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A New Version of Hyper–Wiener Index

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Abstract

The hyper-Wiener index is one of topological descriptors of chemical structures. It is based on distances between vertices. In this paper, we introduce its edge versions and compute these new indices for some well-known graphs such as path, cycle, complete graphs. In addition, we compute these indices for hexagonal chains.

1. Introduction

The ordinary (vertex) Wiener index is one of the oldest molecular-graph-based structure-descriptors [1, 2] and its chemical and mathematical applications are well-documented [3-6]. This version of Wiener index was based on distances between vertices in connected graph G and it is:

$$W(G) = W_v(G) = \sum_{\{x,y\} \subseteq V(G)} d(x,y)$$

where $d(x,y)$ is the distance between vertices x and y.

In addition, the edge versions of Wiener index were introduced by Iranmanesh et al. in 2008 as follow [7]. The first edge-Wiener number is:

$$W_{e0}(G) = \sum_{\{e,f\} \subseteq E(G)} d_0(e,f)$$

where $d_0(e,f) = \begin{cases} d_1(e,f)+1 & e \neq f \\ 0 & e = f \end{cases}$ and

$d_1(e,f) = \min\{d(x,u), d(x,v), d(y,u), d(y,v)\}$ such that $e = xy$ and $f = uv$. In fact we have $W_{e0}(G) = W_v(L(G))$.

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Here, the line graph $L(G)$ is the intersection graph of the edges of G, where vertices correspond to edges of G and vertices in L(G) are adjacent if the corresponding edges share a vertex.

The second edge-Wiener index is:

$$W_{e4}(G) = \sum_{\{e,f\}\subseteq E(G)} d_4(e,f)$$

where $d_4(e,f) = \begin{cases} d_2(e,f) & e \neq f \\ 0 & e = f \end{cases}$ and

$d_2(e,f) = \max\{d(x,u), d(x,v), d(y,u), d(y,v)\}$ such that $e = xy$ and $f = uv$.

The hyper-Wiener index of acyclic graphs was introduced by Milan Randić in 1993. Then Klein et al. [8], generalized Randić's definition for all connected graphs, as a generalization of the Wiener index. It is defined as:

$$WW(G) = WW_v(G) = \frac{1}{2}W_v(G) + \frac{1}{2}\sum_{\{x,y\}\subseteq V(G)} d^2(x,y)$$

where $d^2(x, y) = d(x, y)^2$. We encourage the reader to consult [8–14] for the mathematical properties of hyper-Wiener index and its applications in Chemistry.

In this paper, we introduce its edge versions and compute these new indices for some well-known graphs such as path, cycle, complete graphs. In addition, we compute these indices for hexagonal chains.

2. Some definitions and results

In this section, we introduce the edge versions of desire indices.

Definition 2.1. The edge versions of hyper-Wiener indices are:

$$WW_{ei}(G) = W_{ei}(G) + W_{ei}^{d^2}(G)$$

where $W_{ei}^{d^2}(G) = \frac{1}{2}\sum_{\{e,f\}\subseteq E(G)} d_i^2(e,f)$, $i = 0,4$. Since d_0 and d_4 are distances, $i = 0,4$.

In follows, the edge-hyper Wiener indices of some well-known graphs have been computed . The results have been stated in Table 1 and 2.

Table 1. The first edge-hyper Wiener index of some graphs.

$Graph(G)$	$W_{e0}(G)$	$WW_{e0}(G)$
P_n	$\frac{1}{6}n(n-1)(n-2)$	$\frac{1}{12}n(n-1)(n-2)(n+1)$
C_n , n is even	$\frac{1}{8}n^3$	$\frac{1}{24}n^2(n+1)(n+2)$
C_n , n is odd	$\frac{1}{8}n(n^2-1)$	$\frac{1}{24}n(n-1)(n+1)(n+3)$
K_n	$\frac{1}{4}n(n-1)^2(n-2)$	$\frac{1}{4}n(n-1)(n-2)(3n-5)$

Table 2. The second edge-hyper Wiener index of some graphs.

$Graph(G)$	$W_{e4}(G)$	$WW_{e4}(G)$
P_n	$\frac{1}{6}(n-1)(n-2)(n+3)$	$\frac{1}{12}(n-1)(n-2)(n^2+5n+12)$
C_n , n is even	$\frac{1}{8}n(n^2+4n-8)$	$\frac{1}{24}n(n^3+9n^2+14n-48)$
C_n , n is odd	$\frac{1}{8}n(n^2+4n-13)$	$\frac{1}{24}n(n^3+9n^2-n-57)$
K_n	$\frac{1}{8}n(n-1)(n-2)(n+1)$	$\frac{1}{4}n(n-1)(n-2)(n+1)$

Carbon nanoribbons are mesoscopic systems halfway between aromatic molecules and extended graphite sheets (2D graphite) [15], and have been a subject of great interest due to their properties, which are as interesting as nanotubes' [15–17]. Band structure calculation hows that both zigzag and armchair nanoribbons have electronic properties of their respective nanotubes [16]. A zigzag nanoribbon with the minimum width may be utilized to study both electronic and magnetic properties of other nanoribbons with zigzag edges. The zigzag nanoribbons of minimum width are the polyacenes [$H_2(C_4H_2)_nC_2H_2$] [16], which are linearly arranged organic polymers formed from aromatic molecules [18]. In the last decade, the polyacenes and helical nanotubes have been objects of great interest for their technological applications. Helical nanotubes are nanotubes which hexagons of the tube are arranged along the tube helically.

Therefore, we compute the edge-hyper Wiener indices linear polyacene L_h and heliacene H_h, which are the hexagonal chains. Moreover, with the usage of these computations, we find the lower and upper bounds for edge-hyper Wiener indices of hexagonal chains.

Theorem 2.2. [19] The first edge-Wiener index of the linear polyacene L_h with h hexagons is:

$$W_{e0}(L_h) = \frac{50}{6}h^3 + 12h^2 + \frac{17}{3}h + 1$$

Theorem 2.3. [19] The first edge-Wiener index of H_h with h hexagons is:

$$W_{e0}(H_h) = \frac{25}{6}h^3 + 30h^2 - \frac{115}{6}h + \frac{72}{6}$$

Theorem 2.4. [19] The second edge-Wiener index of the linear polyacene L_h with h hexagons is:

$$W_{e4}(L_h) = \frac{50}{6}h^3 + \frac{47}{2}h^2 + \frac{43}{6}h$$

Theorem 2.5. [19] The second edge-Wiener index of H_h with h hexagons is:

$$W_{e4}(H_h) = \frac{25}{6}h^3 + \frac{85}{2}h^2 - \frac{124}{6}h + \frac{78}{6}$$

Theorem 2.6. The first d^2-edge-Wiener index of the linear polyacene L_h with h hexagons is:

$$W_{e0}^{d^2}(L_h) = 237 - \frac{767}{3}h + \frac{85}{3}h^2 + \frac{92}{3}h^3 + \frac{50}{3}h^4$$

Proof. Suppose L_h is a line hexagonal chain with h hexagonal and $h \geq 3$. We denote the first $(h-1)$ ring by S_1 and the last $(h-1)$ ring by S_2, then $S_i \cong L_{h-1}$ for $i = 1,2$ and $S_1 \cap S_2 \cong L_{h-2}$. Therefore, we have,

$$2W_{e0}^{d^2}(L_h) = \sum_{e,f \in E(L_h)} d_0^2(e,f) = \sum_{e,f \in E(S_1)} d_0^2(e,f) + \sum_{e,f \in E(S_2)} d_0^2(e,f) - \sum_{e,f \in E(S_1 \cap S_2)} d_0^2(e,f)$$

$$+ 2 \sum_{\substack{e \in E(S_1) \setminus E(S_2) \\ f \in E(S_2) \setminus E(S_1)}} d_0^2(e,f) = 4W_{e0}^{d^2}(L_{h-1}) - 2W_{e0}^{d^2}(L_{h-2}) + 2 \sum_{\substack{e \in E(S_1) \setminus E(S_2) \\ f \in E(S_2) \setminus E(S_1)}} d_0^2(e,f) .$$

By Figure 1, it is easy to see that

$$E_1 = \sum_{\substack{e_1 \in E(S_1)-E(S_2) \\ f \in E(S_2)-E(S_1)}} d_0^2(e_1, f) = (2h+1)^2 + 2\left[(2h)^2 + (2h-1)^2)\right]$$

$$E_2 = \sum_{\substack{e_2 \in E(S_1)-E(S_2) \\ f \in E(S_2)-E(S_1)}} d_0^2(e_2, f) = (2h-2)^2 + 2\left[(2h-1)^2 + (2h)^2\right]$$

$$E_3 = \sum_{\substack{e_3 \in E(S_1)-E(S_2) \\ f \in E(S_2)-E(S_1)}} d_0^2(e_3, f) = (2h-3)^2 + 2\left[(2h-2)^2 + (2h-1)^2\right]$$

and thus

$$\sum_{\substack{e \in E(S_1)-E(S_2) \\ f \in E(S_2)-E(S_1)}} {d_0}^2(e, f) = 2[E_1 + 2(E_2 + E_3)] = 200h^2 - 216h + 106 .$$

Therefore, we have $W_{e0}^{d^2}(L_h) = 2W_{e0}^{d^2}(L_{h-1}) - W_{e0}^{d^2}(L_{h-2}) + 200h^2 - 216h + 106$ with $W_{e0}^{d^2}(L_1) = 57$ and $W_{e0}^{d^2}(L_2) = 351$. By solving the above equation, we obtain d^2-edge-Wiener index $W_{e0}^{d^2}(L_h)$, for linear hexagonal chain L_h:

$$W_{e0}^{d^2}(L_h) = 237 - \frac{767}{3}h + \frac{85}{3}h^2 + \frac{92}{3}h^3 + \frac{50}{3}h^4 .$$ ■

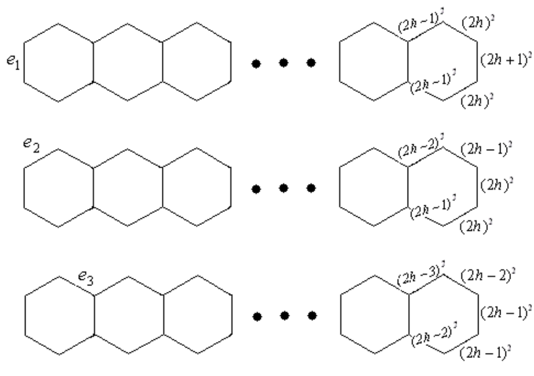

Fig. 1. The distances between special edges of L_h.

Theorem 2.7. The first d^2-edge-Wiener index of H_h with h hexagons is:

$$W_{e0}^{d^2}(H_h) = 397 - 552h + \frac{1007}{6}h^2 + 40h^3 + \frac{25}{6}h^4$$

Proof. Suppose H_h is a linear polyacene with h hexagonal and $h \geq 3$. We denote the first $(h-1)$ ring by S_1 and the last $(h-1)$ ring by S_2, then $S_i \cong H_{h-1}$ for $i = 1,2$ and $S_1 \cap S_2 \cong H_{h-2}$. Therefore, we have,

$$2W_{e0}^{d^2}(H_h) = \sum_{e,f \in E(H_h)} d_0^2(e,f) = 4W_{e0}^{d^2}(H_{h-1}) - 2W_{e0}^{d^2}(H_{h-2}) + 2\sum_{\substack{e \in E(S_1)\backslash E(S_2)\\ f \in E(S_2)\backslash E(S_1)}} d_0^2(e,f).$$

And by similar computations of L_h , we have

$$\sum_{\substack{e \in E(S_1)-E(S_2)\\ f \in E(S_2)-E(S_1)}} d_0^2(e,f) = 50h^2 + 140h + 154\,.$$

Therefore, we have $W_{e0}^{d^2}(H_h) = 2W_{e0}^{d^2}(H_{h-1}) - W_{e0}^{d^2}(H_{h-2}) + 50h^2 + 140h + 154$ with $W_{e0}^{d^2}(H_1) = 57$ and $W_{e0}^{d^2}(H_2) = 351$. By solving the above equation, d^2-edge-Wiener index $W_{e0}^{d^2}(H_h)$, for linear hexagonal chain H_h is

$$W_{e0}^{d^2}(H_h) = 397 - 552h + \frac{1007}{6}h^2 + 40h^3 + \frac{25}{6}h^4\,. \qquad \blacksquare$$

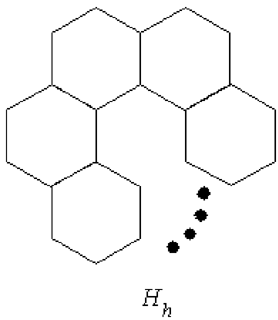

Fig. 2. Two dimensional shape of H_h.

Theorem 2.8. The second d^2-edge-Wiener index of the linear polyacene L_h with h hexagons is:

$$W_{e4}^{d^2}(L_h) = 397 - \frac{1391}{3}h + \frac{277}{3}h^2 + \frac{188}{3}h^3 + \frac{50}{3}h^4$$

Proof. Suppose L_h is a line hexagonal chain with h hexagonal and $h \geq 3$. We denote the first $(h-1)$ ring by S_1 and the last $(h-1)$ ring by S_2, then $S_i \cong L_{h-1}$ for $i = 1,2$ and $S_1 \cap S_2 \cong L_{h-2}$. Therefore, we have,

$$2W_{e4}^{d^2}(L_h) = \sum_{e,f \in E(H_h)} d_4^2(e,f) = 4W_{e4}^{d^2}(L_{h-1}) - 2W_{e4}^{d^2}(L_{h-2}) + 2 \sum_{\substack{e \in E(S_1) \backslash E(S_2) \\ f \in E(S_2) \backslash E(S_1)}} d_4^2(e,f).$$

and

$$\sum_{\substack{e \in E(S_1) - E(S_2) \\ f \in E(S_2) - E(S_1)}} d_4^2(e,f) = 200h^2 - 24h + 42.$$

Therefore, we have $W_{e4}^{d^2}(L_h) = 2W_{e4}^{d^2}(L_{h-1}) - W_{e4}^{d^2}(L_{h-2}) + 200h^2 - 24h + 42$ with $W_{e4}^{d^2}(L_1) = 105$ and $W_{e4}^{d^2}(L_2) = 607$. By solving the above equation, we obtain d^2-edge-Wiener index $W_{e4}^{d^2}(L_h)$, for linear hexagonal chain L_h:

$$W_{e4}^{d^2}(L_h) = 397 - \frac{1391}{3}h + \frac{277}{3}h^2 + \frac{188}{3}h^3 + \frac{50}{3}h^4. \qquad \blacksquare$$

Theorem 2.9. The second d^2-edge-Wiener index of H_h with h hexagons is:

$$W_{e4}^{d^2}(H_h) = 627 - \frac{2687}{3}h + \frac{1877}{6}h^2 + \frac{170}{3}h^3 + \frac{25}{6}h^4$$

Proof. Suppose H_h is a linear polyacene with h hexagonal and $h \geq 3$. We denote the first $(h-1)$ ring by S_1 and the last $(h-1)$ ring by S_2, then $S_i \cong H_{h-1}$ for $i = 1,2$ and $S_1 \cap S_2 \cong H_{h-2}$. Therefore, we have,

$$2W_{e4}^{d^2}(H_h) = \sum_{e,f \in E(H_h)} d_4^2(e,f) = 4W_{e4}^{d^2}(H_{h-1}) - 2W_{e4}^{d^2}(H_{h-2}) + 2 \sum_{\substack{e \in E(S_1) \backslash E(S_2) \\ f \in E(S_2) \backslash E(S_1)}} d_4^2(e,f).$$

and by similar way for computation of L_h, we have

$$\sum_{\substack{e \in E(S_1) - E(S_2) \\ f \in E(S_2) - E(S_1)}} d_4^2(e,f) = 50h^2 + 240h + 344.$$

Therefore, we have $W_{e4}^{d^2}(H_h) = 2W_{e4}^{d^2}(H_{h-1}) - W_{e4}^{d^2}(H_{h-2}) + 50h^2 + 240h + 344$ with $W_{e4}^{d^2}(H_1) = 105$ and $W_{e4}^{d^2}(H_2) = 607$. By solving the above equation, we obtain d^2-edge-Wiener index $W_{e4}^{d^2}(H_h)$, for linear hexagonal chain H_h:

$$W_{e4}^{d^2}(H_h) = 627 - \frac{2687}{3}h + \frac{1877}{6}h^2 + \frac{170}{3}h^3 + \frac{25}{6}h^4$$

Corollary 2.10. The first hyper-edge-Wiener index of the linear polyacene L_h with h hexagons is:

$$WW_{e0}(L_h) = W_{e0}(L_h) + W_{e0}^{d^2}(L_h) = 238 - 250h + \frac{121}{3}h^2 + 39h^3 + \frac{50}{3}h^4$$

Proof. According to Theorems 2-2 and 2-6, the desire result can be concluded. ■

Corollary 2.11. The first hyper-edge-Wiener index of H_h with h hexagons is:

$$WW_{e0}(H_h) = W_{e0}(H_h) + W_{e0}^{d^2}(H_h) = 409 - \frac{3427}{6}h + \frac{1187}{6}h^2 + \frac{265}{6}h^3 + \frac{25}{6}h^4$$

Proof. According to Theorems 2-3 and 2-7, the desire result can be concluded. ■

Corollary 2.12. The second hyper-edge-Wiener index of the linear polyacene L_h with h hexagons is:

$$WW_{e4}(L_h) = W_{e4}(L_h) + W_{e4}^{d^2}(L_h) = 397 - \frac{913}{2}h + \frac{695}{6}h^2 + 71h^3 + \frac{50}{3}h^4$$

Proof. According to Theorems 2-4 and 2-8, the desire result can be concluded. ■

Corollary 2.13. The second hyper-edge-Wiener index of the linear polyacene H_h with h hexagons is:

$$WW_{e4}(H_h) = W_{e4}(H_h) + W_{e4}^{d^2}(H_h) = 640 - \frac{2749}{3}h + \frac{1066}{3}h^2 + \frac{365}{6}h^3 + \frac{25}{6}h^4$$

Proof. According to Theorems 2-5 and 2-9, the desire result can be concluded. ■

Corollary 2-14. The linear polyacene L_h has the maximum edge-hyper Wiener indices and H_h has the minimum edge-hyper Wiener indices among hexagonal chains.

Proof. Since the linear polyacene L_h has the maximum vertex-Wiener index among all benzonoid graphs [20], it has the maximum edge-Wiener indices among all hexagonal chains and then L_h has the maximum edge-hyper Wiener indices among hexagonal chains.

Since the linear polyacene H_h has the minimum vertex-Wiener index among all benzonoid graphs [20], it has the minimum edge-Wiener indices among all hexagonal chains and then H_h has the minimum edge-hyper Wiener indices among hexagonal chains. ■

Theorem 2-15. The bounds of edge-hyper Wiener indices for hexagonal chains G are:

$$WW_{ei}(H_h) \leq WW_{ei}(G) \leq WW_{ei}(L_h), \quad i = 0,4$$

Proof. According to Corollary 2-14, the desire result can be concluded. ■

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