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The proof of a conjecture concerning acyclic molecular graphs with maximal Hosoya index and diameter 4*

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The Hosoya index of a graph is defined as the total number of the matchings of the graph. In this paper, we solve a conjecture in Ou, J. Math. Chem, DOI: 10.1007/S10910-006-9199-1 concerning acyclic molecular graphs with maximal Hosoya index and diameter 4.

KEY WORDS: Hosoya index, tree, diameter

1. Introduction

Given a molecular graph G, the *Hosoya index* $z = z(G)$ is defined as the number of subsets of $E(G)$ in which no edges are incident, i.e., in graph-theoretical terminology, the total number of the matchings of the graph G. Let $m(G, k)$ be the number of k-matchings of G. Then

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

where n is the order of G. It is convenient to define $m(G, 0) = 1$ and $m(G, k) = 0$ when $k \geq \lfloor \frac{n}{2} \rfloor + 1$.

The Hosoya index of a graph was introduced by Hosoya [5] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures (see [3,6,10]). Recently, many authors have investigated the Hosoya index (e.g., see [4, 7, 9, 11, 12]). An important direction is to determine the graphs with maximal or minimal Hosoya indices. Here, we consider the acyclic molecular graphs with maximal Hosoya index. It was established long ago that the path P_n is the unique graph that has maximal Hosoya index and the star S_n is the unique graph that has minimal Hosoya index. One can study structure properties of graphs with maximal Hosoya

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index by considering those graphs that have short diameter (see [8]). Note that $\mathrm{diam}(P_n) = n-1$ and $\mathrm{diam}(S_n) = 2$. In [8], Ou put forward the following conjecture.

Conjecture Let n be a positive integer such that $n-1 = 3k-s$, $s = 0, 1, 2$. If $n \geq 53$, then S_n^k is the unique n-vertex tree of diameter 4 that has maximal Hosoya index.

In this paper, we prove that the the above conjecture is true. Moreover, all acyclic graphs with maximal Hosoya index and diameter 3 are characterized.

In order to discuss our results, we first introduced some terminologies and notations of graphs. Other undefined notations may refer to [1]. Let $G = (V, E)$ be a graph. For a vertex u of G, we denote the neighborhood and the degree of u by $N_G(u)$ and $d_G(u)$, respectively. A *pendant vertex* is a vertex of degree 1. For two vertices u and v, the distance between u and v is the number of edges in a shortest path joining u and v. Let $r(u) = \max\{d(u,v) : v \in V(G)\}$. If $r(u) = \max\{r(v) : v \in V(G)\}$, then we call the vertex u a center of G. The diameter of a graph, denoted by $\mathrm{diam}(G)$, is the maximum distance between any two vertices of G. We also use $G-u$ to denote the graph that arises from G by deleting the vertex $u \in V(G)$.

A tree is called a *double star* $S_{p,q}$ (see figure 1), if it is obtained from $K_{1,p}$ and $K_{1,q-1}$ by identifying a pendent 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 $q = \lceil \frac{n}{2} \rceil$.

Let q, t, m and n be integers such that $q \geq 1, t \geq 2, m \leq t-1$ and $n = qt + m + 1$. Let S_n^t be a tree obtained from a star $K_{1,t}$ by attaching q pendent vertices to m pendent vertices of $K_{1,t}$ and attaching $q-1$ pendent vertices to $t-m$ pendent vertices of $K_{1,t}$, respectively.

2. Lemmas

According to the definition of the Hosoya index, we can get the following results.

Lemma 2.1 (see [3]). Let G be a graph and v be a vertex of G. Then

$$z(G) = z(G-v) + \sum_{u \in N_G(v)} z(G - \{u, v\}).$$

Lemma 2.2 (see [3]). If $G_1, G_2, \ldots, G_t$ are the components of a graph G, then $z(G) = \prod_{i=1}^{t} z(G_i)$.

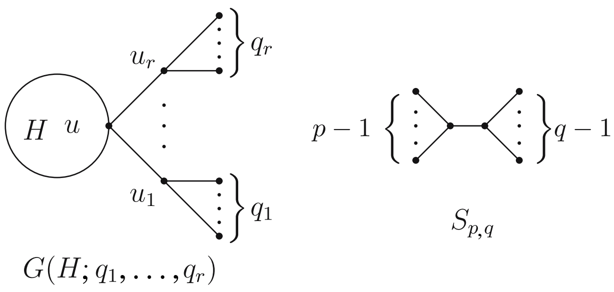

Figure 1. Two special graphs.

Lemma 2.3 (see [2]). Let G and G' be graphs obtained from a graph H by attaching two pendent vertices and attaching a path of order 2 to one vertex u of H, respectively. Then $z(G') > z(G)$.

Definition 2.4 Let $G(H; q_1, q_2, \ldots, q_r)$ (see figure 1) be a connected graph obtained from a graph H by attaching r stars K_{1,q_i}, $1 \leq i \leq r$ to one vertex u of H, respectively.

By Definition 2.4, $S_n^t = G\left(K_1; \underbrace{q, \ldots q}_{t-m}, \underbrace{q-1, \ldots q-1}_{m}\right)$ for $n = (q+1)t - m + 1$. In the following, we denote $\sum_{u' \epsilon N_H(u)} z(H - u - u') = 0$ if $H \cong K_1$ and $u \epsilon V(H)$.

Lemma 2.5 Let $G(H; s, t)$ be a connected graph defined in the above. If $s \geq t+2$ then

$$z(G(H; s-1, t+1)) > z(G(H; s, t)).$$

Proof. Since $s \geq t+2$, $s - t - 1 \geq 1$. By Lemma 2.1, we have

$$\begin{aligned} z(G(H; s, t)) &= z(G(H; s, t) - u) + \sum_{u' \in N_{G(H;s,t)}(u)} z(G(H; s, t) - u - u') \\ &= (s+1)(t+1)z(H-u) + (s+t+2)z(H-u) \\ &\quad + (s+1)(t+1) \sum_{u' \in N_H(u)} z(H - u - u'). \end{aligned}$$

Therefore,

$$\begin{aligned} & z(G(H; s-1, t+1)) - z(G(H; s, t)) \\ &= (s-t-1)\left(z(H-u) + \sum_{u' \in N_H(u)} z(H-u-u')\right) > 0. \end{aligned}$$

□

Lemma 2.6 Let $G(H; q, q, q)$ be a graph (see Definition 2.4). If $q \geq 3$ then

$$z(G(H; q-1, q-1, q-1, 2)) > z(G(H; q, q, q)).$$

Proof. By Lemma 2.1, we have

$$\begin{aligned}
z(G(H; q, q, q)) &= z(G(H; q, q, q) - u) \\
&\quad + \sum_{u' \in N_{G(H;q,q,q)}(u)} z(G(H; q, q, q) - u - u') \\
&= (q+1)^3 z(H-u) + 3(q+1)^2 z(H-u) \\
&\quad + (q+1)^3 \sum_{u' \in N_H(u)} z(H - u - u'), \\
&\quad z(G(H; q-1, q-1, q-1, 2)) \\
&= z(G(H; q-1, q-1, q-1, 2) - u) \\
&\quad + \sum_{u' \in N_{G(H;q-1,q-1,q-1,2)}(u)} z(G(H; q-1, q-1, q-1, 2) - u - u') \\
&= 3q^3 z(H-u) + (q^3 + 3q^2) z(H-u) + 3q^3 \sum_{u' \in N_H(u)} z(H - u - u').
\end{aligned}$$

Therefore,

$$\begin{aligned}
& z(G(H; q-1, q-1, q-1, 2)) - z(G(H; q, q, q)) \\
&\quad = (3q^3 - 3q^2 - 9q - 4) z(H-u) + (2q^3 - 3q^2 - 3q - 1) \sum_{u' \in N_H(u)} z(H - u - u') \\
&\quad > 0.
\end{aligned}$$

□

Lemma 2.7 Let $G(H; q, q)$ be a graph (see Definition 2.4). If $q \geq 3$, then

$$z(G(H; q-1, q-1, 1)) > z(G(H; q, q)).$$

Proof. By Lemma 2.1, we have

$$\begin{aligned}
z(G(H; q, q)) &= z(G(H; q, q) - u) \\
&\quad + \sum_{u' \in N_{G(H;q,q)}(u)} z(G(H; q, q) - u - u')
\end{aligned}$$

$$
\begin{aligned}
&= (q+1)^2 z(H-u) + 2(q+1)z(H-u) \\
&\quad + (q+1)^2 \sum_{u' \in N_H(u)} z(H-u-u'), \\
&\quad z(G(H; q-1, q-1, 1)) \\
&= z(G(H; q-1, q-1, 1) - u) \\
&\quad + \sum_{u' \in N_{G(H; q-1, q-1, 1)}(u)} z(G(H; q-1, q-1, 1) - u - u') \\
&= 2q^2 z(H-u) + (q^2 + 2q) z(H-u) + 2q^2 \sum_{u' \in N_H(u)} z(H-u-u').
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&z(G(H; q-1, q-1, 1)) - z(G(H; q, q)) \\
&\quad = (2q^2 - 4q - 2) z(H-u) + (q^2 - 2q - 1) \sum_{u' \in N_H(u)} z(H-u-u') > 0.
\end{aligned}
$$

□

Lemma 2.8 Let $G(H; 3)$ be a graph (see Definition 2.4). Then

$$z(G(H; 1, 1)) > z(G(H; 3)).$$

Proof. By Lemma 2.1, we have

$$
\begin{aligned}
z(G(H; 3)) &= z(G(H; 3) - u) + \sum_{u' \in N_{G(H;3)}(u)} z(G(H; 3) - u - u') \\
&= 4z(H-u) + z(H-u) + 4 \sum_{u' \in N_H(u)} z(H-u-u'), \\
z(G(H; 1, 1)) &= z(G(H; 1, 1) - u) + \sum_{u' \in N_{G(H;1,1)}(u)} z(G(H; 1, 1) - u - u') \\
&= 4z(H-u) + 4z(H-u) + 4 \sum_{u' \in N_H(u)} z(H-u-u').
\end{aligned}
$$

Therefore,

$$z(G(H; 1, 1)) - z(G(H; 3)) = 3z(H-u) > 0.$$

□

3. Results

From Lemmas 2.1 and 2.2, we can get the following results by calculations.

Lemma 3.1 (i) $z(S_{p,q}) = pq + 1$, where $S_{p,q}$ is a double star of order n; (ii) $z(S_n^k) = 3^{k-s}2^s + (k-s)3^{k-s-1}2^s + s3^{k-s}2^{s-1}$, where $n-1 = 3k-s,\ s = 0, 1, 2$.

By Lemma 3.1, we have the following result.

Lemma 3.2 The Hosoya index of a double star $S_{p,q}$ is monotonously increasing in p.

Proof. By Lemma 3.1, $z(S_{p,q}) - z(S_{p+1,q-1}) = -p + q < 0$ for $p < \lfloor \frac{n}{2} \rfloor$. Thus the lemma holds. □

Note 3.3 The balanced double star $S_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ has the maximum value of Hosoya index among all double stars $S_{p,q}$ with n vertices.

By Lemmas 2.3 and 2.5, we may obtain the following result (given in [8]).

Lemma 3.4 (see [8]). Let G be a tree of order n and diameter 4, and let u be its center. If $n \geq 5$ and $d_G(u) = t \geq 2$, then $z(G) \leq z(S_n^t)$ and equality holds if and only if $G \cong S_n^t$.

Theorem 3.5 Let G be a tree of order n and diameter 4, where $n-1 = 3k-s$, $s = 0, 1, 2$. If $n \geq 53$, then

$$z(G) \leq 3^{k-s}2^s + (k-s)3^{k-s-1}2^s + s3^{k-s}2^{s-1} \tag{1}$$

and equality in (1) holds if and only if $G \cong S_n^k$, that is, S_n^k is the unique n-vertex tree of diameter 4 that has maximal Hosoya index.

Proof. First we note that if $G \cong S_k^n$, then (1) holds by Lemma 3.1.

Now we prove that if G is a tree of order n and diameter 4, where $n-1 = 3k-s,\ s = 0, 1, 2$, then (1) holds and the equality in (1) holds only if $G \cong S_k^n$.

We choose G such that $z(G)$ is as large as possible. Let u be the center of G. By Lemma 3.4, we can assume that $G \cong S_n^t$ ($t \geq 2$), where $t = d_G(u)$. Let $n = (q+1)t - m + 1$ with $0 \leq m \leq t-1$.

We consider two cases.

Case 1 $t > k$.

In this case, $q \leq 2$.

Subcase 1.1 $q = 2$.

In this case, $m \geq s + 3 \geq 3$. Since $n \geq 53$, we have $t > 18$. Note that $G \cong G\left(K_1; \underbrace{2, \ldots, 2}_{t-m}, \underbrace{1, \ldots, 1}_{m}\right)$. Let $G' = G\left(K_1; \underbrace{2, \ldots, 2}_{t-m+2}, \underbrace{1, \ldots, 1}_{m-3}\right)$. If $m = 3$, then

$$z(G') - z(G) = 3^{t-4}(t - 18) > 0.$$

If $m \geq 4$, then

$$\begin{aligned} z(G') - z(G) &= 3^{t-m+2}2^{m-3} + (t - m + 1)3^{t-m+2}2^{m-3} + (m - 3)3^{t-m+2}2^{m-4} \\ &\quad -[3^{t-m}2^{m} + (t - m)3^{t-m+1}2^{m} + m3^{t-m}2^{m-1}] \\ &= 3^{t-m-1}2^{m-4}(2t + m + 36) > 0. \end{aligned}$$

Thus, we have a contradiction with our choice.

Subcase 1.2 $q = 1$.

In this case, $m = 0$. Since $n \geq 53$, we have $t \geq 26$. Then $G \cong G\left(K_1; \underbrace{1, \ldots, 1}_{t}\right)$. By an argument similar to the proof of Subcase 1.1, we have a contradiction with our choice.

Case 2 $t \leq k$.

In this case, $q \geq 2$. If $q = 2$, then $m = s$ and $k = t$, and hence $G \cong S_n^k$. Therefore we assume $q \geq 3$. Thus $t < k$. Note that $G \cong G\left(K_1; \underbrace{q, \ldots, q}_{t-m}, \underbrace{q-1, \ldots, q-1}_{m}\right)$.

If $t - m \geq 3$, then let $G' = G\left(K_1; 2, \underbrace{q, \ldots, q}_{t-m-3}, \underbrace{q-1, \ldots, q-1}_{m+3}\right)$. Thus by Lemma 2.6, we have $z(G') > z(G)$, a contradiction.

If $t - m = 2$, then let $G' = G\left(K_1; 1, \underbrace{q-1, \ldots, q-1}_{t}\right)$. Thus by Lemma 2.7, we have $z(G') > z(G)$, a contradiction.

If $t - m = 1$, then q = 3 and let $G' = G\left(K_1; 1, 1, \underbrace{q-1, \ldots, q-1}_{t-1}\right)$. Thus by Lemma 2.8, we have $z(G') > z(G)$, a contradiction.

Therefore, the proof of the theorem is complete. □

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