MINIMAL ENERGY OF BIPARTITE UNICYCLIC GRAPHS OF A GIVEN BIPARTITION

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Abstract

The energy of a graph is defined as the sum of the absolute values of all the eigenvalues of the graph. In the paper, we characterize the graphs with minimal energy in the class of bipartite unicyclic graphs of a given (p, q)–bipartition, where $q \geq p \geq 2$.

INTRODUCTION

Let G be a graph on n vertices. The characteristic polynomial of G, denoted by $\phi(G)$, is defined as $\phi(G) = \det(xI - A(G))$, where I is the identity matrix of order n and $A(G)$ is the adjacency matrix of G. The n roots of the equation $\phi(G) = 0$, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, are the eigenvalues of the graph G. Since $A(G)$ is symmetric, all

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eigenvalues of G are real. The energy of G, denoted by $E(G)$, is then defined by

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

In chemistry, the energy of a given molecular graph is of interest since it is closely related to the total π–electron energy of the molecular represented by that graph calculated within the Hückel molecular orbital (HMO) approximation [1, 2]. For details on graph–energy concept and a survey of the mathematical properties and results, see [1, 3, 4].

It is well–known that if G is a bipartite graph on n vertices, then $\phi(G)$ can be written as

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

where $b(G, k) \geq 0$ for all $k = 0, 1, \ldots, \lfloor n/2 \rfloor$. Note that $b(G, 0) = 1$ and $b(G, 1)$ is equal to the number of edges of G. Let $m(G, k)$ be number of k–matchings of G. If G is a tree, then [1] $b(G, k) = m(G, k)$ for all k.

In view of the expression for $\phi(G)$, a quasi–order relation can be introduced over the class of all bipartite graphs [5]: if G_1 and G_2 are bipartite graphs, then

$$G_1 \succeq G_2 \Leftrightarrow b(G_1, k) \geq b(G_2, k) \text{ for all } k \geq 0 \,.$$

If $G_1 \succeq G_2$ and there is a k such that $b(G_1, k) > b(G_2, k)$, then we write $G_1 \succ G_2$.

The energy of a bipartite graph G on n vertices can be expressed as the Coulson integral formula [1]

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left(\sum_{k=0}^{\lfloor n/2 \rfloor} b(G, k) x^{2k} \right) dx \,. \tag{1}$$

Let G_1 and G_2 be bipartite graphs. Since $b(G_i, k) \geq 0$ for all k and $i = 1, 2$, from (1) we have the following increasing property of energy:

$$G_1 \succ G_2 \Rightarrow E(G_1) > E(G_2) \,. \tag{2}$$

A connected graph with n vertices and n edges is called a unicyclic graph. If G is a connected bipartite graph, then its vertex set can be uniquely partitioned into V_1 and V_2 such that every edge joins a vertex of V_1 to a vertex of V_2. V_1 and V_2 form a bipartition of vertex set of G. Moreover, if $|V_1| = p$ and $|V_2| = q$, then we say G has a (p, q)–bipartition. Hou [7] determined the unicyclic graphs with minimal energy. Recently, Ye and Chen [8] studied trees of a given bipartition with minimal energy.

In the paper, we will prove that in the class of bipartite unicyclic graphs of a (p, q)–bipartition $(q \geq p \geq 2)$, the graph $B(p, q)$ has minimal energy if $p \geq 4$ or $p = 2$,

the graph $B(3, q)$ or $H(3, q)$ has minimal energy if $p = 3$, where $B(p, q)$ denotes the graph formed by attaching $p - 2$ and $q - 2$ vertices to two adjacent vertices of a quadrangle, respectively, and $H(3, q)$ is the graph formed by attaching $q - 2$ vertices to the pendent vertex of $B(2, 3)$. The graphs $B(p, q)$ $(q \geq 2)$ and $H(3, q)$ $(q \geq p \geq 3)$ are shown in Figure 1.
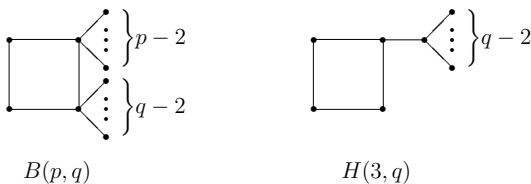

$B(p, q)$ $H(3, q)$

Figure 1. Graphs $B(p, q)$ $(q \geq p \geq 2)$ and $H(3, q)$ $(q \geq 3)$.

RESULTS

Let G be a graph and uv an edge of G, we denote by $G - u$ (resp. $G - uv$) the graph formed from G by deleting the vertex u and the edges incident with u (resp. the edge uv). Denote by P_n the n–vertex path. For two graphs G and H, $G \neq H$ means G and H are not isomorphic.

Lemma 1. *Let G and G' be two bipartite graphs. Suppose that u (resp. u') is a pendent vertex of G (resp. G') and uv (resp. $u'v'$) is the edge of G (resp. G') incident with u (resp. u'). If $G - u \succeq G' - u'$ and $G - u - v \succ G' - u' - v'$; or $G - u \succ G' - u'$ and $G - u - v \succeq G' - u' - v'$, then $G \succ G'$.*

Proof. Since uv is an edge of G with pendent vertex u, we have [6]

$$\phi(G) = x\phi(G - u) - \phi(G - u - v),$$

from which it follows that

$$b(G, k) = b(G - u, k) + b(G - u - v, k - 1). \tag{3}$$

Similarly,

$$b(G', k) = b(G' - u', k) + b(G' - u' - v', k - 1). \tag{4}$$

If $G - u \succeq G' - u'$ and $G - u - v \succ G' - u' - v'$, then by (3) and (4), $b(G, k) \geq b(G', k)$ for all k and there is at least one k such that $b(G, k) > b(G', k)$, and so $G \succ G'$.

Similarly, if $G - u \succ G' - u'$ and $G - u - v \succeq G' - u' - v'$, then $G \succ G'$. The lemma thus holds. □

Lemma 2. [1, 5] *Let T be a tree on n vertices, and $T \neq S_n, Y_n$, where S_n is the n–vertex star, Y_n is formed by attaching a vertex to a pendent vertex of S_{n-1}. Then $T \succ Y_n \succ S_n$.*

Lemma 3. *Let G be a bipartite unicyclic graph of a $(4,4)$–bipartition, and $G \neq B(4,4)$. Then $G \succ B(4,4)$.*

Proof. Since G is bipartite unicyclic graph of a $(4,4)$–bipartition and $G \neq B(4,4)$, G must be isomorphic to one of the sixteen graphs B_i, $i = 1, 2, \ldots, 16$, as shown in Figure 2.
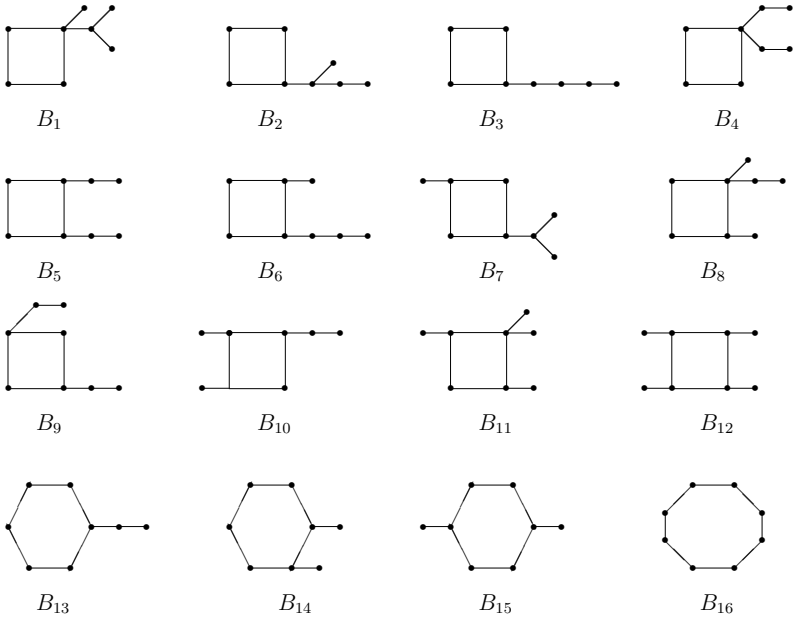

Figure 2. Graphs B_i with $i = 1, 2, \ldots, 16$.

Note that
$$\phi(B_1) = x^8 - 8x^6 + 14x^4 - 4x^2, \quad \phi(B_2) = x^8 - 8x^6 + 16x^4 - 6x^2,$$
$$\phi(B_3) = x^8 - 8x^6 + 17x^4 - 8x^2, \quad \phi(B_4) = x^8 - 8x^6 + 15x^4 - 8x^2,$$
$$\phi(B_5) = x^8 - 8x^6 + 16x^4 - 9x^2, \quad \phi(B_6) = x^8 - 8x^6 + 16x^4 - 8x^2 + 1,$$

$$\phi(B_7) = x^8 - 8x^6 + 15x^4 - 4x^2\,, \qquad \phi(B_8) = x^8 - 8x^6 + 14x^4 - 7x^2 + 1\,,$$

$$\phi(B_9) = x^8 - 8x^6 + 16x^4 - 8x^2\,, \qquad \phi(B_{10}) = x^8 - 8x^6 + 15x^4 - 8x^2 + 1\,,$$

$$\phi(B_{11}) = x^8 - 8x^6 + 13x^4 - 6x^2\,, \qquad \phi(B_{12}) = x^8 - 8x^6 + 14x^4 - 8x^2 + 1\,,$$

$$\phi(B_{13}) = x^8 - 8x^6 + 18x^4 - 13x^2 + 2\,, \quad \phi(B_{14}) = x^8 - 8x^6 + 17x^4 - 11x^2 + 1\,,$$

$$\phi(B_{15}) = x^8 - 8x^6 + 17x^4 - 10x^2 + 1\,, \quad \phi(B_{16}) = x^8 - 8x^6 + 20x^4 - 16x^2 + 2\,,$$

$$\phi(B(4,4)) = x^8 - 8x^6 + 12x^4 - 4x^2\,.$$

It is obvious that $B_i \succ B(4,4)$ for $i = 1, 2, \ldots, 16$. The lemma thus holds. $\quad\square$

Theorem 4. *Let G be a bipartite unicyclic graph of a (p,q)–bipartition $(q \geq p \geq 4)$, and $G \neq B(p,q)$. Then $E(G) > E(B(p,q))$.*

Proof. By the increasing property (2) of energy, it suffices to prove that if G is a bipartite unicyclic graph of a (p,q)–bipartition $(q \geq p \geq 4)$ such that $G \neq B(p,q)$, then $G \succ B(p,q)$. We prove this by induction on $p + q$.

By Lemma 3, the result holds if $p + q = 8$.

Suppose that the result holds for bipartite unicyclic graphs on $p + q - 1$ vertices (of a $(p, q-1)$–bipartition with $q \geq 5$ or a $(p-1, q)$–bipartition with $p \geq 5$) and that G is a bipartite unicyclic graph of a (p,q)–bipartition such that $G \neq B(p,q)$ where $p + q > 8$ and $q \geq p \geq 4$. Let V_1 and V_2 be the bipartition of vertex set of G and $B(p,q)$ with $|V_1| = p$ and $|V_2| = q$.

If G has no pendent vertices, then G is an even cycle with $p = q$, and by Sachs theorem [1],

$$b(B(p,p),2) = m(B(p,p),2) - 2 = (p-2)(p-2) + 4(p-2) + 2 = p^2 - 2\,,$$
$$b(B(p,p),3) = (p-2)^2\,, \quad b(B(p,p),k) = 0 \text{ for all } k \geq 4\,.$$

Note that [1, p. 55]

$$b(G,2) = p(2p-3)\,, \quad b(G,3) = \frac{1}{3}p(2p-4)(2p-5)\,.$$

It can be easily checked that $G \succ B(p,p)$.

In the following, suppose that G has pendent vertices. Note that there is at least a pendent vertex of G in V_2 if $p = 4$. Let u be a pendent vertex and uv the edge incident with u of G, where we may assume that $u \in V_2$ and $v \in V_1$. Then $G - u$ is a bipartite unicyclic graph of a $(p, q-1)$–bipartition (on $p + q - 1$ vertices), and $G - u - v$ is a graph on $p + q - 2$ vertices. Let u' be a pendent vertex and $u'v'$ the edge incident with u' of $B(p,q)$, where $u' \in V_2$ and $v' \in V_1$. Then $B(p,q) - u' = B(p, q-1)$

and $B(p,q) - u' - v' = (q-3)P_1 \cup Y_{P+1}$. It is easy to see that

$$b((q-3)P_1 \cup Y_{p+1}, k) = m((q-3)P_1 \cup Y_{p+1}, k) = \begin{cases} p & \text{if } k=1, \\ p-2 & \text{if } k=2, \\ 0 & \text{if } k \geq 3. \end{cases} \quad (5)$$

First suppose that $p < q$. We denote the degree of v in G by $d_G(v)$. Since $v \in V_1$ and G has a (p,q)–bipartition, we have $d_G(v) \leq q$. Suppose that the cycle of G is C_r with length r.

Case 1 $d_G(v) \leq q-1$. Then $G - u - v$ has at least $p + q - (q-1) = p+1$ edges and so $b(G - u - v, 1) \geq p+1$. We now prove the following:

Claim $G - u - v \succ (q-3)P_1 \cup Y_{p+1}$.

By (5) and the fact that $b(G - u - v, 1) \geq p+1$, to prove the claim we need only to show that $b(G - u - v, 2) \geq p-2$.

Subcase 1.1 $G - u - v$ is acyclic. Then v lies on the cycle C_r and $b(G - u - v, 2) = m(G - u - v, 2)$.

If $G - u - v$ has a unique connected component T which is not an isolated vertex, then T is a tree with at least $p+1$ edges. If T is a star, then $r = 4$ and hence $p = 2$, a contradiction. So T is not a star. By Lemma 2, we have $m(G - u - v, 2) = m(T, 2) \geq m(Y_{p+2}, 2) = p - 1 > p - 2$.

Suppose that there exist s $(s \geq 2)$ connected components $T_1, T_2, \ldots, T_s$ in $G - u - v$ each of which is not an isolated vertex. Then $\sum_{i=1}^{s} e_i \geq p+1$ and $e_i \geq 1$, where e_i denotes the number of edges in T_i for $i = 1, 2, \ldots, s$. Note that $m(G - u - v, 2) = \sum_{i=1}^{s} m(T_i, 2) + \sum_{1 \leq i < j \leq s} e_i e_j$ and that $e_1 e_2 \geq e_1 + e_2 - 1$. We have $m(G - u - v, 2) \geq \sum_{1 \leq i < j \leq s} e_i e_j \geq e_1 + e_2 - 1 + \sum_{i=3}^{s} e_i \geq p > p - 2$.

Hence $b(G - u - v, 2) = m(G - u - v, 2) > p - 2$ if $G - u - v$ is acyclic.

Subcase 1.2 $G - u - v$ is a bipartite graph with exactly one cycle. Then v lies outside C_r. We may choose an edge $e = wz$ in C_r such that $m(G - u - v - w - z, 1) \geq 2$. By Sachs theorem,

$$b(G - u - v, 2) = \begin{cases} m(G - u - v, 2) & \text{if } r > 4, \\ |m(G - u - v, 2) - 2| & \text{if } r = 4. \end{cases}$$

On the other hand,

$$m(G - u - v, 2) = m(G - u - v - e, 2) + m(G - u - v - w - z, 1) \geq m(G - u - v - e, 2) + 2.$$

It follows that

$$b(G - u - v, 2) \geq m(G - u - v - e, 2).$$

If $G - u - v$ has a unique connected component H which is not an isolated vertex, then $H - e$ is not a star, and so by Lemma 2, $b(G - u - v, 2) \geq m(G - u - v - e, 2) = m(H - e, 2) \geq m(Y_{p+1}, 2) = p - 2$.

If there exist s ($s \geq 2$) connected components in $G - u - v$ each of which is not an isolated vertex, then by a similar reasoning as in Subcase 1.1, we have $b(G - u - v, 2) \geq m(G - u - v - e, 2) > p - 2$.

By combining Subcases 1 and 2, the claim holds.

Since $G - u$ is a bipartite unicyclic graph of a $(p, q - 1)$–bipartition (on $p + q - 1$ vertices), we have either $G - u \neq B(p, q - 1)$, and then by induction assumption, $G - u \succ B(p, q - 1)$, or $G - u = B(p, q - 1)$. So we have $G - u \succeq B(p, q - 1)$. By Lemma 1, we have $G \succ B(p, q)$.

Case 2 $d_G(v) = q$. Then $G - u - v$ must be an acyclic graph with at least $p + q - q = p$ edges, and so $b(G - u - v, 1) \geq p$. By a similar reasoning as in Subcase 1.1, we have $b(G - u - v, 2) \geq p - 2$ and hence $G - u - v \succeq (q - 3)P_1 \cup Y_{p+1}$.

Note that $G - u$ is a bipartite unicyclic graph of a $(p, q-1)$–bipartition (on $p + q - 1$ vertices), and that $G - u \neq B(p, q - 1)$ since $G \neq B(p, q)$ and $d_G(v) = q$. By induction assumption, we have $G - u \succ B(p, q - 1)$. Hence by Lemma 1, we have $G \succ B(p, q)$.

Now suppose that $p = q$. Then $G - u$ is a bipartite unicyclic graph of a $(q - 1, q)$–bipartition. By a similar reasoning as above, we can prove that $G \succ B(p, q)$ if $G \neq B(p, q)$.

The theorem is thus proved. □

The following theorem follows from [7, Theorems 4 and 5]. To be more self–contained, a proof is included.

Theorem 5. *Let G be a bipartite unicyclic graph of a $(2, q)$–bipartition ($q \geq 2$), and $G \neq B(2, q)$. Then $G \succ B(2, q)$.*

Proof. It is easy to see that G must be isomorphic to a graph, which is formed by attaching s and $q - 2 - s$ edges to two non–adjacent vertices of a quadrangle, respectively, where $1 \leq s \leq \lfloor q/2 \rfloor - 1$. So $b(G, 1) = q + 2 = b(B(2, q), 1)$, and by Sachs theorem, $b(G, 2) = |m(G, 2) - 2| = 2(q - 2) + s(q - 2 - s) > 2(q - 2) = b(B(2, q), 2)$. Note that $b(B(2, q), k) = 0$ for all $k \geq 3$. The result follows. □

By Theorems 4 and 5, $B(p, q)$ achieves minimal energy in the class of bipartite unicyclic graphs of a (p, q)–bipartition if $q \geq p \geq 4$ or $q \geq p = 2$. In the following we discuss bipartite unicyclic graphs of a $(3, q)$–bipartition if $q \geq 3$.

Lemma 6. *Let G be a bipartite unicyclic graph of a $(3, 3)$–bipartition, and $G \neq$*

$B(3,3), H(3,3)$. Then $G \succ B(3,3)$.

Proof. Note that there are exactly three non–isomorphic bipartite unicyclic graphs of a $(3,3)$–bipartition, $B(3,3)$, $H(3,3)$ and C_6. Since

$$\phi(H(3,3)) = x^6 - 6x^4 + 6x^2, \quad \phi(B(3,3)) = x^6 - 6x^4 + 5x^2 - 1,$$
$$\phi(C_6) = x^6 - 6x^4 + 9x^2 - 2,$$

we have $G = C_6 \succ B(3,3)$. The lemma thus holds. $\square$

Theorem 7. *Let G be a bipartite unicyclic graph of a $(3,q)$–bipartition $(q \geq 3)$, and $G \neq B(3,q), H(3,q)$. Then $E(G) > E(B(3,q))$.*

Proof. By the increasing property (2) of energy, it suffices to prove that if G is a bipartite unicyclic graph of a $(3,q)$–bipartition $(q \geq 3)$ such that $G \neq H(3,q)$, $G \neq B(3,q)$, then $G \succ B(3,q)$. We prove this by induction on q.

By Lemma 6, the result holds if $q = 3$.

Suppose that the result holds for bipartite unicyclic graphs of a $(3,q-1)$–bipartition and that G is a bipartite unicyclic graph of a $(3,q)$–bipartition such that $G \neq B(3,q)$, $H(3,q)$, where $q \geq 4$. Let V_1 and V_2 be the bipartition of vertex set of G and $B(3,q)$ with $|V_1| = 3$ and $|V_2| = q$. Then there is at least a pendent vertex of G in V_2. Choose a pendent vertex $u \in V_2$ such that the shortest distance between u and the vertices of the cycle in G is minimal. Let uv be the edge incident with u of G. Then $v \in V_1$ and $G - u - v$ is a bipartite graph on $3 + q - 2 = q + 1$ vertices. Let u' be a pendent vertex and $u'v'$ the edge incident with u' of $B(3,q)$. Then $B(3,q) - u' = B(3,q-1)$ and $B(3,q) - u' - v' = (q-3)P_1 \cup P_4$. First we prove $G - u - v \succ (q-3)P_1 \cup P_4$.

Case 1 $G - u - v$ has a cycle. Since $G \neq B(3,q), H(3,q)$, G must be isomorphic to G_1 (see Figure 3). So $G - u - v = (q-4)P_1 \cup B(2,3)$. Note that $b(G - u - v, 1) = 5 > 3 = b((q-3)P_1 \cup P_4, 1)$, $b(G - u - v, 2) = 2 > 1 = b((q-3)P_1 \cup P_4, 2)$ and $b((q-3)P_1 \cup P_4, k) = 0$ for all $k \geq 3$. Hence $G - u - v \succ (q-3)P_1 \cup P_4$.

Case 2 $G - u - v$ is an acyclic graph on $q + 1$ vertices. We denote the degree of v in G by $d_G(v)$. Since $v \in V_1$ and G has a $(3,q)$–bipartition, $d_G(v) \leq q$.

Subcase 2.1 $d_G(v) \leq q - 1$. Then $G - u - v$ has at least $q + 3 - (q-1) = 4$ edges, and so $b(G - u - v, 1) = 4 > b((q-3)P_1 \cup P_4, 1) = 3$. Let H be the graph formed from $G - u - v$ by deleting all isolated vertices. If H is star, then v lies on the cycle of G and the length of the cycle is 4 and hence G is a bipartite graph of a $(2, q+1)$–bipartition, a contradiction. So we have $b(G - u - v, 2) = b(H, 2) > b((q-3)P_1 \cup P_4, 2) = 1$. It follows that $G - u - v \succ P_4 \cup (q-3)P_1$.

Subcase 2.2 $d_G(v) = q$. Since $G \neq B(3,q), H(3,q)$, G must be isomorphic to G_2 (see Figure 3). So $G - u - v = (q-4)P_1 \cup P_2 \cup P_3$. It is easy to see that $P_2 \cup P_3 \succ P_1 \cup P_4$

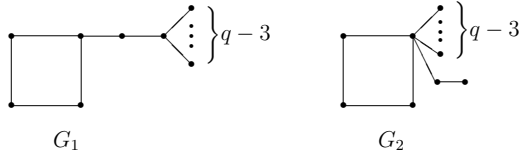and hence $G - u - v = (q - 4)P_1 \cup P_2 \cup P_3 \succ (q - 3)P_1 \cup P_4$.

$$G_1 \qquad\qquad\qquad G_2$$

Figure 3. Graphs G_1 and G_2.

By combining Cases 1 and 2, we have $G - u - v \succ (q - 3)P_1 \cup P_4$. By induction assumption, we have $G - u \succeq B(3, q - 1)$. Hence by Lemma 1, $G \succ B(3, q)$.

The theorem is thus proved. □

For $B(3, q)$ and $H(3, q)$ with $q \geq 3$, we have

$$\phi(B(3, q)) = x^{q+3} - (q + 3)x^{q+1} + (3q - 4)x^{q-1} - (q - 2)x^{q-3},$$
$$\phi(H(3, q)) = x^{q+3} - (q + 3)x^{q+1} + (4q - 6)x^{q-1}.$$

From their characteristic polynomials, we can not order $B(3, q)$ and $H(3, q)$ by using the quasi–order relation, but we can calculate that $E(B(3, 3)) = 7.202 > E(H(3, 3)) = 6.602$ and $E(B(3, 4)) = 3.971 > E(H(3, 4)) = 3.650$ (rounded to three decimal places). We conjecture that $E(B(3, q)) > E(H(3, q))$ for $q \geq 3$. If this is true, then by Theorem 7, $H(3, q)$ will achieve minimal energy in the class of bipartite unicyclic graphs of a $(3, q)$–bipartition $(q \geq 3)$.

References

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

[2] I. Gutman, Total π–electron energy of benzenoid hydrocarbons, *Topics Curr. Chem.* **162** (1992) 29–63.

[3] I. Gutman, The energy of a graph, *Ber. Math.–Statist. Sekt. Forschungszentrum Graz* **103** (1978) 1–22.

[4] I. Gutman, The energy of a graph: old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), *Algebraic Combinatorics and Applications*, Springer–Verlag, Berlin, 2001, 196–211.

[5] I. Gutman, Acyclic system with extremal Hückel π–electron energy, *Theoret. Chim. Acta (Berlin)* **45** (1977) 79–87.

[6] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs*, 3rd edition, Johann Ambrosius Barth, Heidelberg, 1995.

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

[8] 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.

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

[10] B. Zhou, Energy of a graph, *MATCH Commun. Math. Comput. Chem.* **51** (2004) 111–118.