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Edge-Wiener Indices of n-circumscribed Peri-condensed Benzenoid Graphs

Research Article

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Abstract: The cut method demonstrates its usefulness especially for the topological indices that are based on the distances in the molecular graphs without actually calculating the distances between pairs of vertices. The Wiener index is equal to the sum of distances between all pairs of vertices of the connected graph G, whereas the Edge-Wiener index is the sum of distances between all pairs of edges of the connected graph G. In this paper we calculate the Edge-Wiener indices of Circum-polyacenes, Circum-pyrenes and Circum-trizenes.

MSC: 05C12, 05C90, 05C76.

Keywords: Edge-Wiener indices, Cut method, Circum-polyacenes, Circum-pyrenes and Circum-trizenes.

1. Introduction

A benzenoid system or hexagonal system, honeycomb system is a finite connected subgraph of the infinite hexagonal lattice with no cut vertices or non-hexagonal internal face [1]. Topological indices are designed basically by transforming a molecular graph into a number. The oldest and one of the most thoroughly studied distance-based molecular structure-descriptors is the Wiener index was introduced by the Chemist Harold Wiener in 1947, to analyze the chemical properties of alkanes(paraffins). Since then, numerous articles were published [2–9] in the chemical and mathematical literature, devoted to the Wiener index and various methods for its calculation and edge-version [12–15] of the Wiener index eluded the attention of both pure and applied graph theoreticians. The Wiener index is equal to the sum of distances between all pairs of vertices of the connected graph G, whereas the Edge-Wiener index is the sum of distances between all pairs of edges of the connected graph G. Distance properties of molecular graphs play a vital role in chemical graph theory. Topological indices are used in theoretical chemistry for the design of quantitative structure-property relations (QSPR) and quantitative structure-activity relations (QSAR). The cut method demonstrates its usefulness especially for the topological indices that are based on the distances in the molecular graphs without actually calculating the distances between pairs of vertices [10, 11].

2. Basic Concepts and Terminology

A molecular graph is a representation of the structural formula of the chemical compound. Let G be a simple molecular graph which consists of vertices $V(G)$ and a set of edges $E(G)$ respectively such that a collection of vertices representing

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the atoms in the molecule and a set of edges representing the chemical bonds between the carbon atoms.

Proposition 2.1 ([11]). *Let G be a connected graph. Then G admits a partition of $E(G)$ into convex cuts if and only if G is a partial cube.*

Theorem 2.2 ([11]). *Let G be a partial cube and let $F_1, ..., F_k$ be its Θ-classes. Let $m_1(F_i)$ and $m_2(F_i)$ be the number of edges in the two connected components of $G - F_i$. Then $W_e(G) = \sum_{i=1}^{k} m_1(F_i)m_2(F_i)$.*

Corollary 2.3 ([10]). *Let B be a benzenoid graph and $\mathcal{C}$ the set of its orthogonal cuts. For $C \in \mathcal{C}$, let $\eta_1(C)$ and $\eta_2(C)$ be the number of edges in the two components of $G - C$, respectively. Then $W_e(G) = \sum_{C \in \mathcal{C}} \eta_1(C)\eta_2(C)$.*

We rewrite the above corollary for ease of calculation.

Corollary 2.4. *Let G be a benzenoid graph and let $\{S_1, S_2, S_3, ..., S_p\}$, be a partition of $E(G)$ such that each S_i is an edge cut of G and the removal of edges of S_i leaves G into two components, then the Edge-Wiener index of the graph G is given by $W_e(G) = \sum_{i=1}^{p} |m_1(S_i)||m_2(S_i)|$, where $|m_1(S_i)|$ is the number of edges in the first component and $|m_2(S_i)|$ is the number of edges in the second component.*

3. Edge-Wiener Indices of Circum-polyacenes

In this section, we compute exact analytical expressions for the Edge-Wiener indices of various n-Circum-polyacenes. Particular cases of interest are Circum-naphthalenes(n), Circum-anthracenes(n), Circum-tetracenes(n), Circum-pentacenes(n), Circum-hexacenes(n). As detailed proofs for each of these structures take up a large amount of space, we only show one case for each class in sufficient details with mathematical proofs; in this case the proof is given in depth for Circum-hexacenes(n). The proofs of the remaining structures are similar and we have shown the final simplified expressions in Table 1. In the ensuing paragraphs we show mathematical details of how we obtain the final results exemplifying with Circum-hexacenes(n). Let L_m denote a linear chain of m hexagons. See Figure 1(a). Adding k layers of hexagons to the boundary of L_m gives rise to various chemical structures. The structures when m=6 and k=1,2 are Circum-hexacene(1) and Circum-hexacene(2). See Figure 1(b) and Figure 1(c).

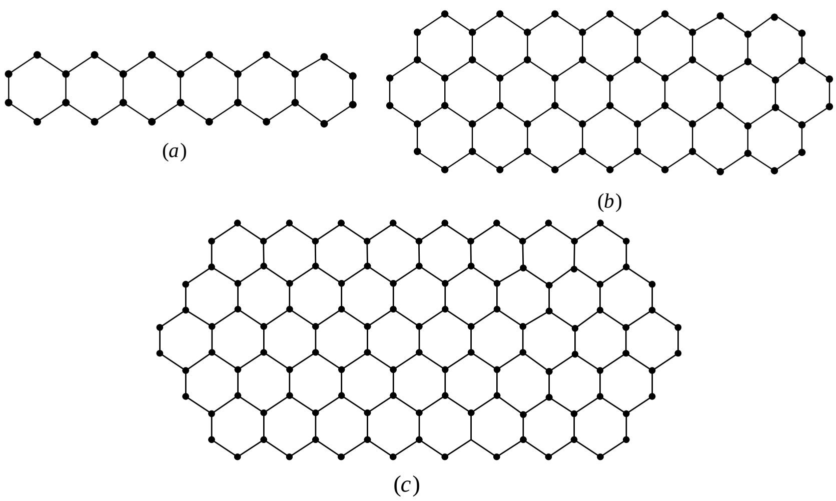

Figure 1 : (a)Linear chain of 6 hexagons (b) Circum-hexacene(1)

(c) Circum-hexacene(2)

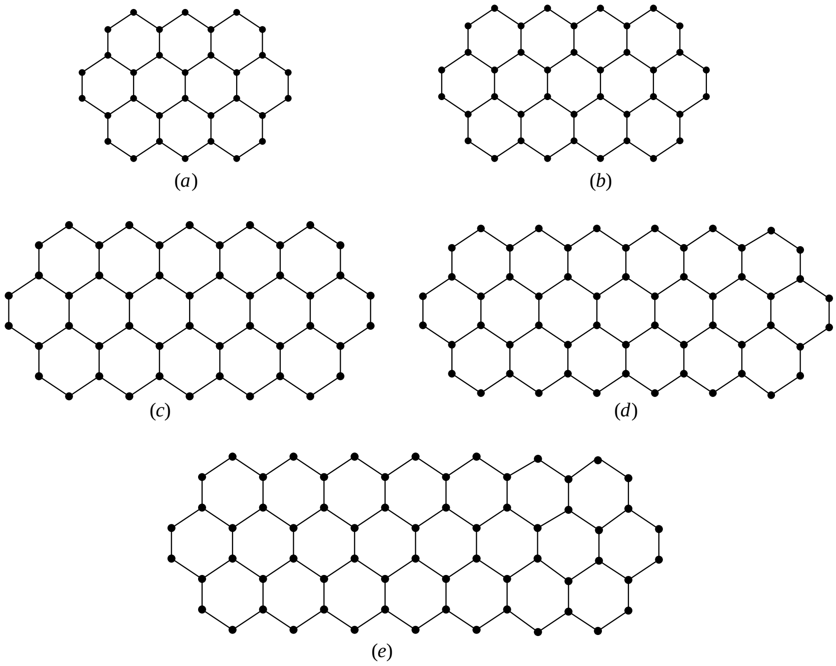

Figure 2 : (a) Circum-naphthalene(1) (b) Circum-anthracene(1)

(c) Circum-tetracene(1) (d) Circum-pentacene(1) (e) Circum-hexacene(1)

3.1. Circum-hexacenes(n) and Linear Polyacenes

Theorem 3.1. *The Edge-Wiener indices of* $Circum-hexacenes(n)$ *is given by*

$$W_e = \frac{[738n^5 + 8820n^4 + 38020n^3 + 72855n^2 + 60687n + 17920)]}{10}.$$

Proof. We use horizontal and diagonal cuts shown in Figure 3 in the edge set of $Circum-hexacene(1)$. Now let S_0 be the horizontal center cut, $\{S_i : 1 \leq i \leq n\}$, $\{S_{-i} : 1 \leq i \leq n\}$ be the horizontal cuts which are parallel to S_0 from the top and bottom respectively as shown in the Figure 3. For $i = 1, 2$, let $\{S_i^j : 1 \leq j \leq n+1\}$ be the diagonal edge cuts from the upper and lower left corners as shown in the Figure 3. Similarly, for $i = 1, 2$, let $\{S_{-i}^j : 1 \leq j \leq n+1\}$ be the diagonal edge cuts from the upper and lower right corners as shown in the Figure 3. Let $\{S_{\pm i}^j : 1 \leq i \leq 2, j = n+2\}$ be the diagonal cuts as shown in the Figure 1.1. Let $\{S_{\pm i}^j : 1 \leq i \leq 2, j = n+3\}$ be the diagonal cuts as shown in the Figure 3.

Removal of S_0 leaves Circum-hexacenes(n) into two components G_{S_i} and G'_{S_i} where $|E(G_{S_i})| = \frac{1}{2}[9n^2+43n+24]$, $|E(G'_{S_i})| = \frac{1}{2}[9n^2 + 43n + 24]$. For $1 \leq i \leq n$, the removal of S_i leaves Circum-hexacenes(n) into two components G_{S_i} and G'_{S_i} where $|E(G_{S_i})| = \sum_{i=1}^{n} \frac{1}{2}[5i^2 + 3i(2n+9) - 2n - 8]$, $|E(G'_{S_i})| = \sum_{i=1}^{n} \frac{1}{2}[18n^2 + 90n - 5i^2 - i(6n+29) + 58]$.

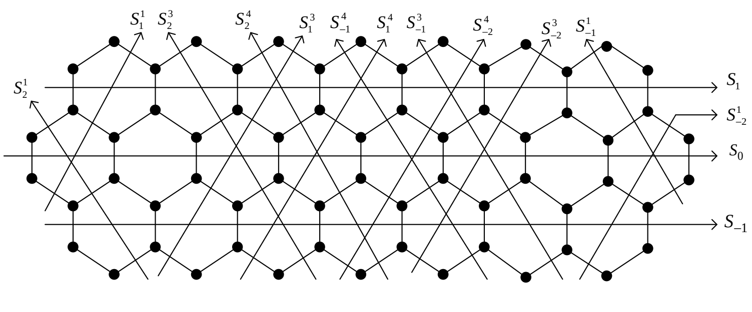

Figure 3 : Circum- hexacene(1) with cuts

For $1 \leq i \leq n$, the removal of S_{-i} leaves Circum-hexacenes(n) into two components $|G_{S_{-i}}$ and $G'_{S_{-i}}$ where $|E(G_{S_{-i}})| = \sum_{i=1}^{n} \frac{1}{2}[5i^2 + 3i(2n+9) - 2n - 8]$, $|E(G'_{S_{-i}})| = \sum_{i=1}^{n} \frac{1}{2}[18n^2 + 90n - 5i^2 - i(6n+29) + 58]$.

For S_i^j, $i = 1, 2$, $1 \leq j \leq n+1$, removal of the edges in S_i^j, leaves Circum-hexacenes(n) into two components $G_{S_i^j}$ and $G'_{S_i^j}$ where $|E(G_{S_i^j})| = \sum_{i=1}^{n+1}[3i^2 + 3i(2n+1) - 2n - 2]$, $|E(G'_{S_i^j})| = \sum_{i=1}^{n+1}[18n^2 + 90n - 3i^2 - i(6n+5) + 62]$.

Similar results hold good when S_{-i}^j, $i = 1, 2$, $1 \leq j \leq n+1$.

For $\{S_{\pm i}^j : 1 \leq i \leq 2, j = n+2\}$, removal of the edges in $S_{\pm i}^j$, leaves Circum-hexacenes(n) into two components $G_{S_{\pm i}^j}$ and $G'_{S_{\pm i}^j}$ where $|E(G_{S_{\pm i}^j})| = 2[9n^2 + 25n + 14]$, $|E(G'_{S_{\pm i}^j})| = 2[9n^2 + 61n + 44]$.

For $\{S_{\pm i}^j : 1 \leq i \leq 2, j = n+3\}$, removal of the edges in $S_{\pm i}^j$, leaves Circum-hexacenes(n) into two components $G_{S_{\pm i}^j}$ and $G'_{S_{\pm i}^j}$ where $|E(G_{S_{\pm i}^j})| = 2[9n^2 + 37n + 24]$, $|E(G'_{S_{\pm i}^j})| = 2[9n^2 + 49n + 34]$.

$$\begin{aligned}
W_e(Circum-hexacenes(n)) &= \frac{1}{2}[9n^2 + 43n + 24]^2 + \sum_{i=1}^{n+1}[(3i^2 + 6ni + 3i - 2n - 2)(18n^2 \\
&+ 90n + 62 - 6ni - 3i^2 - 5i)] + \frac{1}{2}\sum_{i=1}^{n}[(5i^2 + 27i + 6ni - 2n \\
&- 8)(18n^2 - 5i^2 + 90n + 58 - 6ni - 29i)] + [(9n^2 + 25n \\
&+ 14)(9n^2 + 61n + 44)] + [(9n^2 + 37n + 24)(9n^2 + 49n + 34)] \\
&= \frac{[738n^5 + 8820n^4 + 38020n^3 + 72855n^2 + 60687n + 17920)]}{10}
\end{aligned}$$

□

We have employed cuts similar to the ones shown in Figure 3 for simple linear polyacenes containing m hexagons which we denote by L_m. On the basis of the same procedure we obtain the following expression for the Edge-Weiner index, W_e for any L_m as

$$W_e(L_m) = \frac{1}{6}[50m^3 - 6m^2 + 28m]$$

This result matches with a recent result obtained by Chen et al.[16] for the Wiener index of the associated line graph of L_m by the following simplification:

$$\begin{aligned}
W(LG(L_m)) &= \frac{1}{6}[50m^3 + 69m^2 + 43m] \\
&= W_e(L_m) + \binom{m_e}{2}
\end{aligned}$$

where m_e = number of edges of L_m = 5m+1, by substituting this value for m_e back into above equation we get the result for $W_e(L_m)$ as

$$\begin{aligned}
W(LG(L_m)) &= W_e(L_m) + \binom{m_e}{2} \\
&= \frac{1}{6}[50m^3 - 6m^2 + 28m] + \frac{5m(5m+1)}{2} \\
&= \frac{1}{6}[50m^3 + 69m^2 + 43m]
\end{aligned}$$

Thus we obtain W_e for the first 5 members of linear polyacene series as 72, 230, 536, 1040, 1792 for naphthalene, anthracene, tetracene, pentacene and hexacene, respectively. These numbers are identical to the constant terms in our expressions for Circum-L_m listed in Table 1 obtained using cut methods, as the order of circumscribing goes to 0 we get the W_e for linear polyacenes, providing independent confirmations to our technique. These confirmations provide further proof to our technique. We note that the Edge-Wiener index W_e of graphs considered here and the associated Wiener index of the line graph differ by a factor of $\frac{m_e(m_e-1)}{2}$.

4. Edge-Wiener Indices of Circum-pyrenes and Circum-trizenes

In this section, we find Edge-Wiener indices of the structures Circum-pyrenes(n) and Circum-trizenes(n), out of which the proof is given in detail for Circum-pyrenes(n). The proof of the Circum-trizenes(n) is similar and we have given their results in Table 2. Figure 4(a) depicts the graph of Circum-pyrene(1). Circum-pyrene(2) is obtained by adding a layer of hexagons to the boundary of Circum-pyrenes(1) as shown in Figure 4(b). Inductively, Circum-pyrenes(n) is obtained from Circum-pyrenes($n-1$) by adding a layer of hexagons around the boundary of Circum-pyrenes($n-1$). Similar construction follows for Circum-trizenes(n). See Figure 4(c) and Figure 4(d).

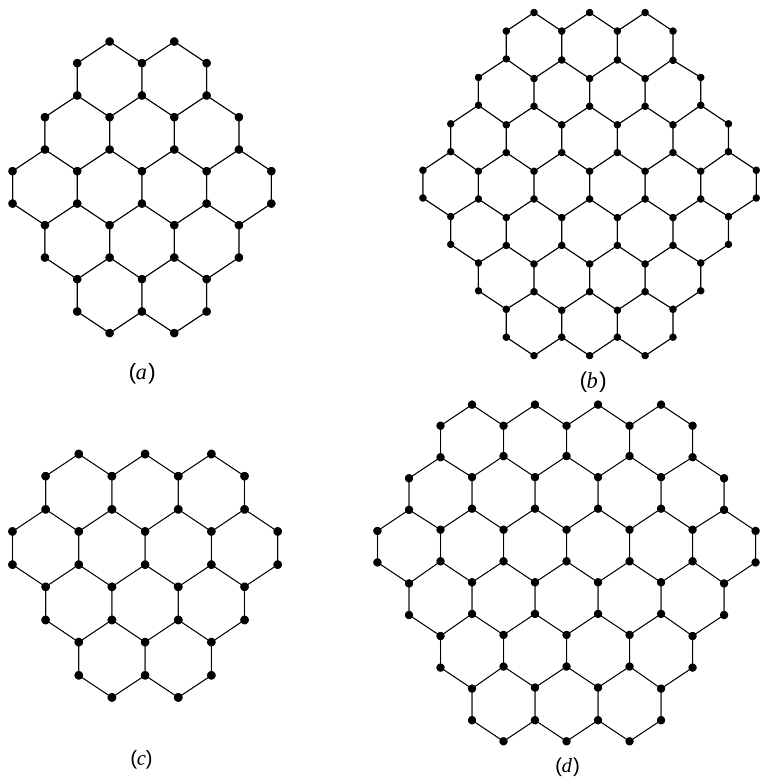

Figure 4 : (a) Circum-pyrene(1) (b) Circum-pyrene(2)

(c) Circum-trizene(1) (d) Circum-trizene(2)

4.1. Circum-pyrenes(n)

Theorem 4.1. *The Edge-Wiener indices of Circum-pyrenes(n) is given by*

$$W_e = \frac{[738n^5 + 5130n^4 + 13960n^3 + 18615n^2 + 12207n + 3160)]}{10}$$

Proof. We use horizontal and diagonal cuts shown in Figure 5 that yield an I-partition of the edge set of Circum-pyrene(1). Now let S_0 be the horizontal center cut, $\{S_i : 1 \leq i \leq n+1\}$, $\{S_{-i} : 1 \leq i \leq n+1\}$ be the horizontal cuts which are parallel to S_0 from the top and bottom respectively as shown in the Figure 5. For $i = 1, 2$, let $\{S_i^j : 1 \leq j \leq n+1\}$

be the diagonal edge cuts from the upper and lower left corners as shown in the Figure 5. Similarly for $i = 1, 2$, let $\{S^j_{-i} : 1 \leq j \leq n+1\}$ be the diagonal edge cuts from the upper and lower right corners as shown in the Figure 5. We observe that S_0, $\{S_i : 1 \leq i \leq n+1\}$, $\{S_{-i} : 1 \leq i \leq n+1\}$, $\{S^j_i : 1 \leq i \leq 2, 1 \leq j \leq n+1\}$ and $\{S^j_{-i} : 1 \leq i \leq 2, 1 \leq j \leq n+1\}$ forms an edge set of Circum-pyrenes(n). Removal of S_0 leaves Circum-pyrenes(n) into two components G_{S_i} and G'_{S_i} where $|E(G_{S_i})| = \frac{1}{2}[9n^2 + 25n + 16]$, $|E(G'_{S_i})| = \frac{1}{2}[9n^2 + 25n + 16]$.

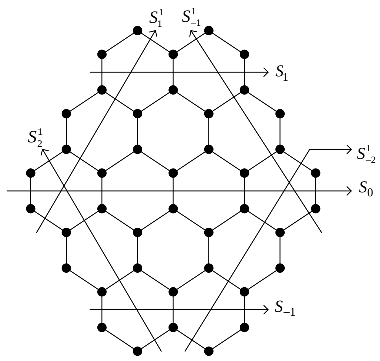

Figure 5 : Circum-pyrene(1)with cuts

For $1 \leq i \leq n+1$, the removal of S_i leaves Circum-pyrenes(n) into two components G_{S_i} and G'_{S_i} where $|E(G_{S_i})| = \sum_{i=1}^{n+1}[\frac{1}{2}(3i^2 + 3i(2n+1) - 2n - 2)]$ $|E(G'_{S_i})| = \sum_{i=1}^{n+1}[\frac{1}{2}(18n^2 + 54n - 3i^2 - i(6n+5) + 38)]$.
For $1 \leq i \leq n+1$, the removal of S_{-i} leaves Circum-pyrenes(n) into two components $G_{S_{-i}}$ and $G'_{S_{-i}}$ where $|E(G_{S_{-i}})| = \sum_{i=1}^{n+1}[\frac{1}{2}(3i^2 + 3i(6n+1) - 2n - 2)]$, $|E(G'_{S_{-i}})| = \sum_{i=1}^{n+1}[\frac{1}{2}(18n^2 + 54n - 3i^2 - i(6n+5) + 38)]$.
For S^j_i, $i = 1, 2$, $1 \leq j \leq n+1$, removal of the edge cuts S^j_i, leaves Circum-pyrenes(n) into two components $G_{S^j_i}$ and $G'_{S^j_i}$ where $|E(G_{S^j_i})| = \sum_{i=1}^{n+1}[3i^2 + i(6n+1) - 2n + 4]$, $|E(G'_{S^j_i})| = \sum_{i=1}^{n+1}[18n^2 + 54n - 3i^2 - 3i(2n+1) + 30]$. Similar results hold good when S^j_{-i}, $i = 1, 2$, $1 \leq j \leq n+1$. Hence,

$$\begin{aligned}
W_e(Circum-pyrenes(n)) &= \frac{1}{2}[9n^2 + 25n + 16]^2 + \sum_{i=1}^{n+1}[3i^2 + i(6n+1) - 2n + 4][18n^2 \\
&+ 54n - 3i^2 - 3i(2n+1) + 30] + \frac{1}{2}\sum_{i=1}^{n+1}[3i^2 + 3i(2n+1) - 2n \\
&- 2][18n^2 + 54n - 3i^2 - i(6n+5) + 38] \\
&= \frac{[738n^5 + 5130n^4 + 13960n^3 + 18615n^2 + 12207n + 3160)]}{10}
\end{aligned}$$

□

Table 1. W_e **of Circum-polyacenes**

Fig. No	Structural Name	Formula
2.a	Circum-naphthalenes(n)	$\frac{[738n^5+3900n^4+7940n^3+7815n^2+3767n+720)]}{10}$
2.b	Circum-anthracenes(n)	$\frac{[738n^5+5130n^4+13480n^3+16785n^2+10017n+2300)]}{10}$
2.c	Circum-tetracenes(n)	$\frac{[738n^5+6360n^4+20340n^3+30135n^2+20787n+5360)]}{10}$
2.d	Circum-pentacenes(n)	$\frac{[738n^5+7590n^4+28520n^3+48585n^2+37277n+10400)]}{10}$
2.e	Circum-hexacenes(n)	$\frac{[738n^5+8820n^4+38020n^3+72855n^2+60687n+17920)]}{10}$

Table 2. W_e **of Circum-pyrenes and Circum-trizenes**

Fig.No.	Structure Name	Formula
4.a	Circum-pyrenes(n)	$\frac{[738n^5+5130n^4+13960n^3+18615n^2+12207n+3160)]}{10}$
4.c	Circum-trizenes(n)	$\frac{[738n^5+4515n^4+10770n^3+12540n^2+7167n+1620)]}{10}$

5. Concluding Remarks

In this paper, we have obtained exact analytical expressions for the Edge-Wiener indices of a number of circumscribed peri-condensed polycyclic aromatic benzenoid hydrocarbons. We have employed cut methods to obtain these expressions which are shown to be polynomials of 5-th degree as a function of n, where n is the order of circumscribing. The current techniques can be extended to obtaining other topological indices such as the Edge-Szeged index, Gutman index, Schultz index etc.,

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