Kragujevac J. Sci. 31 (2009) 45–58. UDC 541.27:541.61

ON THE SPECTRA AND ENERGIES OF DOUBLE–BROOM–LIKE TREES

Renata R. del Vecchio,[a] Ivan Gutman,[b] Vilmar Trevisan,[c] Cybele T. M. Vinagre[a]

[a]*Instituto de Matemática, Universidade Federal Fluminense, Niterói, Brazil*
e-mail: renata@vm.uff.br , cybl@vm.uff.br

[b]*Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia*
e-mail: gutman@kg.ac.rs

[c]*Instituto de Matemática, Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil*
e-mail: trevisan@mat.ufrgs.br

(Received January 2, 2009)

ABSTRACT. Let P_n be the n-vertex path, whose vertices are labelled consecutively by $v_1, v_2, \ldots, v_n$. For $a \geq 1$ and $1 \leq i \leq n$, the *generalized broom* $P_n(i,a)$ is the $(n+a)$-vertex tree, obtained by attaching a pendent vertices to the vertex v_i of P_n . For $a, b \geq 1$ and $1 \leq i < j \leq n$, the *generalized double broom* $P_n(i,a|j,b)$ is the $(n+a+b)$-vertex tree, obtained by attaching a pendent vertices to the vertex v_i of P_n , and b pendent vertices to the vertex v_j of P_n . In this paper we study the spectra and energies of P_n , $P_n(i,a)$, and $P_n(i,a|j,b)$, but some more general results are also pointed out.

INTRODUCTION

The study of eigenvalues and characteristic polynomials of trees is a well-developed part of spectral graph theory [1]. Also since the publication of the seminal monograph [1], numerous results along these lines have been obtained, e. g. [2–9].

If G is a graph on n vertices and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are its eigenvalues, then the energy of G is defined as

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

The first results on the energy of trees were obtained as early as in 1977 [10]. In the meantime scores of results on this topic have accumulated; for some most recent of them see [11–24]. For more detail on graph energy see the recent review [25].

Let P_n be the n-vertex path, whose vertices are labelled by $v_1, v_2, \ldots, v_n$, so that v_i and v_{i+1} are adjacent, $i = 1, 2, \ldots, n-1$. For $a \geq 1$ and $1 \leq i \leq n$, the *generalized broom* $P_n(i, a)$ is the $(n+a)$-vertex tree, obtained by attaching a pendent vertices to the vertex v_i of P_n . We call $P_n(i, a)$ the "generalized broom", because in previous papers [26, 27] the tree $P_n(1, a)$ was named "broom". In [26] it was shown that among all trees with a fixed number of vertices and fixed diameter, $P_n(1, a)$ has minimal energy. In [27] it was shown that $P_n(1, a)$ has minimal energy also among all trees with a fixed number of vertices and fixed number of pendent vertices.

For $a, b \geq 1$ and $1 \leq i < j \leq n$, the *generalized double broom* $P_n(i, a|j, b)$ is the $(n + a + b)$-vertex tree, obtained by attaching a pendent vertices to the vertex v_i of P_n , and b pendent vertices to the vertex v_j of P_n . In view of the above, $P_n(1, a|n, b)$ should be referred to as a "double broom".

ON THE COMPUTATION OF THE CHARACTERISTIC POLYNOMIAL OF A TREE

In this paper we are mainly concerned with *trees* (i. e., connected acyclic graphs) and *forests* (i. e., acyclic, but not necessarily connected graphs). Recall that the *characteristic polynomial* of a graph G is the monic degree-n polynomial [1]

$$\phi(G) = \phi(G, \lambda) = \det(\lambda I_n - A)$$

where A is the adjacency matrix of G.

The roots $\lambda_1, \lambda_2 \ldots, \lambda_n$ of $\phi(G, \lambda)$ are the *eigenvalues* of G, while the set of the eigenvalues is the *spectrum* of G [1].

Denote by $m(G, k)$ the number of k-matchings of the graph G (that is, the number of selection of k independent edges in G). By definition, $m(G, 0) = 1$ and $m(G, 1) =$ number of edges of G.

If T is an n-vertex tree, then [1]

$$\phi(T, \lambda) = \sum_{k \geq 0} (-1)^k \, m(T, k) \, \lambda^{n-2k} \; . \tag{1}$$

We are interested in explicitly constructing the characteristic polynomial of a tree T. One reduction method, first reported by Heilbronner [28, 29], works as follows. Let e be an edge connecting the vertices x_1 and x_2. Then[1]

$$\phi(T) = \phi(T - e) - \phi(T - x_1 - x_2) \; . \tag{2}$$

If x_1 is a pendent vertex of T, and x_2 is its neighbor, then, as a special case of Eq. (2) we have

$$\phi(T) = \lambda \phi(T - x_1) - \phi(T - x_1 - x_2) \; . \tag{3}$$

Two other relations for the characteristic polynomial, that are frequently used in the below considerations, are

$$\phi(G_1 \cup G_2) = \phi(G_1) \, \phi(G_2) \qquad \text{and} \qquad \phi(E_n) = \lambda^n$$

where by $G_1 \cup G_2$ is denoted the graph composed of disjoint components G_1 and G_2, and where E_n is the n-vertex graph without edges.

CHARACTERISTIC POLYNOMIALS OF BROOMS AND DOUBLE BROOMS

Applying Eq. (3) successively to the a pendent vertices of the generalized broom $P_n(i, a)$, we obtain

$$\phi(P_n(i, a)) = \lambda^a \, \phi(P_n) - a \, \lambda^{a-1} \, \phi(P_{i-1}) \, \phi(P_{n-i}) \tag{4}$$

[1] Eq. (2) holds for all graphs, if e is a bridge. Thus, in particular, Eq. (2) holds for any edge of any forest.

which for the simple broom ($i = 1$) reduces to

$$\phi(P_n(1,a)) = \lambda^a \, \phi(P_n) - a \, \lambda^{a-1} \, \phi(P_{n-1}) \ . \tag{5}$$

In a similar manner, by applying Eq. (3) successively to the b pendent vertices of the generalized double broom $P_n(i,a|j,b)$, we get

$$\phi(P_n(i,a|j,b)) = \lambda^b \, \phi(P_n(i,a)) - b \, \lambda^{b-1} \, \phi(P_{j-1}(i,a)) \, \phi(P_{n-j})$$

which combined with (4) yields

$$\begin{aligned} \phi(P_n(i,a|j,b)) &= \lambda^{a+b} \, \phi(P_n) - a \, \lambda^{a+b-1} \, \phi(P_{i-1}) \, \phi(P_{n-i}) \\ &- b \, \lambda^{a+b-1} \, \phi(P_{j-1}) \, \phi(P_{n-j}) + ab \, \lambda^{a+b-2} \, \phi(P_{i-1}) \, \phi(P_{j-i-1}) \, \phi(P_{n-j}) \ . \end{aligned}$$

For the simple double broom ($i = 1$, $j = n$) the above expression is simplified as:

$$\phi(P_n(1,a|n,b)) = \lambda^{a+b} \, \phi(P_n) - (a+b) \, \lambda^{a+b-1} \, \phi(P_{n-1}) + ab \, \lambda^{a+b-2} \, \phi(P_{n-2}) \ . \tag{6}$$

In order to proceed, recall that the Chebyshev polynomial of the first kind, $T_n(x)$, may be defined by the following recurrence relation. Set $T_0(x) = 1$ and $T_1(x) = x$. Then

$$T_n(x) = 2x \, T_{n-1}(x) - T_{n-2}(x) \qquad , \qquad n = 2, 3, \ldots \ .$$

The Chebyshev polynomial of the second kind, $U_n(x)$, may be defined by an analogous recurrence relation,

$$U_n(x) = 2x \, U_{n-1}(x) - U_{n-2}(x) \qquad , \qquad n = 2, 3, \ldots$$

with $U_0(x) = 1$ and $U_1(x) = 2x$.

Consider now the broom $P_n(1,2)$, a tree with $n+2$ vertices.

Proposition 1. The characteristic polynomial of $P_n(1,2)$ satisfies the identity

$$\phi(P_n(1,2)) = 2\lambda \, T_{n+1}(\lambda/2) \ . \tag{7}$$

Proof. Induction on n . Notice that if $n = 0$, then $P_n(1,2)$ is composed by two isolated vertices whose characteristic polynomial is $\lambda^2 = 2\lambda \, T_1(\lambda/2)$. If $n = 1$, then $P_n(1,2)$ is a star with 3 vertices whose characteristic polynomial is $\lambda(\lambda^2-2) = 2\lambda\, T_2(\lambda/2)$. Assuming that the result is true for all $n = 0, 1, \ldots, n'-1$, consider the broom $P_{n'}(1,2)$. Applying the reduction method given by Eq. (3) to the end-vertex $v_{n'}$ of $P_{n'}(1,2)$, and using the induction hypothesis, we obtain

$$\begin{aligned}
\phi(P_{n'}(1,2)) &= \lambda\,\phi(P_{n'-1}(1,2)) - \phi(P_{n'-2}(1,2)) \\
&= \lambda\,[2\lambda\, T_{n'}(\lambda/2)] - [2\lambda\, T_{n'-1}(\lambda/2)] \\
&= 2\lambda\left(2\cdot\frac{\lambda}{2}\, T_{n'}(\lambda/2) - T_{n'-1}(\lambda/2)\right) \\
&= 2\lambda\, T_{n'+1}(\lambda/2)\ .
\end{aligned}$$

Thus, Eq. (7) hods also for $n = n'$, which proves the result. □

Proposition 2. The characteristic polynomial of the path P_n with n is

$$\phi(P_n) = U_n(\lambda/2)\ .$$

Proof. See [1, p. 73]. □

Theorem 1. The characteristic polynomial of the broom $P_n(1,a)$ is

$$\phi(P_n(1,a)) = \lambda^{a-1}\ [U_{n+1}(\lambda/2) - (a-1)U_{n-1}(\lambda/2)]\ .$$

Proof. Combine Proposition 2 with Eq. (5). □

Corollary 1.1. For any integer $n \geq 1$,

$$U_{n+1}(x) - U_{n-1}(x) = 2\,T_{n+1}(x)\ .$$

Proof. This follows by applying the theorem to $P_n(1,2)$ and taking into account Proposition 1. □

Theorem 2. The characteristic polynomial of the double broom $P_n(1,a|n,b)$ is

$$\phi(P_n(1,a|n,b)) = \lambda^{a+b}\, U_n(\lambda/2) - (a+b)\,\lambda^{a+b-1}\, U_{n-1}(\lambda/2) + ab\,\lambda^{a+b-2}\, U_{n-2}(\lambda/2)\ .$$

Proof. Combine Proposition 2 with Eq. (6). □

Corollary 2.1. The characteristic polynomial of the double broom $P_n(1,2|n,2)$ satisfies the identity

$$\phi(P_n(1,2|n,2)) = (\lambda^4 - 4\,\lambda^2)\,U_n(\lambda/2)\ .$$

Proof. In view of Proposition 2, it suffices to show that

$$\phi(P_n(1,2|n,2)) = (\lambda^4 - 4\,\lambda^2)\,\phi(P_n)\ . \tag{8}$$

From (6) we get

$$\begin{aligned}
\phi(P_n(1,2|n,2)) &= \lambda^4\,\phi(P_n) - 4\,\lambda^3\,\phi(P_{n-1}) + 4\,\lambda^2\,\phi(P_{n-2}) \\
&= \lambda^4\,\phi(P_n) - 4\,\lambda^2\,[\lambda\,\phi(P_{n-1}) - \phi(P_{n-2})] \\
&= \lambda^4\,\phi(P_n) - 4\,\lambda^2\,\phi(P_n)
\end{aligned}$$

from which Eq. (8) follows. □

ENERGY OF BROOMS AND DOUBLE BROOMS

Proposition 3.

$$E(P_n) = 2\sum_{k=1}^{n}\left|\cos\frac{k\,\pi}{n+1}\right|\ .$$

Proof. This, otherwise well known result [1, 29], follows from Proposition 2 and the (also well known) fact that the roots of U_n are $\cos[(k\,\pi)/(n+1)]$, $k = 1,\ldots,n$. □

Proposition 4.

$$E(P_n(1,2)) = 2\sum_{k=0}^{n+1}\left|\cos\frac{(2k+1)\pi}{2n+2}\right|\ .$$

Proof. This earlier reported result [30] follows from Proposition 1 and the fact that the roots of T_n are $\cos[(2k+1)\pi/(2n)]$, $k = 0,\ldots,n-1$. □

Proposition 5. $E(P_n(1,2|n,2)) = E(P_n) + 4$.

Proof. See the proof of Corollary 2.1. □

In a number of papers, published in the 1970s and 1980s [10, 31–38], one of the present authors and Fuji Zhang considered the relation $T_1 \succ T_2$ between two trees T_1 and T_2 (as well as an analogous relation between bipartite graphs).

Definition. Let the quantities $m(T,k)$ be same as in Eq. (1). If T_1 and T_2 are two trees, and if $m(T_1,k) \geq m(T_2,k)$ holds for all $k \geq 0$, then we write $T_1 \succeq T_2$. If $m(T_1,k) > m(T_2,k)$ for at least one k, then we write $T_1 \succ T_2$.

The importance of the relation $\succ$ lies in the fact [10] that the energy of a tree T is a monotonically increasing function of the coefficients $m(T,k)$. Therefore, we have [10]:

Proposition 6. $T_1 \succeq T_2$ implies $E(T_1) \geq E(T_2)$. $T_1 \succ T_2$ implies $E(T_1) > E(T_2)$.

In the papers [10, 31–38] the relation $\succ$ was established for a variety of pairs of trees and other types of graphs. Here we point out only one of these results.

Proposition 7. [37] Let, as before, P_n be the n-vertex path, whose vertices are consecutively labelled by $v_1, v_2, \ldots, v_n$. Let T be an arbitrary tree and v its arbitrary (but fixed) vertex. Let $P_n(i,T)$ be the graph obtained by identifying the vertex v_i of P_n with the vertex v of T. Then for $n = 4k+h$, $h \in \{-1,0,1,2\}$, $k \geq 1$,

$$\begin{aligned} P_n(1,T) &\succ P_n(3,T) \succ \cdots \succ P_n(2k+1,T) \succ P_n(2k,T) \\ &\succ P_n(2k-2,T) \succ \cdots \succ P_n(2,T) \ . \end{aligned}$$

It should be noted that the Proposition 7 remains valid if the tree T is replaced by an arbitrary graph G [37].

Applying Propositions 6 and 7 to the generalized brooms we obtain:

Theorem 3. Let $P_n(i|a)$ be the generalized broom and let $n = 4k+h$, $h \in \{-1,0,1,2\}$, $k \geq 1$. Then

$$\begin{aligned} E(P_n(1,a)) &> E(P_n(3,a)) > \cdots > E(P_n(2k+1,a)) > E(P_n(2k,a)) \\ &> E(P_n(2k-2,a)) > \cdots > E(P_n(2,a)) \ . \end{aligned}$$

A less straightforward result of the same kind is:

Theorem 4. Using an analogous notation as in Proposition 7, let T' and T'' be arbitrary trees, v' an arbitrary (but fixed) vertex of T', and v'' an arbitrary (but fixed) vertex of T''. Let $P_n(i, T'|j, T'')$ be the graph obtained by identifying the vertex v_i of P_n with the vertex v' of T' and by identifying the vertex v_j of P_n with the vertex v'' of T''. Then for $3 \leq i < j \leq n-2$,

$$P_n(1, T'|n, T'') \succ P_n(i, T'|j, T'') \succ P_n(2, T'|n-1, T'') .$$

Proof.

In view of Eq. (1), the Heilbronner formula (2) is tantamount to

$$m(T, k) = m(T - e, k) + m(T - x_1 - x_2, k - 1) \qquad \text{for all } k \geq 1 . \tag{9}$$

Applying the Eq. (9) to the edge connecting the vertices v_{j-1} and v_j of the tree $P_n(i, T'|j, T'')$, we get

$$m(P_n(i, T'|j, T''), k) = m(P_{j-1}(i, T') \cup X, k) + m(P_{j-2}(i, T') \cup Y, k - 1) \tag{10}$$

where $X = P_{n-j+1}(1, T'')$ and $Y = P_{n-j+1}(1, T'') - v_1$.

Assume now that the parameter j in $(P_n(i, T'|j, T'')$ is fixed. If so, then the structure of the subgraphs X and Y is also fixed. Then from Proposition 7 we conclude that both terms $m(P_{j-1}(i, T') \cup X, k)$ and $m(P_{j-2}(i, T'') \cup Y, k-1)$ will be maximal (resp. minimal) if $i = 1$ (resp. $i = 2$). Then by Eq. (10), for fixed value of j, the term $m(P_n(i, T'|j, T''), k)$ will be maximal and minimal for $i = 1$ and $i = 2$, respectively, i. e.,

$$m(P_n(1, T'|j, T''), k) \geq m(P_n(i, T'|j, T''), k) > m(P_n(2, T'|j, T''), k)$$

holds for all values of $k \geq 0$ and for $3 \leq i < j$.

By symmetry, for fixed value of the parameter i,

$$m(P_n(i, T'|n, T''), k) \geq m(P_n(i, T'|j, T''), k) > m(P_n(i, T'|n-1, T''), k)$$

holds for all values of $k \geq 0$ and for $i < j \leq n-2$.

Theorem 4 follows by combining the above two results. $\square$

Corollary 4.1. For the trees $P_n(i,T'|j,T'')$ specified in Theorem 4, and for $3 \leq i < j \leq n-2$,

$$E(P_n(1,T'|n,T'')) > E(P_n(i,T'|j,T'')) > E(P_n(2,T'|n-1,T'')) \ .$$

Corollary 4.2. Let $P_n(i,a|j,b)$ be the generalized double broom. Then for $3 \leq i < j \leq n-2$,

$$P_n(1,a|n,b) \succ P_n(i,a|j,b) \succ P_n(2,a|n-1,b)$$

and

$$E(P_n(1,a|n,b)) > E(P_n(i,a|j,b)) > E(P_n(2,a|n-1,b)) \ .$$

Extending Theorem 4 to specifying the trees $P_n(i,T'|j,T'')$ with second–maximal and second–minimal energy seems to be a less easy task. It is not difficult to envisage that the species with second–maximal energy could be either $P_n(3,T'|n,T'')$ or $P_n(1,T'|n-2,T'')$, but the complete answer may depend on the actual structure of T' and T''.

As for the energy of the double broom $P_n(1,a|n,b)$ we can say something more.

Theorem 5. Among the double brooms $P_n(1,a|n,b)$ with fixed number p of pendent vertices ($p = a+b$), the double broom $P_n(1,p-2|n,2)$ has minimal whereas $P_n(1,\lceil p/2 \rceil|n,\lfloor p/2 \rfloor)$ has maximal energy.

Proof. Assume that $a \geq b$. Applying Eq. (9) to one of the pendent edges incident to the vertex v_n of $P_n(1,a|n,b)$ results in:

$$m(P_n(1,a|n,b),k) = m(P_n(1,a|n,b-1),k) + m(P_{n-1}(1,a),k-1) \ .$$

Applying Eq. (9) to one of the pendent edges incident to the vertex v_1 of the double broom $P_n(1,a+1|n,b-1)$ results in:

$$m(P_n(1,a+1|n,b-1),k) = m(P_n(1,a|n,b-1),k) + m(P_{n-1}(1,b),k-1) \ .$$

Then

$$\begin{aligned} & m(P_n(1,a|n,b),k) - m(P_n(1,a+1|n,b-1),k) \\ = \ & m(P_{n-1}(1,a),k-1) - m(P_{n-1}(1,b),k-1) \ . \end{aligned} \qquad (11)$$

If $a = b$ then the right–hand side Eq. (11) is equal to zero for all values of k. If $a > b$ then the broom $P_{n-1}(1, b)$ is a proper subgraph of the broom $P_{n-1}(1, a)$ and therefore the right–hand side of (11) is non-negative for all k and positive at least for $k = 2$. Consequently,

$$m(P_n(1, a|n, b), k) \geq m(P_n(1, a+1|n, b-1), k) \qquad \text{for all } k \geq 0$$

i. e.,

$$P_n(1, a|n, b) \succ P_n(1, a+1|n, b-1) \ .$$

Theorem 5 follows. □

Theorem 6. Among the double brooms $P_n(1, a|n, b)$ with fixed number N vertices $(N = n + a + b)$, $P_{N-4}(1, 2|N-4, 2)$ has maximal whereas $P_2(1, N-4|2, 2)$ has minimal energy.

Proof. Denote by S_n the n-vertex star, and by E_n the n-vertex graph without edges. Apply Eq. (9) to the edge between the vertices v_{n-1} and v_n of $P_n(1, a|n, b)$. This yields:

$$m(P_n(1, a|n, b), k) = m(P_{n-1}(1, a) \cup S_{b+1}, k) + m(P_{n-2}(1, a) \cup E_b, k-1) \ .$$

Apply now Eq. (9) to the edge between the vertices v_{n-1} and v_n of $P_{n+1}(1, a|n+1, b-1)$. This yields:

$$m(P_{n+1}(1, a|n+1, b-1), k) = m(P_{n-1}(1, a) \cup S_{b+1}, k) + m(P_{n-2}(1, a) \cup S_b, k-1) \ .$$

Therefore

$$\begin{aligned} & m(P_{n+1}(1, a|n+1, b-1), k) - m(P_n(1, a|n, b), k) \\ = \ & m(P_{n-2}(1, a) \cup S_b, k-1) - m(P_{n-2}(1, a) \cup E_b, k-1) \ . \end{aligned}$$

The right–hand side of the latter equality is evidently positive for some and zero for the other values of k, implying

$$P_{n+1}(1, a|n+1, b-1) \succ P_n(1, a|n, b)$$

and

$$E(P_{n+1}(1, a|n+1, b-1)) > E(P_n(1, a|n, b)) \ .$$

In other words, extending the diameter of the double broom on the expense of the number of pendent vertices, increase the energy. Hence the maximal–energy double broom will have a minimal number of pendent vertices (= 2) on each of its side.

The minimal–energy double broom will have smallest possible diameter, i. e., $n = 2$. The requirement that the difference between the parameters a and b be as large as possible follows from Theorem 5. $\square$

The energy of the maximal–energy N-vertex double broom $P_{N-4}(1,2|n,2)$ is determined by Proposition 5. By an easy calculation we find that for the minimal–energy N-vertex double broom $E(P_2(1,N-4|2,2) = 2\sqrt{N-1+\sqrt{8N-32}}$. Thus we arrive at:

Corollary 6.1. For $n \geq 2$, $a \geq 2$, $b \geq 2$, the energy of the double broom $P_n(1,a|n,b)$ satisfies the inequalities

$$2\sqrt{n+a+b-1+\sqrt{8n+8a+8b-40}} \leq E(P_n(1,a|n,b)) \leq 4 + E(P_{n+a+b-4})$$

with equality on the left–hand side if and only if $n = 2$ and $a = 2$ or $b = 2$, and with equality on the right–hand side if and only if $a = b = 2$.

Acknowledgement. Part of this work was supported by the Serbian Ministry of Science, through Grant no. 144015G.

REFERENCES

[1] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, Academic Press, New York, 1980; 2nd revised ed.: Barth, Heidelberg, 1995.

[2] G. H. Fricke, S. T. Hedetniemi, D. P. Jacobs, V. Trevisan, *Reducing the adjacency matrix of a tree*, El. J. Lin. Algebra **1** (1996) 34–43.

[3] D. P. Jacobs, V. Trevisan, *The determinant of a tree's neighborhood matrix*, Lin. Algebra Appl. **256** (1997) 235–249.

[4] D. P. Jacobs, C. M. S. Machado, V. Trevisan, *An $O(n^2)$ algorithm for the characteristic polynomial of a tree*, J. Comb. Math. Comb. Comput. **54** (2005) 213–221.

[5] O. Rojo, R. Soto, *The spectra of the adjacency matrix and Laplacian matrix for some balanced trees*, Lin. Algebra Appl. **403** (2005) 97–117.

[6] O. Rojo, *The spectra of some trees and bounds for the largest eigenvalue of any tree*, Lin. Algebra Appl. **414** (2006) 199-217.

[7] O. Rojo, M. Robbiano, *An explicit formula for eigenvalues of Bethe trees and upper bounds on the largest eigenvalue of any tree*, Lin. Algebra Appl. **427** (2007) 138–150.

[8] 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. Sci. Math. Natur.) **137** (2008) 59–81.

[9] O. Rojo, L. Medina, *Spectra of generalized Bethe trees attached to a path*, Lin. Algebra Appl. **430** (2009) 483–503.

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

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

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

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

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

[15] W. H. Wang, *Ordering of Hückel trees according to minimal energies*, Lin. Algebra Appl. **430** (2009) 703–717.

[16] S. Li, N. Li, *On minimal energies of acyclic conjugated molecules*, MATCH Commun. Math. Comput. Chem. **61** (2009) 341–349.

[17] M. Robbiano, R. Jiménez, L. Medina, *The energy and an approximation to Estrada index of some trees*, MATCH Commun. Math. Comput. Chem. **61** (2009) 369–382.

[18] S. Li, X. Li, *The fourth maximal energy of acyclic graphs*, MATCH Commun. Math. Comput. Chem. **61** (2009) 383–394.

[19] O. Miljković, B. Furtula, S. Radenković, I. Gutman, *Equienergetic and almost–equienergetic trees*, MATCH Commun. Math. Comput. Chem. **61** (2009) 451–461.

[20] J. Ou, *On acyclic molecular graphs with maximal Hosoya index, energy, and short diameter*, J. Math. Chem., in press.

[21] X. Li, X. Yao, J. Zhang, I. Gutman, *Maximum energy trees with two maximum degree vertices*, J. Math. Chem. **45** (2009) 962–973.

[22] C. Heuberger, S. G. Wagner, *Chemical trees minimizing energy and Hosoya index*, J. Math. Chem. **46** (2009) 214–230.

[23] J. Zhang, B. Zhou, *Minimal energies of non-starlike trees with given number of pendent vertices*, MATCH Commun. Math. Comput. Chem. **62** (2009) 481–490.

[24] C. Heuberger, S. G. Wagner, *On a class of extremal trees for various indices*, MATCH Commun. Math. Comput. Chem. **62** (2009) 437–464.

[25] 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, pp. 145–174.

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

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

[28] E. Heilbronner, *Das Kompositions–Prinzip: Eine anschauliche Methode zur elektronen–theoretischen Behandlung nicht oder niedrig symmetrischer Molekeln im Rahmen der MO–Theorie*, Helv. Chim. Acta **36** (1953) 170–188.

[29] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.

[30] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, *Graph theory and molecular orbitals. XII. Acyclic polyenes*, J. Chem. Phys. **62** (1975) 3399–3405.

[31] I. Gutman, *Partial ordering of forests according to their characteristic polynomials*, in: A. Hajnal, V. T. Sós (Eds.), *Combinatorics*, North–Holland, Amsterdam, 1978, pp. 429–436.

[32] I. Gutman, *Graphs with greatest number of matchings*, Publ. Inst. Math. (Beograd) **27** (1980) 67–76.

[33] F. Zhang, *Two theorems of comparison of bipartite graphs by their energy*, Kexue Tongbao **28** (1983) 726–730.

[34] F. Zhang, Z. Lai, *The totally ordered subset in a sort of Hasse graphs of trees*, J. Xinjiang Univ. (1983) 35–36.

[35] F. Zhang, Z. Lai, *Three theorems of comparison of trees by their energy*, Science Exploration **3** (1983) 12–19.

[36] I. Gutman, F. Zhang, *On a quasiordering of bipartite graphs*, Publ. Inst. Math. (Beograd) **40** (1986) 11–15.

[37] I. Gutman, F. Zhang, *On the ordering of graphs with respect to their matching numbers*, Discr. Appl. Math. **15** (1986) 25–33.

[38] Y. Zhang, F. Zhang, I. Gutman, *On the ordering of bipartite graphs with respect to their characteristic polynomials*, Coll. Sci. Papers Fac. Sci. Kragujevac **9** (1988) 9–20.