

Minimal Spectrum-Sums of Bipartite Graphs with Exactly Two Vertex-Disjoint Cycles

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The spectrum-sum of a graph is defined as the sum of the absolute values of its eigenvalues. The graphs with minimal spectrum-sums in the class of connected bipartite graphs with exactly two vertex-disjoint cycles, in the class of connected bipartite graphs with exactly two vertex-disjoint cycles whose lengths are congruent with 2 modulo 4, and in the class of connected bipartite graphs with exactly two vertex-disjoint cycles one of which has length congruent with 2 modulo 4, are determined, respectively.

INTRODUCTION

Let G be a simple graph with n vertices.¹ The characteristic polynomial of G is the characteristic polynomial of its adjacency matrix, denoted by $\phi(G, \lambda)$.^{2,3} The eigenvalues of G denoted by $\lambda_1, \dots, \lambda_n$, are the roots of $\phi(G, \lambda) = 0$. The set of graph-eigenvalues is also called the spectrum of the graph.⁴ The spectrum-sum of G is defined as the sum of the absolute values of all elements in the graph-spectrum:

$$E(G) = |\lambda_1| + |\lambda_2| + \dots + |\lambda_n|.$$

In the literature, the energy of a graph is usually employed for the spectrum-sum, *e.g.*, Refs. 5–8. This term was introduced by Gutman⁹ and an explanation why he had chosen this term is given in Ref. 10. We choose the

term spectrum-sum since in physical sciences energy represents a measurable quantity.

If G is the molecular graph of a conjugated hydrocarbon, often called the Hückel graph,¹¹ then the corresponding set of eigenvalues is called the Hückel spectrum.¹² The connection between the graph spectrum and Hückel spectrum and the role of Hückel spectrum in the theory of conjugated molecules were discussed in detail elsewhere.^{13,14} The use of the Hückel spectrum in chemistry has been recently presented, for example, in this journal.¹⁵

For a bipartite graph G (depicting the alternant structures)¹⁶ with n vertices, its characteristic polynomial can be written as:

$$\phi(G, \lambda) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k b_k(G) \lambda^{n-2k},$$

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where $b_k(G) \geq 0$ for $k = 0, 1, \dots, \left\lfloor \frac{n}{2} \right\rfloor$. For convenience, let $b_k(G) = 0$ for $k < 0$ or $k > \left\lfloor \frac{n}{2} \right\rfloor$. We also note that the spectrum-sum can be calculated by the Coulson integral formula:¹⁷

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \log \left[1 + \sum_{k=1}^{\lfloor n/2 \rfloor} b_k(G) x^{2k} \right] dx.$$

Thus, one can define a quasi-order relation over the class of all bipartite graphs: if G and G' are bipartite graphs with n vertices, then:

$$G \succeq G' \Leftrightarrow b_k(G) \geq b_k(G') \text{ for } k = 0, 1, \dots, \left\lfloor \frac{n}{2} \right\rfloor.$$

If $G \succeq G'$ and there is a k_0 such that $b_{k_0}(G) > b_{k_0}(G')$, then we write $G \succ G'$. According to the Coulson integral formula for energy, for bipartite graphs G and G' , we have:

$$G \succ G' \Rightarrow E(G) > E(G') \quad (1)$$

Gutman¹⁸ determined acyclic conjugated structures (trees) with extremal Hückel π -electron energies (spectrum-sums). That work triggered interest in determining graphs with minimal or maximal spectrum sums.^{5–8,19–26} In the present report, we join these efforts by studying graphs with minimal spectrum-sums in the class of bipartite graphs with exactly two vertex-disjoint cycles. Examples of these graphs are shown in Figure 1.

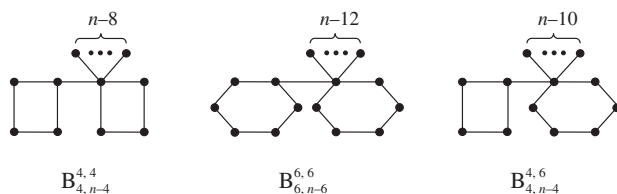


Figure 1. Examples of graphs with minimal spectrum-sums in the class of bipartite graphs with exactly two vertex-disjoint cycles.

PRELIMINARIES

Let P_n and C_n be the path and cycle with n vertices, respectively. Let U_n^l be the graph obtained by attaching $n-l$ pendent vertices to a vertex of the cycle C_l . The vertex-disjoint union of graphs G and H is denoted by $G \cup H$, $[p]G$ denotes the vertex-disjoint union of p copies of G .

Lemma 1.¹⁰ – Let G be a bipartite graph and let uv be a bridge of G . Then:

$$b_k(G) = b_k(G - uv) + b_{k-1}(G - u - v).$$

According to Lemma 1, it is easy to see that the following two lemmas hold.

Lemma 2. – Let G be a bipartite graph and let uv be a bridge of G . Then $G \succ G - uv$.

For example, if an acyclic graph G with n vertices contains a subgraph H with $t < n$ vertices, then according to Lemma 2, we have $G \succ H \cup [n-t]P_1$.

Lemma 3. – Let G and G' be two bipartite graphs with n vertices. Let uv be a bridge of G and $u'v'$ be a bridge of G' . If $G - uv \succeq G' - u'v'$ and $G - u - v \succ G' - u' - v'$, or $G - uv \succ G' - u'v'$ and $G - u - v \succeq G' - u' - v'$ then $G \succ G'$.

According to Theorems 4 and 5 in Ref. 5 and Theorem 4 in Ref. 6, we have:

Lemma 4.^{5,6} – Let G be an n -vertex bipartite unicyclic graph whose unique cycle length is l . If $G \neq U_n^l$, then $G \succ U_n^l$. If $l > 4$ then $U_n^l \succ U_n^4$. If $l > 6$ then $U_n^l \succ U_n^6$.

Lemma 5.²⁶ – Let G_1 and G_2 be two vertex-disjoint bipartite graphs. Then for any $k \geq 0$,

$$b_k(G_1 \cup G_2) = \sum_{i=0}^k b_i(G_1) b_{k-i}(G_2).$$

Proof: Let $n_i = |V(G_i)|$ for $i = 1, 2$. Note that:

$$\begin{aligned} & \sum_{i=0}^{\lfloor n/2 \rfloor} (-1)^k b_k(G_1 \cup G_2) x^{n-2k} = \\ & \phi(G_1 \cup G_2, x) = \\ & \phi(G_1, x) \phi(G_2, x) = \\ & \sum_{i=0}^{\lfloor n_1/2 \rfloor} (-1)^i b_i(G_1) x^{n_1-2i} \sum_{i=0}^{\lfloor n_2/2 \rfloor} (-1)^i b_i(G_2) x^{n_2-2i}. \end{aligned}$$

The result follows directly. \square

RESULTS

Let $B_{n_1, n_2}^{l_1, l_2}$ be the graph obtained by adding an edge between the vertex of maximal degree in $U_{n_1}^{l_1}$ and the vertex of maximal degree in $U_{n_2}^{l_2}$. Let G be an n -vertex connected bipartite graph with exactly two vertex-disjoint cycles. Then there are two vertex-disjoint cycles $C^{(1)}$ and $C^{(2)}$ in G with lengths l_1 and l_2 , respectively, and there is a unique path P connecting a vertex say $u = u_1$ in $C^{(1)}$ and a vertex say v in $C^{(2)}$, such that each edge in P is a bridge of G , where l_1 and l_2 are even and at least four. Let u_2 be the unique neighbor of u_1 in P . Then $G - u_1 u_2$ consists of two components G_1 containing the cycle $C^{(1)}$ and G_2 containing the cycle $C^{(2)}$. Let $n_i = |V(G_i)|$, $i = 1, 2$. Obviously, $n_1 + n_2 = n$.

Theorem 6. – Let G be an n -vertex connected bipartite graph with exactly two vertex-disjoint cycles, where $n \geq 9$. If $G \neq B_{4, n-4}^{4,4}$ then $G \succ B_{4, n-4}^{4,4}$.

Proof: According to Lemma 4, $G_i \succeq U_{n_i}^4$ for $i = 1, 2$. According to Lemma 5:

$$G - u_1 u_2 = G_1 \cup G_2 \succeq U_{n_1}^4 \cup U_{n_2}^4.$$

Now we consider the graph $G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2)$. Note that $G_1 - u_1$ is an acyclic graph containing a path P_3 . According to Lemma 2, $G_1 - u_1 \succeq P_3[n_1 - 4]P_1$, and if u_2 lies on the cycle $C^{(2)}$, then $G_2 - u_2 \succeq P_3 \cup [n_2 - 4]P_1$. Suppose that u_2 lies outside the cycle $C^{(2)}$. According to Lemma 2, $G_2 - u_2 \succeq C_{l_2} \cup [n_2 - 1 - l_2]P_1$. It is easily seen that:

$$b_1(C_{l_2} \cup [n_2 - 1 - l_2]P_1) = l_2 > 2 = b_1(P_3 \cup [n_2 - 4]P_1),$$

and $b_k(C_{l_2} \cup [n_2 - 1 - l_2]P_1) \geq 0 = b_k(P_3 \cup [n_2 - 4]P_1)$ for all $k \geq 2$. Thus, we have $G_2 - u_2 \succeq C_{l_2} \cup [n_2 - 1 - l_2]P_1 \succ P_3 \cup [n_2 - 4]P_1$. It follows that $G_2 - u_2 \succeq P_3 \cup [n_2 - 4]P_1$ whether u_2 lies on the cycle $C^{(2)}$ or not. Thus we have proved that: $G_1 - u_1 \succeq P_3 \cup [n_1 - 4]P_1$ and $G_2 - u_2 \succeq P_3 \cup [n_2 - 4]P_1$. Now according to Lemma 5:

$$G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2) \succeq [2]P_3 \cup [n - 8]P_1.$$

If $\min\{n_1, n_2\} = 4$ say $n_1 = 4$ then since $G \neq B_{4,n-4}^{4,4}$ we have $G_2 - u_2$ containing the path or the star on four vertices as a subgraph, and so $b_1(G - u_1 - u_2) = b_1(G_1 - u_1) + b_1(G_2 - u_2) \geq 2 + 3 > 4 = b_1([2]P_3 \cup [n - 8]P_1)$, implying:

$$G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2) \succ [2]P_3 \cup [n - 8]P_1.$$

According to Lemma 3, we have $G \succ B_{n_1, n_2}^{4,4}$ and if $\min\{n_1, n_2\} = 4$, then $G \succ B_{n_1, n_2}^{4,4} = B_{4, n-4}^{4,4}$ and so the result follows. By direct calculation:

$$\begin{aligned} \phi(U_{n_1}^4 \cup U_{n_2}^4, \lambda) &= [\lambda^{n_1 - n_1} \lambda^{n_1 - 2} + (2n_1 - 8)\lambda^{n_1 - 4}] \times \\ &\quad [\lambda^{n_2 - n_2} \lambda^{n_2 - 2} + (2n_2 - 8)\lambda^{n_2 - 4}] = \\ &\quad [\lambda^n - n\lambda^{n-2} + (n_1 n_2 + 2n - 16)\lambda^{n-4} - \\ &\quad 4(n_1 n_2 - 2n)\lambda^{n-6} + \\ &\quad 4(n_1 n_2 - 4n + 16)\lambda^{n-8}]. \end{aligned}$$

Suppose that $\min\{n_1, n_2\} > 4$. Then $n_1 n_2 > 4(n - 4)$. Thus $b_2(U_{n_1}^4 \cup U_{n_2}^4) = n_1 n_2 + 2n - 16 > 4(n - 4) + 2n - 16 \geq b_2(U_{n_1}^4 \cup U_{n_2}^4)$. Similarly, $b_k(U_{n_1}^4 \cup U_{n_2}^4) > b_k(U_{n_1}^4 \cup U_{n_2}^4)$ for $k = 3, 4$. Note that $b_k(U_{n_1}^4 \cup U_{n_2}^4) = b_k(U_{n_1}^4 \cup U_{n_2}^4) = 0$ for $k \geq 4$. It follows that $U_{n_1}^4 \cup U_{n_2}^4 \succ U_{n_1}^4 \cup U_{n_2}^4$. According to Lemma 3, $B_{n_1, n_2}^{4,4} \succ B_{4, n-4}^{4,4}$. It follows that $G \succeq B_{n_1, n_2}^{4,4} \succ B_{4, n-4}^{4,4}$. \square

Theorem 7. – Let G be an n -vertex connected bipartite graph with exactly two vertex-disjoint cycles, where $n \geq 13$. If both cycle lengths of G are congruent with 2 modulo 4 and $G \neq B_{6, n-6}^{6,6}$, then $G \succ B_{6, n-6}^{6,6}$.

Proof: According to Lemma 4, $G_i \succeq U_{n_i}^6$ for $i = 1, 2$. According to Lemma 5, $G - u_1 u_2 = G_1 \cup G_2 \succeq U_{n_1}^6 \cup U_{n_2}^6$.

Now we consider the graph $G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2)$. According to Lemma 2, $G_1 - u_1 \succeq P_5 \cup [n_1 - 6]P_1$, and if u_2 lies on the cycle $C^{(2)}$ then $G_2 - u_2 \succeq P_5 \cup [n_2 - 6]P_1$.

Suppose that u_2 lies outside the cycle $C^{(2)}$. According to Lemma 2, $G_2 - u_2 \succeq C_{l_2} \cup [n_2 - 1 - l_2]P_1$. It is easily seen that:

$$b_1(C_{l_2} \cup [n_2 - 1 - l_2]P_1) = l_2 > 4 = b_1(P_5 \cup [n_2 - 6]P_1),$$

$$b_2(C_{l_2} \cup [n_2 - 1 - l_2]P_1) = \frac{l_2(l_2 - 3)}{2} > 3 = b_2(P_5 \cup [n_2 - 6]P_1),$$

and $b_k(C_{l_2} \cup [n_2 - 1 - l_2]P_1) \geq 0 = b_k(P_5 \cup [n_2 - 6]P_1)$ for all $k \geq 3$. Thus, we have $G_2 - u_2 \succeq C_{l_2} \cup [n_2 - 1 - l_2]P_1 \succ P_5 \cup [n_2 - 6]P_1$. It follows that $G_2 - u_2 \succeq P_5 \cup [n_2 - 6]P_1$ whether u_2 lies on the cycle $C^{(2)}$ or not. According to Lemma 5:

$$G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2) \succeq [2]P_5 \cup [n - 12]P_1.$$

If $\min\{n_1, n_2\} = 6$ say $n_1 = 6$, then since $G \neq B_{6, n-6}^{6,6}$ we have $G_2 - u_2$ containing a subgraph formed by attaching a pendent vertex to the path P_5 , and so $b_1(G - u_1 - u_2) = b_1(G_1 - u_1) + b_1(G_2 - u_2) \geq 4 + 5 > 8 = b_1([2]P_5 \cup [n - 12]P_1)$, implying:

$$G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2) \succ [2]P_5 \cup [n - 12]P_1.$$

According to Lemma 3, we have $G \succeq B_{n_1, n_2}^{6,6}$, and if $n_1 = 6$, then $G \succ B_{n_1, n_2}^{6,6} = B_{6, n-6}^{6,6}$, and so the result follows. By direct calculation:

$$\begin{aligned} \phi(U_{n_1}^6 \cup U_{n_2}^6, \lambda) &= \\ &[\lambda^{n_1 - n_1} \lambda^{n_1 - 2} + (4n_1 - 5)\lambda^{n_1 - 4} - (3n_1 - 18)\lambda^{n_1 - 6}] \times \\ &[\lambda^{n_2 - n_2} \lambda^{n_2 - 2} + (4n_2 - 5)\lambda^{n_2 - 4} - (3n_2 - 18)\lambda^{n_2 - 6}] = \\ &\lambda^n - n\lambda^{n-2} + (n_1 n_2 + 4n - 30)\lambda^{n-4} - \\ &(8n_1 n_2 - 12n - 36)\lambda^{n-6} + (22n_1 n_2 - 78n + 225)\lambda^{n-8} - \\ &(24n_1 n_2 - 117n + 540)\lambda^{n-10} + (9n_1 n_2 - 54n - 324)\lambda^{n-12}. \end{aligned}$$

If $\min\{n_1, n_2\} > 6$ then $n_1 n_2 > 6(n - 6)$, and from the characteristic polynomial above, we have $U_{n_1}^6 \cup U_{n_2}^6 \succ U_{n_1}^6 \cup U_{n_2}^6$. According to Lemma 3, we have $G \succeq B_{n_1, n_2}^{6,6} = B_{6, n-6}^{6,6}$. \square

The following theorem was reported in Ref. 26. Here we give an alternate proof.

Theorem 8. – Let G be an n -vertex connected bipartite graph with exactly two vertex-disjoint cycles, where $n \geq 11$. If one cycle length of G is congruent with 2 modulo 4 and $G \neq B_{4, n-4}^{4,6}$, then $G \succ B_{4, n-4}^{4,6}$.

Proof: Suppose without loss of generality that $l_2 \equiv 2 \pmod{4}$. According to Lemma 4, $G_1 \succeq U_{n_1}^4$ and $G_2 \succeq U_{n_2}^6$. According to Lemma 5, $G - u_1 u_2 = G_1 \cup G_2 \succeq U_{n_1}^4 \cup U_{n_2}^6$.

Now we consider the graph $G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2)$. According to Lemma 2, $G_1 - u_1 \succeq P_3 \cup [n_1 - 4]P_1$, and if u_2 lies on the cycle $C^{(2)}$, then $G_2 - u_2 \succeq P_5 \cup [n_2 - 6]P_1$.

Suppose that u_2 lies outside the cycle $C^{(2)}$. According to Lemma 2, $G_2 - u_2 \succeq C_{l_2} \cup [n_2 - 1 - l_2]P_1$. It is easily seen that:

$$b_1(C_{l_2} \cup [n_2 - 1 - l_2]P_1) = l_2 > 4 = b_1(P_5 \cup [n_2 - 6]P_1),$$

$$b_2(C_{l_2} \cup [n_2 - 1 - l_2]P_1) = \frac{l_2(l_2 - 3)}{2} > 3 = b_2(P_5 \cup [n_2 - 6]P_1),$$

and $b_k(C_{l_2} \cup [n_2 - 1 - l_2]P_1) \geq 0 = b_k(P_5 \cup [n_2 - 6]P_1)$ for all $k \geq 3$. Thus, we have $G_2 - u_2 \succeq C_{l_2} \cup [n_2 - 1 - l_2]P_1 \succ P_5 \cup [n_2 - 6]P_1$. It follows that $G_2 - u_2 \succeq P_5 \cup [n_2 - 6]P_1$ whether u_2 lies either on the cycle $C^{(2)}$ or not. According to Lemma 5:

$$G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2) \succeq P_3 \cup P_5 \cup [n - 10]P_1.$$

If $n_1 = 4$ then since, $G \neq B_{4,n-4}^{4,6}$, we have $G_2 - u_2$ containing a subgraph formed by attaching a pendent vertex to the path P_5 and so $b_1(G - u_1 - u_2) = b_1(G_1 - u_1) + b_1(G_2 - u_2) \geq 2 + 5 > 6 = b_1(P_3 \cup P_5 \cup [n - 10]P_1)$, implying:

$$G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2) \succ P_3 \cup P_5 \cup [n - 10]P_1.$$

According to Lemma 3, we have $G \succeq B_{n_1, n_2}^{4,6}$, and if $n_1 = 4$, then $G \succ B_{n_1, n_2}^{4,6} = B_{4, n-4}^{4,6}$, and so the result follows. By direct calculation:

$$\begin{aligned} \phi(U_{n_1}^4 \cup U_{n_2}^6, \lambda) &= \lambda^n - n\lambda^{n-2} + (n_1 n_2 + 2n_2 + 2n - 23)\lambda^{n-4} - \\ &\quad (6n_1 n_2 + 10n_2 - 15n - 18)\lambda^{n-6} + \\ &\quad (11n_1 n_2 + 16n_2 - 48n + 120)\lambda^{n-8} - \\ &\quad (6n_1 n_2 + 12n_2 - 36n + 144)\lambda^{n-10}. \end{aligned}$$

If $n_1 > 4$ then $f(n_1, n_2) = an_1 n_2 + bn_2 > f(4, n-4)$ for $(a, b) = (1, 2)$, $(6, 10)$, $(11, 16)$, $(6, 12)$ and thus from the characteristic polynomial above, we have $U_{n_1}^4 \cup U_{n_2}^6 \cup U_4^4 \cup U_{n-4}^6$. According to Lemma 3, we have $G \succeq B_{n_1, n_2}^{4,6} \succ B_{4, n-6}^{4,6}$. \square

Let G be an n -vertex connected bipartite graph with exactly two vertex-disjoint cycles, where $n \geq 9$. According to Theorems 6, 7 and 8, and using (1), we have:

- (i) If $G \neq B_{4, n-4}^{4,4}$ then $E(G) > E(B_{4, n-4}^{4,4})$.
- (ii) If both cycle lengths of G are congruent with 2 modulo 4 and $G \neq B_{6, n-6}^{6,6}$ where $n \geq 13$ then $E(G) > E(B_{6, n-6}^{6,6})$.

- (iii) If one cycle length of G is congruent with 2 modulo 4 and $G \neq B_{4, n-4}^{4,6}$, where $n \geq 11$ then $E(G) > E(B_{4, n-4}^{4,6})$.

For the graphs $B_{4, n-4}^{4,4}$, $B_{4, n-4}^{4,6}$ and $B_{6, n-6}^{6,6}$ with $n \geq 12$, it may be easily checked by Lemmas 3 and 4 or by the characteristic polynomials that $E(B_{4, n-4}^{4,4}) < E(B_{4, n-4}^{4,6}) < E(B_{6, n-6}^{6,6})$.

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REFERENCES

1. R. J. Wilson, *Introduction to Graph Theory*, Oliver & Boyd, Edinburgh, 1972, p. 9.
2. N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, FL, 1992, Chapter 5.
3. D. Janežič, A. Miličević, S. Nikolić, and N. Trinajstić, *Graph-Theoretical Matrices in Chemistry*, University of Kragujevac, Kragujevac, 2007, Chapter 2.
4. D. Cvetković, M. Doob, and H. Sachs, *Spectra of Graphs – Theory and Application*, 3rd ed., Johann Ambrosius Barth, Heidelberg, 1995.
5. Y. Hou, *J. Math. Chem.* **29** (2001) 163–168.
6. A. Chen, A. Chang, and W. C. Shiu, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 95–102.
7. Y. Hou, *Lin. Multilin. Algebra* **49** (2002) 347–354.
8. I. Gutman, B. Furtula, and H. Hua, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 85–92.
9. I. Gutman, *Ber. Math.-Stat. Sket. Forschungszentrum Graz* **103** (1978) 1–22.
10. I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, 1986, pp. 139–139.
11. A. Graovac and N. Trinajstić, *Croat. Chem. Acta* **59** (1975) 95–104.
12. N. Trinajstić, in: *Chemical Graph Theory – Introduction and Fundamentals*, Gordon and Breach, New York, 1991, pp. 235–279.
13. A. Graovac, I. Gutman, and N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer-Verlag, Berlin, 1977.
14. N. Trinajstić, Z. Mihalić, and A. Graovac, in: *Graph-Theoretical Approaches to Chemical Reactivity*, Kluwer, Dordrecht, 1994, pp. 37–72.
15. S. Nikolić, A. Miličević, and N. Trinajstić, *Croat. Chem. Acta* **79** (2006) 155–159.
16. N. Trinajstić, in: G. A. Segal (Ed.), *Modern Theoretical Chemistry. 7. Semiempirical Methods of Electronic Structure Calculations. Part A: Techniques*, Plenum Press, New York, 1977, pp. 1–28.
17. C. A. Coulson, *Proc. Cambridge Phil. Soc.* **36** (1940) 201–206.
18. I. Gutman, *Theoret. Chim. Acta* **45** (1977) 79–87.
19. F. Zhang and H. Li, *Discr. Appl. Math.* **92** (1999) 71–84.
20. H. Li, *J. Math. Chem.* **25** (1999) 145–169.
21. J. Zhang and B. Zhou, *J. Math. Chem.* **37** (2005) 423–431.

22. J. Zhang and B. Zhou, *Appl. Math. J. Chinese Univ. Ser. A* **20** (2005) 233–238.
23. W. Lin, X. Guo, and H. Li, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 363–378.
24. J. Rada, *Discr. Appl. Math.* **92** (2005) 437–443.
25. Y. Yang and B. Zhou, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 321–342.
26. Z. Liu and B. Zhou, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 381–396.

SAŽETAK

Minimalne spektralne sume bipartitnih grafova s točno dva prstena razmaknuta jednim bridom

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Spektralna suma grafa definirana kao zbroj apsolutnih vrijednosti svih elemenata u spektru grafa. Pronađeni su grafovi s minimalnim spektralnim sumama u klasi bipartitnih grafova s točno dva prstena razmaknuta jednim bridom gdje su veličine prstenova sukladno s 2 modulo 4 i u klasi bipartitnih grafova s točno dva prstena razmaknuta jednim bridom gdje je veličina jednoga prstena sukladana s 2 modulo 4.