Journal of Mathematical Chemistry, Vol. 43, No. 1, January 2008 (© 2006)
DOI: 10.1007/s10910-006-9199-1

On acyclic molecular graphs with maximal Hosoya index, energy, and short diameter

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Received 27 May 2006; revised 10 September 2006

The total number of matchings of a graph is defined as its Hosoya index. Conjugated and non-conjugated acyclic graphs that have maximal Hosoya index and short diameter are characterized in this paper, explicit expressions of the Hosoya indices of these extremal graphs are also presented.

KEY WORDS: Energy, Hosoya index, acyclic graph, matching

1. Introduction

Hosoya index of a graph G, written as $Z(G)$, is defined as the total number of its matchings [1], where a matching M of graph G is a set of its edges that share no common endpoints. If denote by $m(G,k)$ the number of k-matchings, matching that consists of k edges, of G, then

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

where n is the order of G, the number of its vertices, and $\lfloor n/2 \rfloor$ is the integer part of $n/2$. It is convenient to define $m(G,0) = 1$ and $m(G,k) = 0$ when $k \geqslant \lfloor n/2 \rfloor + 1$.

As a chemical structure descriptor, Hosoya index plays an important role in the so-called inverse structure–property relationship problems. For details, the readers are suggested to refer to Gutman and Polansky [2] and Skvortsova et al. [3] and their references. On the other hand, Hosoya index of an acyclic molecular graph G has a close relationship with its energy $E(G)$, the sum of the absolute values of all eigenvalues of its adjacency matrix $A(G)$ [4], since $E(G)$ can be expressed in terms of Coulson integral [2]:

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} x^{-2} \ln \left(1 + \sum_{k=1}^{\lfloor n/2 \rfloor} m(G,k) x^{2k} \right) dx.$$

Extremal molecular graphs that have maximal or minimal Hosoya index draw a lot of attention [5–8]. The authors present an ordering of conjugated acyclic graphs according to their maximal energy (or Hosoya indices) in [9]. Extremal unicyclic molecular graphs with minimal Hosoya index and prescribed girth are characterized in [10], explicit expressions of their Hosoya indices are also presented there.

Let G be a conjugated n-vertex tree and M be its perfect matching. Then a k-matching of G consists of two disjoint parts: an i-matching M_1 of $G - M$ and a subset M_2 of M such that no edges of M_1 and M_2 share common endpoints, and vice versa. If $G - M$ is connected, then for any i-matching of $G - M$ there are $2i$ edges in M that cannot be chosen to form together with this i-matching of $G - M$ a k-matching of G. And so

$$m(G,k) = \sum_{i=1}^{k} m(G - M, i) \times \binom{n/2 - 2i}{k - i}.$$

If $G - M$ is disconnected, then for any given i-matching of $G - M$ there exist $i - 1$ to $2i$ edges in M that cannot be chosen to form together with this i-matching a k-matching of G. Let $m_j(G - M, i)$ stand for the number of i-matchings of $G - M$ that shares common endpoints with exactly j edges of M each. Then

$$m(G,k) = \sum_{i=0}^{k} \sum_{j=i-1}^{2i} m_j(G - M, i) \times \binom{n/2 - j}{k - j}.$$

From the above two formulas, we conclude that when G has maximal Hosoya index, under the condition that the size of every component of $G - M$ is given, each component of $G - M$ should have maximal Hosoya index, and that the endpoints of edges of M that join different components of $G - M$ are 1-degree vertices of the corresponding components. Noting that each component of $G - M$ has shorter diameter than G, the previous reasoning shows that one can study structure properties of graphs with maximal Hosoya index by considering those graphs that have short diameter.

In section two of this paper, we present explicit expressions of maximal Hosoya indices of trees with diameter four and characterize those trees whose center has any given degree. A conjecture on the structure property of extremal n-vertex trees is presented there. Extremal conjugated trees with diameter five are characterized in section three, the expression of their Hosoya indices are also presented there.

For graph-theoretical symbols and terminologies not defined here, we follow that of Ref. [11].

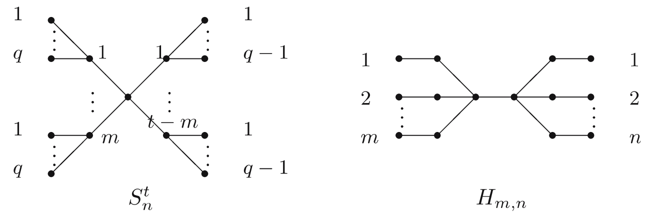

Figure 1. Two special graphs.

2. Trees of diameter four

Before presenting the main results of this section, let us define a class of trees at first. For two vertices u and v of a connected graph G, we denote by $d(u, v)$ the distance between u and v (namely the number of edges of a shortest path between u and v); write $r(u) = \mathrm{Max}\{d(u, v) : v \in V(G)\}$ and call vertex u a center of graph G if $r(u) = \mathrm{Min}\{r(v) : v \in V(G)\}$, where $V(G)$ is the vertex-set of G. A classic graph-theoretical result says that a connected graph contains exactly one center if it has even diameter or two centers otherwise, in the latter case these two centers are also called bicenters.

Let q, t, m, and n be four nonnegative integers such that $q \geqslant 1, t \geqslant 2$, $m \leqslant t-1$ and $n = qt + m + 1$. Let S_n^t stand for the tree with order n and diameter 4 that is obtained as follows: join every center of m copies of the complete bipartite graph $K_{q,1}$ and $t - m$ copies of the complete bipartite graph $K_{q-1,1}$ each by an edge to a new vertex u. Clearly, S_n^t contains u as its unique center with degree(valence) $d(u) = t$. For clarity, this graph is depicted in figure 1 (the other graph is employed in section 3).

Lemma 2.1. Let G be a tree with order n and diameter 4. If its center has degree t, then $m(G, k) \leqslant m(S_n^t, k)$ with equality holding for every nonnegative integer k if and only if $G = S_n^t$.

Proof. Let u be the center of G and $N(u) = \{v_1, v_2, \ldots, v_t\}$ be its neighborhood; let $d(v_i) = x_i + 1$ be the degree of vertex v_i, $i = 1, \ldots, t$. Assume without loss of generality that $x_1 \geqslant x_2 \geqslant \cdots \geqslant x_t$. If $x_1 \geqslant x_t + 2$, after deleting from G a pendant vertex (1-degree vertex) adjacent to v_1 and attaching an edge to vertex v_t, we construct a new graph G'. When $1 \leqslant k \leqslant t$, the k-matchings of G are partitioned into two classes: those that saturate the center u and those not. And so, when $2 \leqslant k \leqslant t$ we have

$$m(G, k) = (t - k + 1) \sum_{1 \leqslant i_1 < i_2 < \cdots < i_{k-1} \leqslant t} x_{i_1} x_{i_2} x_{i_{k-1}} + \sum_{1 \leqslant i_1 < i_2 < \cdots < i_k \leqslant t} x_{i_1} x_{i_2} x_{i_k},$$

where $\{i_1, i_2, \ldots, i_k\} \subset \{1, 2, \ldots, t\}$. When $4 \leqslant k \leqslant t$, we have

$$\begin{aligned} m(G', k) - m(G, k) = (t - k + 1)(x_1 - x_t - 1) &\sum_{1<i_1<\cdots<i_{k-3}<t} x_{i_1} x_{i_2} \cdots x_{i_{k-3}} \\ +(x_1 - x_t - 1) &\sum_{1<i_1<\cdots<i_{k-2}<t} x_{i_1} x_{i_2} \cdots x_{i_{k-2}}. \end{aligned} \tag{1}$$

When $k \leqslant 3$, we have

$$m(G', k) - m(G, k) = \begin{cases} 0, & \text{if } k = 0 \text{ or } 1, \\ x_1 - x_t - 1, & \text{if } k = 2, \\ (x_1 - x_t - 1)(t - 2 + \sum_{i=2}^{t-1} x_i), & \text{if } k = 3. \end{cases} \tag{2}$$

Since $x_1 \geqslant x_t + 2$, it follows from the combination of Eqs. (1) and (2) that $m(G', k) \geqslant m(G, k)$ holds for every nonnegative integer k. The equality in previous formula holds for every nonnegative integer k if and only if $x_1 = x_t + 1$. The lemma follows from above discussion. $\square$

Lemma 2.2. Let t, n be two nonnegative integers such that $n \geqslant 5$ and $2 \leqslant t \leqslant n - 1$. Then $Z(S_n^t) = (\lfloor (n-1)/t \rfloor + 1)^{n-2-t\lfloor (n-1)/t \rfloor} \times \lfloor (n-1)/t \rfloor^{t-n+t\lfloor (n-1)/t \rfloor} \times ((\lfloor (n-1)/t \rfloor + 1)(t + \lfloor (n-1)/t \rfloor) - n + 1 + t\lfloor (n-1)/t \rfloor)$.

Proof. Assume k, m be two nonnegative integers such that $n - 1 = kt + m, m \leqslant t - 1$. Then $k = \lfloor (n-1)/t \rfloor$, $m = n - 1 - \lfloor (n-1)/t \rfloor$.

Case 1 $m = 0$. Let us label any $k - 1$ pendant vertices and their common neighbour with $1, 2, \ldots, k - 1$ and k, respectively, at first, and then label any other $k - 1$ pendant vertices and their common neighbor with $k + 1, \ldots, 2k$, respectively, etc. Finally, label with n the center of S_n^t. Write $B = (b_{ij})$ for the neighbor matrix of S_n^t, where $b_{ij} = 1$ if and only if either $i = j$ or vertex i is adjacent to vertex j. Then

$$B = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ \vdots \\ k-1 \\ k \\ k+1 \\ \vdots \\ n \end{array} \begin{array}{c} \begin{array}{cccccccccccc} 1 & 2 & 3 & \cdots & k-1 & k & k+1 & \cdots & 2k-1 & 2k & \cdots & n \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 1 & 1 & 1 & \cdots & 1 & 1 & 0 & \cdots & 0 & 0 & \cdots & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 1 & \cdots & 1 \end{pmatrix} \end{array}.$$

Since S_n^t is an acyclic graph, a classic result says $Z(S_n^t) = \mathrm{Per}(B)$. Expanding the permanent $\mathrm{Per}(B)$ of matrix B along its first k rows, if denote by B_1 the $\binom{1,\ldots,k}{1,\ldots,k}$-minor of B, B_2 the $\binom{k+1,\ldots,n}{k+1,\ldots,n}$-minor, B_3 the $\binom{1,\ldots,k}{1,\ldots,k-1,n}$-minor, and B_4 the $\binom{k+1,\ldots,n}{k,\ldots,n-1}$-minor, we have

$$\mathrm{Per}(B) = \mathrm{Per}(B_1)\mathrm{Per}(B_2) + \mathrm{Per}(B_3)\mathrm{Per}(B_4) \tag{3}$$

Noting that B_1 and B_2 is the neighbor matrix of $K_{1,k-1}$ and S_{n-k}^{t-1}, respectively, we have $\mathrm{Per}(B_1) = k$. On the other hand, the $\binom{1,\ldots,n-k-1}{2,\ldots,n-k}$-minor of B_4 is the neighbor matrix of graph $(t-1)K_{1,k-1}$, the union of $t-1$ copies of $K_{1,k-1}$. Since the Hosoya index of the union of two vertex-disjoint graphs equals to the product of the Hosoya indices of these two graphs, if expanding $\mathrm{Per}(B_4)$ along its first column we get

$$\mathrm{Per}(B_4) = (Z(K_{1,k-1}))^{t-1}. \tag{4}$$

Since $\mathrm{Per}(B_1) = k$ and B_2 is the neighbor matrix of S_{n-k}^{t-1}, it follows from the combination of (3) and (4) that

$$\begin{aligned}\mathrm{Per}(B) &= kZ(S_{n-k}^{t-1}) + k^{t-1}\\ &= k(kZ(S_{n-2k}^{t-2}) + k^{t-2}) + k^{k-1}\\ &= k^2 Z(S_{n-2k}^{t-2}) + 2k^{t-1}\\ &\quad\ldots\\ &= k^{t-1}(k+1) + (t-1)k^{t-1} = tk^{t-1} + k^t.\end{aligned}$$

The first part of the lemma follows.

Case 2 $m \geqslant 1$. Label at first the k-degree neighbors of the center and their pendent neighbors just as in case 1, and then the $(k+1)$-degree neighbors of the center and their pendent neighbors. Finally label the center with n. Expanding the permanent of this neighbor matrix along its first k arrows, we obtain $\mathrm{Per}(B) = kZ(S_{n-k}^{t-1}) + (k+1)^m k^{t-m-1}$. Expand similarly the permanent of the neighbor matrix of S_{n-k}^{t-1} if its center has a k-degree neighbor, etc. Finally, we stop at getting the permanent of the neighbor matrix of $S_{n-(t-m)k}^m$. Hence,

$$\begin{aligned}\mathrm{Per}(B) &= kZ(S_{n-k}^{t-1}) + (k+1)^m k^{t-m-1}\\ &= k(kZ(S_{n-2k}^{t-2}) + (k+1)^m k^{t-m-2}) + (k+1)^m k^{t-m-1}\\ &= k^2 Z(S_{n-2k}^{t-2}) + 2(k+1)^m k^{t-m-1}\\ &\quad\ldots\\ &= k^{t-m} Z(S_{n-(t-m)k}^m) + (t-m)(k+1)^m k^{t-m-1}\\ &= k^{t-m}(m(k+1)^{m-1} + (k+1)^m) + (t-m)(k+1)^m k^{t-m-1}\\ &= (k+1)^{m-1}k^{t-m-1}((k+1)(k+t) - m).\end{aligned}$$

The lemma follows from above formula. □

Theorem 2.3 follows directly from the combination of lemmas 2.1 and 2.2, corollary 2.4 follows from lemma 2.1, and corollary 2.5 follows from theorem 2.3.

Theorem 2.3. Let t and n be two nonnegative integers such that $n \geqslant 5$ and $2 \leqslant t \leqslant n-1$. Let G be an n-vertex tree of diameter 4 with center having degree t. Then $Z(G) \leqslant (\lfloor (n-1)/t \rfloor + 1)^{n-2-t\lfloor (n-1)/t \rfloor} \times \lfloor (n-1)/t \rfloor^{t-n+t\lfloor (n-1)/t \rfloor} \times ((\lfloor (n-1)/t \rfloor + 1)(t + \lfloor (n-1)/t \rfloor) - n + 1 + t\lfloor (n-1)/t \rfloor)$. The equality holds if and only if $G = S_n^t$.

Corollary 2.4. Let G be an n-vertex tree of diameter 4 and vertex u be its center. If $n \geqslant 5$ and $d(u) = t \geqslant 2$, then $E(G) \leqslant E(S_n^t)$ with the equality holding if and only if $G = S_n^t$.

Corollary 2.5. If $n \geqslant 5$, then the maxmal Hosoya index of n-vertex trees of diameter 4 is Max $\{Z(S_n^t) : 2 \leqslant t \leqslant n-1\}$.

Remark 1. Employing MATLAB 6.5 we determine, according to the formulas listed in lemma 2.2 and corollary 2.5, some trees of diameter 4 that have maximal Hosoya indices. A very interesting phenomenon is also found. We employ the following MATLAB program to calculate the maximal Hosoya index of trees of order n and the degree x of their centers. At first for any given integer $n \geqslant 5$ we input the following program in the command window:

```
>> clear
>> fun = ' − ((fix((n − 1)/x) + 1)(n − 2 − x*(fix((n − 1)/x)))*(fix((n − 1)/x))
   +(x − n)x*(fix((n − 1)/x)))*((fix((n − 1)/x) + 1)*(x + fix((n − 1)/x)) − n + 1
   +x*fix((n − 1)/x)))',
>> [X,fval] = fminbnd(fun, 2, n − 1).
```

After running this program we obtain the value of x. And then, for above given n we substitute $\lfloor x \rfloor$ and $\lfloor x \rfloor + 1$, respectively, for x in the following program to get the values of '-fval'. The greater value of these two '-fval's is the maximal Hosoya index, and its corresponding value of $\lfloor x \rfloor$ or $\lfloor x \rfloor + 1$ is the degree of the center.

```
>> (fix((n − 1)/x) + 1) ^ (n − 2 − x*(fix((n − 1)/x)))*(fix((n − 1)/x))(x − n + x*
(fix((n − 1)/x)))*((fix((n − 1)/x) + 1)*(x + fix((n − 1)/x)) − n + 1 + x*fix((n − 1)/x)).
```

Table 1
Degree of the center of S_n^x that has maximal Hosoya index.

n	x	n	x	n	x	n	x	n	x	n	x	n	x
5	2	19	9	33	14	47	16,17	61	20	75	25	497	166
6	3	20	9	34	14	48	17	62	21	76	25	498	166
7	3	21	10	35	14	49	17	63	21	77	26	499	166
8	3,4	22	10	36	14	50	17	64	21	78	26	500	167
9	4	23	11	37	14,15	51	17	65	22	79	26	899	300
10	4	24	11	38	15	52	17,18	66	22	89	30	900	300
11	5	25	12	39	15	53	18	67	22	90	30	901	300
12	5	26	12	40	15	54	18	68	23	91	30	1499	500
13	6	27	12,13	41	15	55	18	69	23	119	40	1500	500
14	6	28	13	42	15,16	56	19	70	23	120	40	1501	500
15	7	29	13	43	16	57	19	71	24	121	40		
16	7	30	13	44	16	58	19	72	24	229	100		
17	8	31	13	45	16	59	20	73	24	300	100		
18	8	32	13,14	46	16	60	20	74	25	301	100		

Table 1 lists some degrees of the centers of n-vertex trees of diameter 4 that have maximal Hosoya index. All these values of x are obtained by above two programs.

Table 1 shows that when $n = 8, 27, 32, 42, 47, 52$ there exist two non-isomorphic n-vertex trees G and H of diameter 4 that are not m-comparable, namely there exist two distinct positive integers k_1 and k_2 such that $m(G, k_1) > m(H, k_1)$ and $m(G, k_2) < m(H, k_2)$. But they have same maximal Hosoya indices. Its seems by table 1 that if $n \geqslant 53$ and $n - 1 = 3k - s$, $s = 0, 1, 2$, then S_n^k is the unique n-vertex trees of diameter 4 that has maximal Hosoya indices. And so we put forward the following conjucture.

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

Remark 2. An anonunous referee puts forward an interesting problem as follows: to characterize acyclic graphs with maximal Hosoya index, graphs with how short diameter need we determine at first? Or conversely, if acyclic graphs with diameter no more than s are all characterized, the structure properties of acyclic graphs with diameter at least how long can be determined?

3. Conjugated trees of diameter 5 or less

Note that no trees of diameter 2 contain a perfect matching, and that other conjugated trees with diameter $d \leqslant 4$ are uniquely determined by their order: they are isolated edge when $d = 1$; 4-vertex path P_4 when $d = 3$ and $B_m^\star$ when

$d = 4$ [4], where $B_m^{\star}$ is obtained by attaching an edge to every vertex of the star $K_{1,m}$. In this section, we characterize extremal conjugated trees of diameter 5 that have maximal energies and present explicit expressions of their Hosoya indices. Let us denote by $H_{m,n}$ the tree obtained by joining at first with an edge the centers of stars $K_{1,m}$ and $K_{1,n}$ and then attaching an edge to every 1-degree vertex of the resulting graph, refer to figure 1 for clarity.

Lemma 3.1. Let G be a conjugated tree of order n and diameter 5. Then $m(G,k) \leqslant m(H_{m,m},k)$ when $n = 4m+2$ and $m(G,k) \leqslant m(H_{m,m-1},k)$ when $n = 4m$, with the equality holding if and only if G is isomorphic to the corresponding graph.

Proof. Let $M(G)$ be the unique perfect matching of graph G. When $n = 4m+2$, since G has diameter 5, the subgraph G' that is induced by the edges of $G - M(G)$ contains at most two components, none of which contains 2-matching (or equivalently each of the two components is a star) when there exists two components. Since G' contains precisely $2m$ edges, it follows that $m(G',2) \leqslant m^2$, with the equality holding if and only if G' consists of two stars $K_{1,m}$.

Recall that every k-matching of G is formed by an i-matching S_1 of G' and a $(k-i)$-order subset S_2 of $M(G)$ such that no edges of S_1 and S_2 share a common endpoint. Since the perfect matching $M(G)$ must cover every vertex of G', every 1-matching of G' is adjacent to two edges of $M(G)$ and every 2-matching is adjacent to at least three edges of $M(G)$. Furthermore, every 2-matching of G is adjacent to three edges of $M(G)$ if and only if G' consists of two stars. Denote by s_3 and s_4, respectively, the number of 2-matchings of G' that is adjacent to three and four edges each. Then

$$\begin{aligned}
m(G,k) &= m(G',0)\binom{2m+1}{k} + m(G',1)\binom{2m-1}{k-1} \\
&\quad + s_1\binom{2k-2}{k-2} + s_2\binom{2k-3}{k-2} \\
&\leqslant \binom{2m+1}{k} + 2m\binom{2m-1}{k-1} + (s_1+s_2)\binom{2k-2}{k-2} \\
&\leqslant \binom{2m+1}{k} + 2m\binom{2m-1}{k-1} + m^2\binom{2k-2}{k-2} \\
&= m(H_{m,m},k).
\end{aligned} \tag{5}$$

As is pointed out before, the first inequality becomes equality if and only if G' consists of two stars, and the equality in the second inequality holds if and only if these two star are both isomorphic to $K_{1,m}$. The first part of lemma 3.1 follows, and the second one also follows similarly. □

Lemma 3.2. For every positive integer m, $Z(H_{m,m}) = 2^{2m-2}(m^2 + 4m + 8)$ and $Z(H_{m,m-1}) = 2^{2m-3}(m^2 + 3m + 6)$.

Proof. Notice that $H_{m,m}$ has a unique perfect matching M with size $2m + 1$. Every k-matching of $H_{m,m}$ consists of an i-matching M_1 of $H_{m,m} - M$ and a subset M_2 of order $k-i$ of M such that no edges of M_1 is incident with any edges of M_2. Conversely, any two such edge-sets form a k-matching of $H_{m,m}$. Since every 1-matching of $H_{m,m} - M$ is incident with two edges of M and every 2-matching is incident with three edges in total of M, it follows that

$$m(H_{m,m}, k) = \binom{2m+1}{k} + \binom{2m}{1}\binom{2m-1}{k-1} + \binom{m}{1}\binom{m}{1}\binom{2m-2}{k-2}.$$

And so

$$\begin{aligned} Z(H_{m,m}) &= \sum_{k=0}^{2m+1} m(H_{m,m}, k) \\ &= \sum_{k=0}^{2m+1} \binom{2m+1}{k} + \sum_{k=1}^{2m-1} 2m\binom{2m-1}{k-1} + \sum_{k=2}^{2m-2} m^2\binom{2m-2}{k-2} \\ &= 2^{2m-2}(m^2 + 4m + 8). \end{aligned}$$

The first part of lemma 3.2 follows and the second one can be shown with a similar technique. □

The following theorem follows directly from the combination of lemma 3.1 and 3.2; corollary 3.4 follows directly from lemma 3.1 and the expression of $E(G)$ (in terms of Coulson integral).

Theorem 3.3. Let G be a conjugated tree with order n and diameter 5. Then $Z(G) \leqslant 2^{2m-2}(m^2 + 4m + 8)$ when $n = 4m + 2$, with the equality holding if and only if $G = H_{m,m}$; $Z(G) \leqslant 2^{2m-3}(m^2 + 3m + 6)$ when $n = 4m$, with the equality holding if and only if $G = H_{m,m-1}$.

Corollary 3.4. Let G be a conjugated tree with order n and diameter 5. Then $E(G) \leqslant E(H_{m,m})$ when $n = 4m + 2$, with the equality holding if and only if $G = H_{m,m}$; $E(G) \leqslant E(H_{m,m-1})$ when $n = 4m$, with the equality holding if and only if $G = H_{m,m-1}$.

Acknowledgements

Thank the anonymous referees for their valuable suggestions, one of which is written as remark 2 in section two. Supported by National Natural

Science Foundation of China (10271105); Natural Science Foundation of Fujian (A0510021); Education Ministry of Fujian (JA03147).

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