MATCH
Communications in Mathematical
and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **62** (2009) 473-480

ISSN 0340 - 6253

On the minimal energy of trees with a given number of vertices of degree two *

Xiaoxia Lin [a,b,†] Xiaofeng Guo [a]

[a] School of Mathematical Sciences, Xiamen University, Xiamen Fujian 361005, China

[b] School of Sciences, Jimei University, Xiamen Fujian 361021, China

(Received February 9, 2009)

Abstract

The energy of a molecular graph is a popular parameter that is defined as the sum of the absolute values of eigenvalues of the graph. It is well known that in the case of trees the energy is related to the matching polynomial and thus also to the Hosoya index via a certain Coulson integral. Ye and Yuan [On the minimal energy of trees with a given number of pendent vertices, MATCH Commun. Math. Comput. Chem. 57 (2007) 193-201.] and Yu and Lv [Minimum energy on trees with k pendent vertices, Lin. Algebra Appl. 418 (2006) 625-633] independently characterized the trees with the minimal energy among the trees with a given number of pendent vertices (that is, vertices of degree one). Let $\mathcal{T}_{n,t}$ be the set of trees of order n with at least t vertices of degree two. In the present paper, we characterize the tree with minimal energy or Hosoya index in $\mathcal{T}_{n,t}$.

* The project supported by NSFC (10831001).

† Corresponding author. E-mail: lxx@jmu.edu.cn

1 Introduction

Gutman [2,4] defined the energy of a graph G with n vertices, denoted by $E(G)$. The energy is a graph parameter stemming from the Hückel molecular orbital (HMO) approximation for the total π-electron energy. It is defined as the sum of the absolute values of eigenvalues of a graph: if $\lambda_1, \lambda_2, \cdots, \lambda_n$ denote the spectrum of a graph G, then

$$E(G) = \sum_{i=1}^{n} |\lambda_i| \ .$$

The Hosoya index of a graph G with n vertices, denoted by $Z(G)$, is defined as

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

where $m(G,r)$ denotes the number of matchings with r edges in G.

Let T be a tree with n vertices, and let $V(T) = 1, 2, ..., n$ denote the set of vertices of T. The adjacency matrix $A(T)$ of T is the square matrix $A(T) = (a_{ij})$ of order n, where $a_{ij} = 1$ if i and j are adjacent and 0 otherwise. The characteristic polynomial of T, denoted here by $\phi(T,x)$, is defined as $\phi(T,x) = det(xI - A(T))$, where I is the identity matrix of order n. It is well known [1] that if T is a tree with n vertices then

$$\phi(T,x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k m(T,k) x^{n-2k} \ , \tag{1}$$

where $m(T,k)$ equals the number of matchings with k edges in T, and $\lfloor \frac{n}{2} \rfloor$ denotes the largest integer no more than $\frac{n}{2}$.

It follows from (1) that the energy can actually be computed by means of Coulson integral [5,6,7].

$$E(T) = \frac{2}{\pi} \int_0^{\infty} x^{-2} log(\sum_k m(T,k) x^{2k}) dx \tag{2}$$

The fact that $E(T)$ is a strictly monotonously increasing function of all matching numbers $m(T,k)$, $k = 0, 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$, provides a way of comparing the energies of pair of trees. Gutman [3] introduced a quasi-ordering relation " $\succeq$ "(i.e. reflexive and transitive relation) on the set of all forests (acyclic graphs) with n vertices: if T_1 and T_2 are two forests with n vertices and characteristic polynomials in the form (1), then

$$T_1 \succeq T_2 \Longleftrightarrow m(T_1,k) \geq m(T_2,k)$$

for all $k = 0, 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$.

If $T_1 \succeq T_2$ and there exists a k such that $m(T_1, k) > m(T_2, k)$ then $T_1 \succ T_2$. Hence, by (2),

$$T_1 \succeq T_2 \Longrightarrow E(T_1) \geq E(T_2) \tag{3}$$

$$T_1 \succ T_2 \Longrightarrow E(T_1) > E(T_2) \tag{4}$$

This quasi-ordering has been successfully applied in the study of the extremal values of energy over a significant class of graph (see [8-28, 31-38]). In [4] Gutman determined the tree with n vertices and the maximal energy, namely, the path P_n. Furthermore, he obtained the following result.

$$E(X_n) < E(Y_n) < E(Z_n) < E(W_n) < E(T)$$

for any tree $T \neq X_n, Y_n, Z_n, W_n$ with n vertices, where X_n is a star $K_{1,n-1}$, Y_n is the graph obtain by attaching a pendent edge to a pendent vertex of $K_{1,n-2}$, Z_n by attaching two pendent edge to a pendent vertex of $K_{1,n-3}$, and W_n by attaching a P_3 (here P_m denotes a path with m vertices) to a pendent vertex of $K_{1,n-3}$. Fig. 1 shows the trees X_9, Y_9, Z_9, W_9.

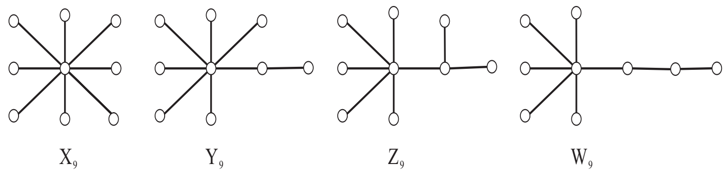

Fig. 1: The trees X_9, Y_9, Z_9 and W_9

Zhang et al [25] determined the trees with maximal energy and minimal energy [24], respectively, among the hexagonal chains. Lin et al [16] determined the tree with maximal energy among the trees with order n and maximum degree $\Delta(3 \leq \Delta \leq n-2)$ and the tree with minimal energy among the trees with order n and maximum degree $\Delta(\lceil \frac{n+1}{3} \rceil \leq \Delta \leq n-2)$. Zhou et al [28] determined the minimal energy of trees of a prescribed diameter. Ye et al [22] and Yu et al [27] determined the minimal energy of trees with a given number of pendent vertices (that is, vertices of degree one), respectively. In the present paper, we will consider the minimal energy of trees with a given number of vertices of degree two.

In order to formulate our results, We need to define a tree $T_{n,t}$ with n vertices as follows: $T_{n,t}$ is obtained from a path P_{t+2} with $t+2$ vertices by attaching $n-t-2$ pendent edges to an end vertex of P_{t+2}. $T_{n,t}$ is called a broom (see Brualdi and Goldwasser [29]).

Fig.2 shows the broom $T_{n,t}$. Obviously, the largest length of a path of $T_{n,t}$ is $t+2$ and $T_{n,0}$ is a star $K_{1,n-1}$. Let $\mathcal{T}_{n,t}$ be the set of trees of order n with at least t vertices of degree two. Clearly, $T_{n,t} \in \mathcal{T}_{n,t}$.

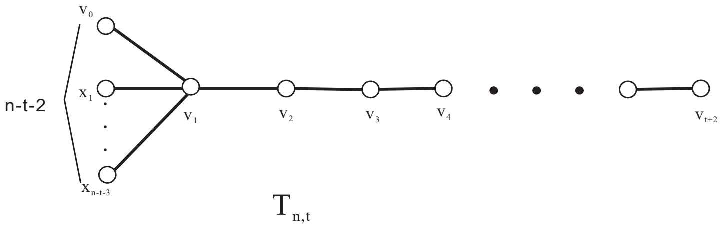

Fig. 2: The broom $T_{n,t}$

Let T be a tree of order n, and $n \geq 3$. Let $e = uv$ be a nonpendent edge of T, and let T_1 and T_2 be the two components of $T - e$, $u \in V(T_1)$, $v \in V(T_2)$. Let T_0 be the tree obtained from T in the following way.

(1) Contract the edge (i.e. identify u of T_1 with v of T_2).

(2) Attach a pendent vertex to the vertex u $(= v)$.

The procedures (1) and (2) are called [30] the *edge-growing transformation* of T (on edge $e = uv$), or e.g.t of T (on edge $e = uv$) for short.

The following lemmas will be used in the proof of our main result.

Lemma 1.1 [16] *Let T be a tree of order n with at least a nonpendent edge, and $n \geq 3$. If T_0 can be obtained from T by one step of e.g.t, then $T \succ T_0$ and $E(T) > E(T_0)$.*

Lemma 1.2 [21] *Let T and T' be two trees of order n. Suppose that uv (resp. $u'v'$) is a pendent edge of T (resp. T') and u (resp. u') is a pendent vertex of T (resp. T'). Let $T_1 = T - u$, $T_2 = T - u - v$, $T_1' = T' - u'$, and $T_2' = T' - u' - v'$. If $T_1 \succeq T_1'$ and $T_2 \succ T_2'$; or $T_1 \succ T_1'$ and $T_2 \succeq T_2'$, then $T \succ T'$.*

It is obvious that, in Lemma 1.2, if $T_1 \succeq T_1'$ and $T_2 \succeq T_2'$ then $T \succeq T'$.

Lemma 1.3 [22] *Let T be an acyclic graph with n vertices $(n > 1)$ and T' a spanning subgraph (resp. a proper spanning subgraph) of T. Then $T \succeq T'$ (resp. $T \succ T'$).*

In this paper, we prove the following.

Theorem 1.4 *Let n and t be two positive integers with $n \geq t+2 \geq 2$, and let T be a tree with n vertices in which there are at least t vertices of degree two. Then $E(T) \geq E(T_{n,t})$ with equality if and only if T is the broom $T_{n,t}$.*

Corollary 1.5 *Let n be a positive integer $n \geq 2$,and $t \geq 0$, and let T be a tree with n vertices and with at least t vertices of degree two. Then $Z(T) \geq Z(T_{n,t})$ with equality if and only if T is the broom $T_{n,t}$, where $Z(T)$ denotes the Hosoya index of T.*

2 Proofs of the main results

Now we are in the position to prove our main results.

Proof of Therorem 1.4. By (3) and (4), it suffice to prove $T \succ T_{n,t}$ for any tree $T \ncong T_{n,t}$ in $\mathcal{T}_{n,t}$. We will prove it by induction on n and t.

If $t = 0$ and $T \ncong T_{n,0}$, by a number of e.g.t, T can be transformed to a star which is just $T_{n,0}$. By Lemma 1.1, $T \succ T_{n,0}$.

For any tree $T \in \mathcal{T}_{n,t}$, $n \geq t+2$. So a tree with t vertices of degree two and with a minimum number of vertices has exactly $t+2$ vertices which is just a path P_{t+2} isomorphic to $T_{t+2,t}$. Thus if $n = t+2$, then $T \cong T_{t+2,t}$ and $E(T) = E(T_{t+2,t})$.

Now we suppose that $n > t+2 > 2$ and that, for any tree $T' \in \mathcal{T}_{n',t'}$ with either $n' \leq n$ and $t' < t$ or $n' < n$ and $t' \leq t$, $T' \succeq T_{n',t'}$, and $E(T') = E(T_{n',t'})$ if and only if $T' \cong T_{n',t'}$.

Denote the diameter of T by d. Let $P_{d+1} = u_0u_1 \cdots u_d$ be a longest path in T. Then $d_T(u_0) = d_T(u_d) = 1$, where $d_T(u_i)$ denotes the degree of the vertex u_i in T. Let $d_T(u_1) = s \geq 2$, and $u_0, w_1, w_2, \cdots, w_{s-2}, u_2$ the adjacent vertices of u_1. Since P_{d+1} is a longest path in T, $d_T(w_j) = 1$ for $j = 1, 2, \cdots, s-2$. Let T_0 be the component of $T - u_1$ containing u_2. Then T_0 contains at least $t+1$ vertices, in which at least one pendent vertex of T and at least t vertices having degree two in T. $T - u_1 - u_2$ consists of T_0 and $s-2$ isolated vertices.

Note that $T_{n,t}$ consists of a path $P_{t+2} = v_1v_2 \cdots v_{t+2}$ and $n-t-2$ pendent vertices $v_0, x_1, x_2, \cdots, x_{n-t-3}$ adjacent to v_1 (see Fig. 2).

We can assert that $s = d_T(u_1) \leq d_{T_{n,t}}(v_1) = n-t-1$. Otherwise, $s \geq n-t \geq 3$. Then T_0 would have at most t vertices in which at least two pendent vertices of T_0 and at most $t-2$ vertices of degree two. Thus T would have at most $t-1$ vertices of degree two, a contradiction.

Case 1. $d_T(u_1) = s = 2$. Then $T - u_0$ is a tree with $n-1$ vertices and with at least $t-1$ vertices of degree two, $T - u_0 - u_1$ is a tree with $n-2$ vertices and with at least $t-2$ vertices of degree two. By induction hypothesis, $T - u_0 \succeq T_{n-1,t-1} \cong T_{n,t} - v_{t+2}$, $T - u_0 - u_1 \succeq T_{n-2,t-2} \cong T_{n,t} - v_{t+2} - v_{t+1}$. In addition, $E(T - u_0) = E(T_{n,t} - v_{t+2})$ if and only if $T - u_0 \cong T_{n,t} - v_{t+2}$, and $E(T - u_0 - u_1) = E(T_{n,t} - v_{t+2} - v_{t+1})$ if and only if $T - u_0 - u_1 \cong T_{n,t} - v_{t+2} - v_{t+1}$. Since $T \ncong T_{n,t}$, either $T - u_0 \succ T_{n,t} - v_{t+2}$ or $T - u_0 - u_1 \succ T_{n,t} - v_{t+2} - v_{t+1}$. By Lemma 1.2, we have $T \succ T_{n,t}$.

Case 2. $d_T(u_1) = s \geq 3$. Then $T - u_0$ is a tree with $n-1$ vertices in which there are at least t vertices of degree two, $T - u_0 - u_1$ consists of $s-2$ isolated vertices and a tree T_0 with $n-s$ vertices in which there are at least $t-1$ vertices of degree two. By induction hypothesis, $T - u_0 \succeq T_{n-1,t} \cong T_{n,t} - v_0$, $T - u_0 - u_1 \succeq T_0 \succeq T_{n-s,t-1}$. Since $s \leq n-t-1$, we have that $n-s \geq t+1$ and $T_{n-s,t-1}$ contains a subgraph P_{t+1}. By Lemma 1.3, $T_{n-s,t-1} \succeq P_{t+1}$. On the other hand, $T_{n,t} - v_0 - v_1$ consists of $n-t-3$ isolated vertices and a path P_{t+1}, so $P_{t+1} \succeq T_{n,t} - v_0 - v_1$. Therefore, $T - u_0 - u_1 \succeq P_{t+1} \succeq T_{n,t} - v_0 - v_1$. Since $T \ncong T_{n,t}$, either $T - u_0 \succ T_{n,t} - v_0$ or $T - u_0 - u_1 \succ T_{n,t} - v_0 - v_1$. By Lemma 1.2, we also have $T \succ T_{n,t}$. $\square$

Proof of Corollary 1.5. Note that for any tree T with n vertices, the Hosoya index $Z(G) = \sum_{r=0}^{\lfloor \frac{n}{2} \rfloor} m(G,r)$. Hence, if T_1 and T_2 are two trees with n vertices such that $T_1 \succeq T_2$ then $Z(T_1) \geq Z(T_2)$. Now it follows from Therorem 1.4 that $Z(T) \geq Z(T_{n,t})$. $\square$

References

[1] D. M. Cvetković, M. Doob , H. Sachs, Spectra of Graphs, Academic Press, New York, 1980.

[2] I. Gutman, The energy of a graph, Ber. Math.-Statist. Sekt. Forsch. Graz. 103 (1978) 1-22.

[3] I. Gutman, Acyclic conjugated molecules, trees and their energies, J. Math. Chem. 1 (1987) 123-143.

[4] I. Gutman, Acyclic systems with extremal Hückel π-electron energy, Theor. Chim. Acta 45 (1977) 79-87.

[5] I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.

[6] I. Gutman, M. Mateljević, Note on the Coulson integral formula, J. Math. Chem. 39 (2006) 259–266.

[7] M. Mateljević, I. Gutman, Note on the Coulson and Coulson–Jacobs integral formulas, MATCH Commun. Math. Comput. Chem. 59 (2008) 257–268.

[8] I. Gutman, Y. Hou, Bipartite unicyclic graphs with greatest energy, MATCH Commun. Math. Comput. Chem. 43 (2001) 17-28.

[9] Y. Hou, On acyclic systems with minimal Hosoya index, Discrete Appl. Math. 119 (2002) 251-257.

[10] Y. Hou, Unicyclic graphs with minimal energy, J. Math. Chem. 29 (2001) 163-168.

[11] Y. Hou, Bicyclic graphs with minimal energy, Linear Multilinear Algebra 49 (2002) 347-354.

[12] Y. Hou, I. Gutman, C. W. Wou, Unicyclic graphs with maximal energy, Linear Algebra Appl. 356 (2002) 27-36.

[13] G. Indulal, A. Vijayakumar, On a pair of equienergetic graphs, MATCH Commun. Math. Comput. Chem. 55 (2006) 83-90.

[14] H. Li, On minimal energy ordering of acyclic conjugated molecules, J. Math. Chem. 25 (1999) 145-169.

[15] F. Li, B. Zhou, Minimal energy of bipartite unicyclic graphs of a given bipartition, MATCH Commun. Math. Comput. Chem. 54 (2005) 379-388.

[16] W. Lin, X. Guo, H. Li, On the extremal energies of trees with a given maximum degree, MATCH Commun. Math. Comput. Chem. 54 (2005) 363-378.

[17] J. Rada, A. Tineo, Polygonal chains with minimal energy, Linear Algebra Appl. 372 (2003) 333-344.

[18] W.-H. Wang , A. Chang , L. Z. Zhang , D. Q. Lu , Unicyclic Hückel molecular graphs with minimal energy, J. Math. Chem. 39 (2006) 231-241.

[19] W. Yan , L. Ye , On the minimal energy of trees with a given diameter, Appl. Math. Lett. 18 (2005) 1046-1052.

[20] W. Yan , L. Ye , On the maximal energy and the Hosoya index of a type of trees with many pendent vertices, MATCH Commun. Math. Comput. Chem. 53 (2005) 449-459.

[21] L. Ye , R. Chen, Ordering of trees with a given bipartition by their energies and Hosoya indices, MATCH Commun. Math. Comput. Chem. 52 (2004) 193-208.

[22] L. Ye , Yuan X., On the minimal energy of trees with a given number of pendent vertices. MATCH Commun. Math. Comput. Chem. 57 (2007) 193-201.

[23] F. Zhang , H. Li, On acyclic conjugated molecules with minimal energies, Discrete Appl. Math. 92 (1999) 71-84.

[24] F. Zhang , Z. Li, Li. Wang, Hexagonal chains with minimal total π-energy, Chem. Phys. Lett. 337 (2001) 125-130.

[25] F. Zhang , Z. Li, L. Wang, Hexagonal chains with maximal total π-energy, Chem. Phys. Lett. 337 (2001) 131-137.

[26] Y. Yang , B. Zhou, Minimum energy of bicyclic graphs of a given diameter. MATCH Commun. Math. Comput. Chem. 59 (2008) 321-342.

[27] A. Yu , X. Lv , Minimum energy on trees with k pendent vertices, Linear Algebra Appl. 418 (2006) 625-633.

[28] B. Zhou , F. Li, On minimal energies of trees of a prescribed diameter. J. Math. Chem. 39 (2006) 465-473.

[29] E. A. Brualdi, J. L. Goldwasser, Permanent of the Laplacian matrix of trees and bipartite graphs, Discrete Math. 48 (1984) 1-12.

[30] G. H. Xu, On the spectral radius of trees with perfect matching, in: Combinatorics and Graph Theory, World Scientific, Singapore, 1997.

[31] I. Gutman, S. Radenković, Hypoenergetic molecular graphs, Indian J. Chem. 46A (2007) 1733–1736.

[32] N. Li, S. Li, On the extremal energy of trees, MATCH Commun. Math. Comput. Chem. 59 (2008) 291–314.

[33] I. Gutman, S. Radenković, N. Li, S. Li, Extremal energy of trees, MATCH Commun. Math. Comput. Chem. 59 (2008) 315–320.

[34] V. Nikiforov, The energy of C_4-free graphs of bounded degree, Lin. Algebra Appl. 428 (2008) 2569–2573.

[35] I. Gutman, X. Li, Y. Shi, J. Zhang, Hypoenergetic trees, MATCH Commun. Math. Comput. Chem. 60 (2008) 415–426.

[36] M. Robbiano, I. Gutman, R. Jiménez, B. San Martín, Spectra of copies of Bethe trees attached to path and applications, Bull. Acad. Serbe Sci. Arts (Cl. Math. Natur.) 137 (2008) 59–81.

[37] J. M. Guo, On the minimal energy ordering of trees with perfect matchings, Discr. Appl. Math. 156 (2008) 2598–2605.

[38] I. Gutman, X. Li, J. Zhang, Graph energy, in: M. Dehmer, F. Emmert–Streib (Eds.), Analysis of Complex Networks. From Biology to Linguistics, Wiley–VCH, Weinheim, 2009, 145–174.