$. Since, there exist 3 orthogonal cuts and implies that $nu_1=7$, $nv_1=47$, $nu_2=16$, $nv_2=38$, $nu_3=27$, and $nv_3=33$, see Figure 3. The number of repetition of first, second and third orthogonal cuts are equal to 6, 6 and 3, respectively. Hence,

$$PI_v(H_3) = \sum_{e\in E(H_3)} \left(n_u(e|H_3) + n_v(e|H_3)\right) = 6\times 4(7+47) + 6\times 5(16+38) + 3\times 6(27+27) = 3888.$$

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