k-membered ring spiro chains with extremal hyper-Wiener index

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Abstract In this paper, we compute the hyper-Wiener index of arbitrary k-membered ring spiro chain. We also determine the extremal k-membered ring spiro chains for hyper-Wiener index.

Keywords Hyper-Wiener index; k-membered ring spiro chain; k-membered ring

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1 Introduction

The Wiener index, one of the on widely used descriptors of molecular topology, was introduced by H. Wiener [1] in 1947

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as the sum of distances between all pairs of vertices of the graph. The Wiener index is well correlated with certain physico-chemical properties of organic compound from which the graph is derived. The hyper-Wiener index of acyclic graphs was introduced by Milan Randić [2] in 1993. Then D. J. Klein et al. [3] generalized Randić's definition for all connected graphs as a generalization of the Wiener index. Suppose that $G = (V(G), E(G))$ is a connected graph and that $d(u,v)$ is the distance between u and v in the graph G. Then *hyper-Wiener index* is defined as $WW(G) = \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}(d(u,v) + d^2(u,v))$. I. Gutman et al. [4-9] studied the mathematical properties of hyper-Wiener index and its applications in chemistry. M. H. Khalifeh et al. [10] computed the hyper-Wiener indices of some graph operations such as Cartesian product, composition, join and disjunction of graphs. T. Mansour and M. Schork [11] computed the exact formulae of hyper-Wiener of bridge and chain graphs. Recently, X. Chen et al. [12] studied the six-membered spiro chains having extremal values of Merrifield-Simmons index and Hosoya index.

A *k-membered ring spiro chain* is a kind of graph consisting of n k-membered rings $B_1, B_2, ..., B_n$ with the properties that (i) for any $1 \leq i < j \leq n$, B_i and B_j are linked by a spiro union (two k-membered rings have only one common vertex, this linkage is called *spiro union*, the common vertex is designated as *spiro* *vertex*) if and only if $j = i + 1$, and (ii) the spiro vertex should be the vertex with degree four in the k-membered ring spiro chains.

In this paper, we compute the hyper-Wiener index of arbitrary k-membered ring spiro chain and determine the k-membered ring spiro chains having extremal values of hyper-Wiener index.

2 Main results

Suppose that u is a vertex of a graph G and that $d(u|G) = \sum_{v \in G} d(u,v)$ and $d^2(u|G) = \sum_{v \in G} d^2(u,v) = \sum_{v \in G} (d(u,v))^2$. Then the hyper-Wiener index can also be defined as $WW(G) = \frac{1}{4}\sum_{u \in V(G)} (d(u|G) + d^2(u|G))$. Now we give the following important theorem.

Theorem 2.1. *Let G be a connected graph with a cut-vertex u_0 such that G_1 and G_2 are two connected subgraphs of G having u_0 as the only common vertex and $G_1 \cup G_2 = G$. Then*

$$WW(G) = WW(G_1) + WW(G_2) + \frac{1}{2}(|V(G_2)| - 1)(d(u_0|G_1) + d^2(u_0|G_1)) + \frac{1}{2}(|V(G_1)| - 1)(d(u_0|G_2) + d^2(u_0|G_2)) + d(u_0|G_1)d(u_0|G_2).$$

Proof. By the definition of the hyper-Wiener index, we have

$$WW(G) = \frac{1}{2}\sum_{\{u,v\} \subseteq V(G_1)} (d(u,v) + d^2(u,v)) + \frac{1}{4}\sum_{u \in V(G_1)} \sum_{v \in V(G_2) \setminus u_0}$$

$$(d(u,v)+d^2(u,v))+\frac{1}{4}\sum_{v\in V(G_2)\backslash u_0}\sum_{u\in V(G_1)}(d(u,v)+d^2(u,v))$$
$$+\frac{1}{2}\sum_{\{u,v\}\subseteq V(G_2)\backslash u_0}(d(u,v)+d^2(u,v)).$$

Since $d(u,v) = d(u,u_0) + d(u_0,v)$. Therefore, substituting the identity in the above equation and by a simple combinatorial argument we can prove that the result is true. □

The number of k-membered rings in a k-membered ring spiro chain is called its *length*. Denote by $\mathcal{G}(n)$ the set of all k-membered ring spiro chains of length n. A k-membered ring B in a k-membered ring spiro chain is *internal* if it contains two spiro vertices, and the others *terminal*. Two vertices u and v on k-membered ring B are *t-position* if $d(u,v) = t$. An internal k-membered ring B is *t-position* if the two spiro vertices on B are t-position. A *t-position-k-membered ring spiro chain* is called if all internal k-membered rings are t-position. Denote by G_n^t the t-position-k-membered ring spiro chain of length n, then clearly $G_n^t \in \mathcal{G}(n)$, $t = 1 \le t \le \lfloor\frac{k}{2}\rfloor$.

Theorem 2.2. *Let $G_n^t \in \mathcal{G}(n)$ be a t-position-k-membered ring spiro chain. Then*

$$WW(G_n^t) = \frac{k^2(k+1)(k+2) - 3(1-\hat{k})k(k+1)}{48}n + \frac{1}{2}(\lfloor\frac{k}{2}\rfloor^4 +$$
$$(\frac{8}{3} - 2\hat{k})\lfloor\frac{k}{2}\rfloor^3 + (\hat{k}^2 - 3\hat{k} + k + 1)\lfloor\frac{k}{2}\rfloor^2 - ((k-1)(\hat{k}-1)$$

$$-\frac{1}{3})\lfloor\frac{k}{2}\rfloor)(n+1)(n-2)+\frac{1}{6}(k-1)t(\lfloor\frac{k}{2}\rfloor^2-(\hat{k}-1)\lfloor\frac{k}{2}\rfloor$$
$$+\frac{k-1}{2})n(n-1)(n-2)+\frac{1}{6}(k-1)t(\lfloor\frac{k}{2}\rfloor^2-(\hat{k}-1)\lfloor\frac{k}{2}\rfloor)(n$$
$$-2)(n^2+2n+3)+\frac{1}{24}(k-1)^2t^2n(n-1)^2(n-2)+(k-$$
$$1)(\frac{2}{3}\lfloor\frac{k}{2}\rfloor^3+(2-\hat{k})\lfloor\frac{k}{2}\rfloor^2+(\frac{4}{3}-\hat{k})\lfloor\frac{k}{2}\rfloor)+(\lfloor\frac{k}{2}\rfloor^2-(\hat{k}-1)\lfloor\frac{k}{2}\rfloor)^2,$$

where

$$\hat{k}=\begin{cases}0, & \text{if } k \text{ is odd;}\\ 1, & \text{if } k \text{ is even.}\end{cases}$$

Proof. G_n^t can be obtained from $G_{n-1}^t \in \mathcal{G}(n-1)$ by attaching a k-membered ring B_n to the terminal k-membered ring B_{n-1}, so that $G_n^t = G_{n-1}^t \cup B_n$. Let $x_1, x_2, \cdots, x_{n-1}$ denote the spiro vertices, as shown in Fig. 1. By Theorem 2.1, we have

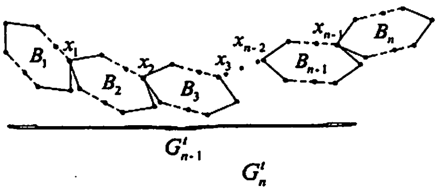

Fig.1

$$\begin{aligned}WW(G_n^t) &= WW(G_{n-1}^t)+WW(B_n)\\ &+\frac{1}{2}(|V(G_{n-1}^t)|-1)(d(x_{n-1}|B_n)+d^2(x_{n-1}|B_n))\\ &+\frac{1}{2}(|V(B_n)|-1)(d(x_{n-1}|G_{n-1}^t)+d^2(x_{n-1}|G_{n-1}^t))\\ &+d(x_{n-1}|G_{n-1}^t)d(x_{n-1}|B_n).\end{aligned}$$

Since $G^t_{n-1} = B_1 \cup B_2 \cup \cdots \cup B_{n-1}$, we have

$$\begin{aligned}
d(x_{n-1}|G^t_{n-1}) &= d(x_{n-1}|B_{n-1}) + d(x_{n-1}|B_{n-2}\backslash x_{n-2}) + \cdots \\
&+ d(x_{n-1}|B_2\backslash x_2) + d(x_{n-1}|B_1\backslash x_1) \\
&= d(x_{n-1}|B_{n-1}) + ((k-1)t + d(x_{n-2}|B_{n-2})) + \cdots + \\
&((k-1)(n-3)t + d(x_2|B_2)) + ((k-1)(n-2)t + d(x_1|B_1)) \\
&= \sum_{i=1}^{n-1} d(x_i|B_i) + \frac{(k-1)t(n-1)(n-2)}{2}, \\
d^2(x_{n-1}|G^t_{n-1}) &= d^2(x_{n-1}|B_{n-1}) + d^2(x_{n-1}|B_{n-2}\backslash x_{n-2}) + \cdots \\
&+ d^2(x_{n-1}|B_2\backslash x_2) + d^2(x_{n-1}|B_1\backslash x_1) \\
&= d^2(x_{n-1}|B_{n-1}) + \sum_{u \in V(B_{n-2}\backslash x_{n-2})} (t + d(x_{n-2}, u))^2 + \cdots \\
&+ \sum_{u \in V(B_2\backslash x_2)} ((n-3)t + d(x_2, u))^2 \\
&+ \sum_{u \in V(B_1\backslash x_1)} ((n-2)t + d(x_1, u))^2 \\
&= \sum_{i=1}^{n-1} d^2(x_i|B_i) + 2t\sum_{i=1}^{n-2}(n-1-i)d(x_i|B_i) \\
&+ \frac{(k-1)t^2(n-2)(n-1)(2n-3)}{6}.
\end{aligned}$$

Note that $|V(G^t_{n-1})| = (k-1)(n-1)+1$ and $|V(B_n)| = k$. Thus we have

$$\begin{aligned}
WW(G^t_n) &= WW(G^t_{n-1}) + WW(B_n) \\
&+ \frac{1}{2}(k-1)(n-1)(d(x_{n-1}|B_n) + d^2(x_{n-1}|B_n)) \\
&+ \frac{1}{2}(k-1)(\sum_{i=1}^{n-1} d(x_i|B_i) + \frac{(k-1)t(n-1)(n-2)}{2}
\end{aligned}$$

$$+\sum_{i=1}^{n-1} d^2(x_i|B_i) + 2t\sum_{i=1}^{n-2}(n-1-i)d(x_i|B_i)$$
$$+\frac{(k-1)t^2(n-2)(n-1)(2n-3)}{6}) + (\sum_{i=1}^{n-1} d(x_i|B_i)$$
$$+\frac{(k-1)t(n-1)(n-2)}{2})d(x_{n-1}|B_n).$$

Set

$$\hat{k} = \begin{cases} 0, & \text{if } k \text{ is odd;} \\ 1, & \text{if } k \text{ is even.} \end{cases}$$

By a simple combinatorial argument, we easily obtain $WW(B_n) = \frac{k^2(k+1)(k+2)-3(1-\hat{k})k(k+1)}{48}$, $d(x_i|B_i) = \lfloor\frac{k}{2}\rfloor^2 - (\hat{k}-1)\lfloor\frac{k}{2}\rfloor$, and $d^2(x_i|B_i) = \frac{\lfloor\frac{k}{2}\rfloor(\lfloor\frac{k}{2}\rfloor+1)(2\lfloor\frac{k}{2}\rfloor+1)}{3} - \hat{k}\cdot\lfloor\frac{k}{2}\rfloor^2$ $(i = 1, 2, \cdots, n-1)$. Substituting these identities in $WW(G_n^t)$, we have

$$WW(G_n^t) - WW(G_{n-1}^t) = \frac{k^2(k+1)(k+2) - 3(1-\hat{k})k(k+1)}{48}$$
$$+ (\lfloor\frac{k}{2}\rfloor^4 + (\frac{8}{3} - 2\hat{k})\lfloor\frac{k}{2}\rfloor^3 + (\hat{k}^2 - 3\hat{k} + k + 1)\lfloor\frac{k}{2}\rfloor^2$$
$$- ((k-1)(\hat{k}-1) - \frac{1}{3})\lfloor\frac{k}{2}\rfloor)(n-1) + \frac{1}{2}(k-1)t(\lfloor\frac{k}{2}\rfloor^2$$
$$- (\hat{k}-1)\lfloor\frac{k}{2}\rfloor + \frac{k-1}{2})(n-1)(n-2) + \frac{1}{2}(k-1)t(\lfloor\frac{k}{2}\rfloor^2$$
$$- (\hat{k}-1)\lfloor\frac{k}{2}\rfloor)n(n-1) + \frac{1}{12}(k-1)^2t^2(n-2)(n-1)(2n-3).$$

Note that $WW(G_2^t) = \frac{k^2(k+1)(k+2)-3(1-\hat{k})k(k+1)}{24} + (k-1)(\frac{2}{3}\lfloor\frac{k}{2}\rfloor^3 + (2-\hat{k})\lfloor\frac{k}{2}\rfloor^2 + (\frac{4}{3}-\hat{k})\lfloor\frac{k}{2}\rfloor) + (\lfloor\frac{k}{2}\rfloor^2 - (\hat{k}-1)\lfloor\frac{k}{2}\rfloor)^2$. Since $\sum_{n=3}^{n}(WW(G_n^t) - WW(G_{n-1}^t)) = WW(G_n^t) - WW(G_2^t)$, substituting $WW(G_2^t)$ into it, we can obtain the assertion. □

Corollary 2.3. *Let $G_n^t \in \mathcal{G}(n)$ $(n > 2, t = 1, 2, \cdots, \lfloor \frac{k}{2} \rfloor)$ be a t-position-k-membered ring spiro chain. Then*

$$WW(G_n^1) < WW(G_n^2) < \cdots < WW(G_n^{\lfloor \frac{k}{2} \rfloor - 1}) < WW(G_n^{\lfloor \frac{k}{2} \rfloor}).$$

Proof. In Theorem 2.2, denote the equation on the right hand by function $f(t)$, $1 \leq t \leq \lfloor \frac{k}{2} \rfloor$. We can prove that $f(t)$ is an increasing function of t for all $1 \leq t \leq \lfloor \frac{k}{2} \rfloor$ by some manipulations. Hence that $f(1) < f(2) < \cdots < f(\lfloor \frac{k}{2} \rfloor - 1) < f(\lfloor \frac{k}{2} \rfloor)$. This proves the assertion. □

A para- and ortho-k-membered ring spiro chains of length n are called if all internal k-membered rings are $\lfloor \frac{k}{2} \rfloor$- and 1-position, denoted by $L_n = G_n^{\lfloor \frac{k}{2} \rfloor}$ and $O_n = G_n^1$, respectively.

Theorem 2.4. *Let $G \in \mathcal{G}(n)$ be a k-membered ring spiro chain. Then*

$$WW(O_n) \leq WW(G) \leq WW(L_n),$$

with the left equality if and only if $G \cong O_n$ and the right equality if and only if $G \cong L_n$.

Proof. Suppose that $G_i \in \mathcal{G}(n_i)$ is a subgraph of the k-membered ring spiro chain G that has the common vertex v_i $(i = 1, 2)$ with the k-membered ring B so that $G = G_1 \cup B \cup G_2$, as shown in Fig. 2. If v_1 and v_2 are t-position ($1 \le t \le \lfloor \frac{k}{2} \rfloor$), then, by Theorem 2.1, we have

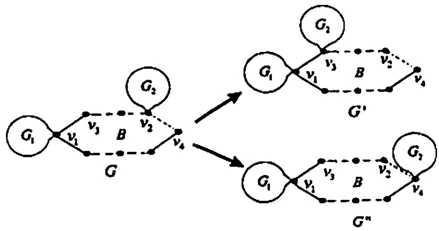

Fig.2

$$
\begin{aligned}
WW(G) &= WW(G_1 \cup B) + WW(G_2) \\
&+ \frac{1}{2}(|V(G_1 \cup B)| - 1)(d_G(v_2|G_2) + d_G^2(v_2|G_2)) \\
&+ \frac{1}{2}(|V(G_2)| - 1)(d_G(v_2|G_1 \cup B) + d_G^2(v_2|G_1 \cup B)) \\
&+ d_G(v_2|G_1 \cup B)d_G(v_2|G_2) \\
&= WW(G_1) + WW(B) \\
&+ \frac{1}{2}(|V(G_1)| - 1)(d_G(v_1|B) + d_G^2(v_1|B)) \\
&+ \frac{1}{2}(|V(B)| - 1)(d_G(v_1|G_1) + d_G^2(v_1|G_1)) \\
&+ d_G(v_1|G_1)d_G(v_1|B) + WW(G_2) \\
&+ \frac{1}{2}(|V(G_1 \cup B)| - 1)(d_G(v_2|G_2) + d_G^2(v_2|G_2)) \\
&+ \frac{1}{2}(|V(G_2)| - 1)(d_G(v_2|G_1 \cup B) + d_G^2(v_2|G_1 \cup B)) \\
&+ d_G(v_2|G_1 \cup B)d_G(v_2|G_2).
\end{aligned}
$$

If v_1 and v_3 are 1-position, we transform G_2 from v_2 to v_3, and denote the resulting graph by G' as shown in Fig. 2. Then, by Theorem 2.1, we have

$$\begin{aligned}WW(G') &= WW(G_1) + WW(B) + \frac{1}{2}(|V(G_1)| - 1)(d_{G'}(v_1|B) \\ &+ d^2_{G'}(v_1|B)) + \frac{1}{2}(|V(B)| - 1)(d_{G'}(v_1|G_1) + d^2_{G'}(v_1|G_1)) \\ &+ d_{G'}(v_1|G_1)d_{G'}(v_1|B) + WW(G_2) + \frac{1}{2}(|V(G_1 \cup B)| \\ &- 1)(d_{G'}(v_3|G_2) + d^2_{G'}(v_3|G_2)) + \frac{1}{2}(|V(G_2)| - 1)\cdot \\ &(d_{G'}(v_3|G_1 \cup B) + d^2_{G'}(v_3|G_1 \cup B)) \\ &+ d_{G'}(v_3|G_1 \cup B)d_{G'}(v_3|G_2).\end{aligned}$$

Note that $d_G(v_1|B) = d_{G'}(v_1|B)$, $d_G(v_1|G_1) = d_{G'}(v_1|G_1)$ and $d^2_G(v_1|G_1) = d^2_{G'}(v_1|G_1)$. Considering the difference of $WW(G)$ and $WW(G')$, we have

$$\begin{aligned}WW(G) - WW(G') &= \frac{1}{2}(|V(G_1 \cup B)| - 1)(d_G(v_2|G_2) \\ &- d_{G'}(v_3|G_2) + d^2_G(v_2|G_2) - d^2_{G'}(v_3|G_2)) + \frac{1}{2}(|V(G_2)| \\ &- 1)(d_G(v_2|G_1 \cup B) - d_{G'}(v_3|G_1 \cup B) + d^2_G(v_2|G_1 \cup B) \\ &- d^2_{G'}(v_3|G_1 \cup B)) + d_G(v_2|G_1 \cup B)d_G(v_2|G_2) \\ &- d_{G'}(v_3|G_1 \cup B)d_{G'}(v_3|G_2).\end{aligned}$$

Through simple combinatorial argument, we easily obtain $d_G(v_2|G_2) > d_{G'}(v_3|G_2)$ and $d_G(v_2|G_1 \cup B) > d_{G'}(v_3|G_1 \cup B)$. Note that $d_G(v_2|G_2) = d_{G'}(v_3|G_2)$. Then we have $WW(G) - WW(G') > 0$ namely $WW(G) > WW(G')$.

If v_1 and v_4 are $\lfloor \frac{k}{2} \rfloor$-position, we transform G_2 from v_2 to v_4, and denote the resulting graph by G'' as shown in Fig.

2. Analogously, we can obtain $WW(G'') > WW(G)$.Hence $WW(G') < WW(G) < WW(G'')$. Therefore, when all internal k-membered rings of G are $\lfloor \frac{k}{2} \rfloor$- and 1-position, the hyper-Wiener index is largest and smallest, respectively. Hence the assertion is obtained. □

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