Extremal Wiener-Hosoya Index Of Acyclic Graphs With Short Diameter*

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Abstract

The Wiener-Hosoya index was firstly introduced by M. Randić in 2004. For any tree T, the Wiener-Hosoya index is defined as

$$WH(T) = \sum_{e \in E(T)} (h(e) + h[e])$$

where $e = uv$ is an arbitrary edge of T, and $h(e)$ is the product of the numbers of the vertices in each component of $T - e$, and $h[e]$ is the product of the numbers of the vertices in each component of $T - \{u, v\}$. We shall investigate the Wiener-Hosoya index of trees with diameter not larger than 4, and characterize the extremal graphs in this paper.

1 Introduction

Numbers reflecting certain structural features of organic molecules that are obtained from the molecular graph are usually called graph invariants or more commonly topological indices. Among topological indices, the Wiener index [1] is certainly the most important one, which was introduced by the chemist Harold Wiener, more than 60 years ago. Historical details and further bibliography on the chemical applications of the Wiener index can be found in the literature [3,4].

Let $G = (V, E)$ be a simple connected graph with vertex set V and edge set E. The Wiener index of G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v) \tag{1}$$

where $d_G(u, v)$ is the distance between u and v(i.e., the smallest length of any $u - v$ path in G).

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The Hosoya index $Z(G)$ [2] of a graph is the total number of its matchings, namely

$$Z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G,k) \tag{2}$$

where $\lfloor \frac{n}{2} \rfloor$ stands for the integer part of $\frac{n}{2}$ and $m(G,k)$ is the number of k-matching of graph G. An elegant composition principle for calculating Z was found by Hosoya et al [5], expressed as the following:

$$Z(G) = Z(G-e) + Z(G-ee) \tag{3}$$

The Wiener-Hosoya index is one of the recently introduced distance based molecular structure descriptors. It was put forward in 2004 by Randić et al [6], in parallel with the symbol W for the Wiener index, the Wiener-Hosoya index is traditionally denoted by WH, and it is defined as:

$$WH(T) = \sum_{e \in E(T)} (h(e) + h[e]) \tag{4}$$

where $e = uv$ is an arbitrary edge of T, $h(e)$ is the product of the numbers of the vertices in each component of $T-e$, and $h[e]$ is the product of the numbers of the vertices in each component of $T - \{u,v\}$; $h[e] = 0$ if e is a pendent edge. The Wiener-Hosoya index has some different properties. For example, the Wiener-Hosoya index has a visibly lower degeneracy than many other known simple topological indices by examining degenerate cases of the graphs among octanes, nonanes and decane isomers, for details, see [6]. Some most recent mathematical studies about the Wiener-Hosoya index, see [8-9].

In this paper, we shall investigate the Wiener-Hosoya index of trees with diameter not more than 4, and determine the extremal Wiener-Hosoya index of these trees.

2 Preliminaries

A tree is called a *a double star* $S_{p,q}$(see Figure 1(a)), if it is obtained from $K_{1,p}$ and $K_{1,q-1}$ by identifying a pendant vertex of $K_{1,p}$ with the center of $K_{1,q-1}$, where $1 < p \leq q$. Then for a double star $S_{p,q}$ with n vertices, we have $p+q=n$, and $p \leq \lfloor \frac{n}{2} \rfloor$. We call a double star $S_{p,q}$ *balanced*, if $p = \lfloor \frac{n}{2} \rfloor$ and $q = \lceil \frac{n}{2} \rceil$.

Definition. Let $(c_1, c_2, \cdots, c_d)$ be a partition of n, the *starlike tree* [7] is constructed in the following way:

(1) Let $S_1, S_2, \cdots, S_d$ be the stars with edge number $c_1-1, c_2-1, \cdots, c_d-1$ respectively, and $v_1, v_2, \cdots, v_d$ be their center vertices;

(2) Add a vertex v_0, which join the center vertices $v_1, v_2, \cdots, v_d$ of $S_1, S_2, \cdots, S_d$ respectively.

Then, we can obtain a tree T with diameter not more than 4. The degrees of $v_1, v_2, \cdots, v_d$ are $c_1, c_2, \cdots, c_d$, resp. $|V(T)| = n+1$, $|E(T)| = d + (c_1 - 1) + (c_2 - 1) + \cdots + (c_d - 1) = c_1 + c_2 + \cdots + c_d = n$. We denote it by $S(c_1, c_2, \cdots, c_d)$, and it is shown in Figure 1(b).

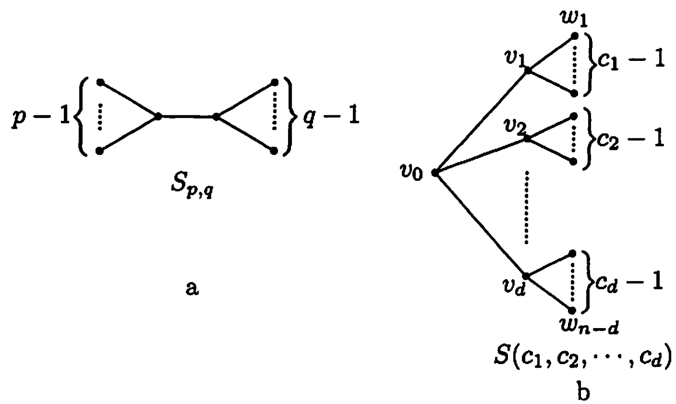

Figure 1. double star $S_{p,q}$ and starlike tree $S(c_1, c_2, \cdots, c_d)$

3 Extremal Wiener-Hosoya index of starlike trees

Firstly, we shall determine the Wiener-Hosoya index of starlike trees.

Theorem 1. Let $S(c_1, c_2, \cdots, c_d)$ be the graph depicted in Fig 1(b). Then

$$WH(S(c_1, c_2, \cdots, c_d)) = 2n^2 - nd + n - \sum_{i=1}^{d} c_i^2 + \prod_{k=1}^{d} c_k \cdot \sum_{k=1}^{d} \frac{1}{c_k}$$

Proof. Let $T = S(c_1, c_2, \cdots, c_d)$; we divide the edges of $S(c_1, c_2, \cdots, c_d)$ into two groups, i.e., $E = E_1 \bigcup E_2$.

(1) Let $E_1 = \{e | e = v_i w_j\}(v_i \sim w_j$,i.e., v_i adjacent to the pendant vertex w_j, $i = 1, 2, \cdots, d$; $j = 1, 2, \cdots, n-d)$, i.e., E_1 are pendant edges. The contribution of these edges to the Wiener-Hosoya index is

$$\sum_{e \in E_1} (h(e) + h[e]) = (n-d)n$$

(2) Let $E_2 = \{e | e = v_0 v_i\}(v_0 \sim v_i$,i.e., v_0 adjacent to v_i, $i = 1, 2, \cdots, d)$. All the edges for the contribution to the Wiener-Hosoya index are

$$\begin{aligned}
&\sum_{e\in E_2}(h(e)+h[e])\\
=\;&\sum_{i=1}^{d} c_i(n+1-c_i)+\prod_{k=1}^{d} c_k\cdot\sum_{k=1}^{d}\tfrac{1}{c_k}\\
=\;&n(n+1)-\sum_{i=1}^{d} c_i^2+\prod_{k=1}^{d} c_k\cdot\sum_{k=1}^{d}\tfrac{1}{c_k}
\end{aligned}$$

Summing up, the Wiener-Hosoya index of T is

$$\begin{aligned}
&WH(T)\\
=\;&\sum_{e\in E_1}(h(e)+h[e])+\sum_{e\in E_2}(h(e)+h[e])\\
=\;&2n^2-nd+n-\sum_{i=1}^{d} c_i^2+\prod_{k=1}^{d} c_k\cdot\sum_{k=1}^{d}\tfrac{1}{c_k}
\end{aligned}$$

The next section will be devoted to the characterization of the star-like tree of extremal Wiener-Hosoya index. Firstly, we introduce a lemma in the following:

Lemma 2. If a partition contains two parts c_i, c_j such that $c_i \geq c_j+2$, the corresponding Wiener-Hosoya index of $S(c_1, c_2, \cdots, c_d)$ increases if they are replaced by c_i-1, c_j+1

Proof. Obviously, if n and d remain unchanged, the terms in the Wiener-Hosoya index of $S(c_1, c_2, \cdots, c_d)$ that change are the sum $\sum_{i=1}^{d} c_i^2$ and $\prod_{k=1}^{d} c_k \cdot \sum_{k=1}^{d} \frac{1}{c_k}$. Let

$$A = c_1 c_2 \cdots c_{i-1} c_{i+1} \cdots c_{j-1} c_{j+1} \cdots c_d;$$

$$B = \frac{1}{c_1}+\frac{1}{c_2}+\cdots+\frac{1}{c_{i-1}}+\frac{1}{c_{i+1}}+\cdots+\frac{1}{c_{j-1}}+\frac{1}{c_{j+1}}+\cdots+\frac{1}{c_d}$$

then by Theorem 1, the difference is

$$\begin{aligned}
&WH(S(c_1,\cdots,c_i-1,\cdots,c_j+1,\cdots,c_d))-WH(S(c_1,\cdots,c_i,\\
&\cdots,c_j,\cdots,c_d))\\
=\;&-(c_i-1)^2-(c_j+1)^2+c_i^2+c_j^2+c_1c_2\cdots c_{i-1}c_{i+1}\cdots c_{j-1}c_{j+1}\\
&\cdots c_d(c_i-1)(c_j+1)(\tfrac{1}{c_1}+\tfrac{1}{c_2}+\cdots+\tfrac{1}{c_{i-1}}+\tfrac{1}{c_{i+1}}+\cdots+\\
&\tfrac{1}{c_{j-1}}+\tfrac{1}{c_{j+1}}+\cdots+\tfrac{1}{c_d}+\tfrac{1}{c_i-1}+\tfrac{1}{c_j+1})-c_1c_2\cdots c_{i-1}c_{i+1}\cdots\\
&c_{j-1}c_{j+1}\cdots c_dc_ic_j(\tfrac{1}{c_1}+\tfrac{1}{c_2}+\cdots+\tfrac{1}{c_{i-1}}+\tfrac{1}{c_{i+1}}+\cdots+\tfrac{1}{c_{j-1}}+\tfrac{1}{c_{j+1}}\\
&+\cdots+\tfrac{1}{c_d}+\tfrac{1}{c_i}+\tfrac{1}{c_j})\\
=\;&2(c_i-c_j-1)+A(c_i-1)(c_j+1)(B+\tfrac{1}{c_i-1}+\tfrac{1}{c_j+1})-Ac_ic_j(B+\\
&\tfrac{1}{c_i}+\tfrac{1}{c_j})\\
=\;&2(c_i-c_j-1)+AB(c_i-1)(c_j+1)+A(c_i+c_j)-ABc_ic_j\\
&-A(c_i+c_j)\\
=\;&(AB+2)(c_i-c_j-1)>0
\end{aligned}$$

Therefore, if a partition satisfies the condition of the lemma, its Wiener-Hosoya index cannot be maximal. So we only have to consider partitions consisting of two different parts k and $k+1$ for the maximal case.

Let $\mathcal{A}(n,d) = \{S(c_1,c_2,\cdots,c_d) | \sum_{i=1}^{d} c_i = n\}$ be the set of all starlike trees $S(c_1,c_2,\cdots,c_d)$ with fixed partition length d, then

Theorem 3. Let $G \in \mathcal{A}(n,d)$, then $S(n-d+1,1,1,\cdots,1)$; $S(n-d,2,1,1,\cdots,1)$, if $2 \leq d \leq n-2$; $S(n-d-1,3,1,1,\cdots,1)$, if $2 \leq d \leq n-4$ or $S(2,2,2,1,\cdots,1)$, if $d=n-3$; $S(k+1,k+1,\cdots,k+1,k,k,\cdots,k), k = \lfloor \frac{n}{d} \rfloor$ has the smallest, the second smallest, the third smallest and the largest Wiener-Hosoya index, respectively.

Proof. Let $G \in \mathcal{A}(n,d)$, and choose G such that $WH(G)$ is as large as possible. If the partition is different from $(k+1,k+1,\cdots,k+1,k,k,\cdots,k)$, we can find parts c_i, c_j such that $c_i \geq c_j+2$, and if we replace them by c_i-1, c_j+1, we obtain a graph G'. After that operation, the Wiener-Hosoya index increases by Lemma 2, such that $WH(G') > WH(G)$, which contradicts the choice of G. Analogously, we choose G such that $WH(G)$ is as small as possible. If a partition is different from $(n-d+1,1,1,\cdots,1)$, and we replace them by c_i+1, c_j-1, we obtain a graph G', the Wiener-Hosoya index will decreases by Lemma 2, such that $WH(G') < WH(G)$, which contradicts the choice of G as well. This proves the statements for maximum and minimum.

For $d=n-1$ and $d=1$, the partition is uniquely determined by its length. Thus there is no second smallest Wiener-Hosoya index in this case. Therefore, we consider the case $2 \leq d \leq n-2$. Now, suppose that there is a graphs G, and the partition of G is different from $(n-d+1,1,1,\cdots,1)$ and $(n-d,2,1,1,\cdots,1)$, and that $WH(G)$ is as small as possible, and the partition must contain either two parts $c_i \geq c_j \geq 3$ or three parts $c_i \geq c_j \geq c_k \geq 2$. In both case, we replace c_i, c_j by c_i+1, c_j-1, then we obtain a partition different from $(n-d+1,1,1,\cdots,1)$, and the Wiener-Hosoya index decreases in this case. Repeating this operation, we shall get the partition $(n-d,2,1,1,\cdots,1)$, which gives the second smallest Wiener-Hosoya index.

If $d \geq n-2$ or $d=1$, there are no further partitions. If $d=n-3$, there is only one partition remaining, namely $(2,2,2,1,\cdots,1)$. Thus it is also the partition giving the third smallest Wiener-Hosoya index. Eventually, if $1 \leq d \leq n-4$, Similar to the discussion of the above two cases, we obtain a partition $(n-d-1,3,1,1,\cdots,1)$, which gives us the third smallest Wiener-Hosoya index. It follows that $S(n-d-1,3,1,1,\cdots,1)$, if $2 \leq d \leq n-4$ or $S(2,2,2,1,\cdots,1)$, if $d=n-3$ attains the third smallest Wiener-Hosoya index.

The proof of the theorem is completed.

Theorem 4. The Wiener-Hosoya index of a double star $S_{p,q}$ is monotonous increasing in p.

Proof. Similar to the above proof, by simple calculation, we have

$$\begin{aligned} & WH(S_{p,q}) \\ = & (n-2)(n-1)+pq+1 \\ = & n^2-3n+3+pq \end{aligned}$$

From the definition of $S_{p,q}$, we have $p+q=n, 1<p\leq q$, thus,

$$WH(S_{p,q}) = -p^2+np+n^2-3n+3$$

and since $\frac{\partial(WH(S_{p,q}))}{\partial p} = n-2p \geq 0$, $WH(S_{p,q})$ is monotonously increasing in p. Thus, the Theorem holds.

Corollary 5. The balanced double star $S_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ and $S_{2,n-2}$ have the maximum and minimum values of Wiener-Hosoya index among all double stars $S_{p,q}$ with n vertices, *resp.*

References

[1] H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc. 69(1947)17-20.

[2] Hosoya H. Topological index, a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons. Bull. Chem. Soc. Japan. 44(1971)2322-2339.

[3] A. A. Dobrynin, R. Entringer and I. Gutman, Wiener index of trees: theory and applications, Acta Appl. Math. 66(2001)211-249.

[4] A. A. Dobrynin, I. Gutman, S. Klavžar and P. Žigert, Wiener Index of Hexagonal Systems, Acta Appl. Math. 72(2002)247-294.

[5] Hosoya H. K. Kawasaki and K. Mizutani, Topological index thermodynamics properties, Empirical rules on the boiling points of saturated hydrocarbons. Bull. Chem. Soc. Japan. 45(1972)3415.

[6] M. Randić, Wiener-Hosoya index-A novel graph theoretical molecular descriptor. J.Chem.Inf.Comput.Sci. 44(2004)373-377.

[7] S. G. Wagner, A class of trees and its Wiener index, Acta Appl. Math. 91(2006)119-132.

[8] H. Feng, J.Qian, Minimum Trees With Respect To Wiener-Hosoya Index. Journal Of Mathematical Study (Chinese). 39(2006)117-123.

[9] H. Feng, J.Qian, Minimum Trees With Respect To Wiener-Hosoya Index. Journal Of Zhangzhou Normal University (Nat. Sci) (Chinese). 58(2007)25-30.