MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **58** (2007) 75-82

ISSN 0340 - 6253

BIPARTITE UNICYCLIC GRAPHS WITH MAXIMAL, SECOND–MAXIMAL, AND THIRD–MAXIMAL ENERGY

Ivan Gutman,[a] Boris Furtula[a] and Hongbo Hua[b]

[a] *Faculty of Science, University of Kragujevac,*
P. O. Box 60, 34000 Kragujevac, Serbia
e-mail: gutman@kg.ac.yu ; boris.furtula@gmail.com

[b] *Department of Computing Science, Huaiyin Institute of Technology,*
Huaian, Jiangsu 223000, P. R. China
e-mail: hongbo.hua@gmail.com

(Received February 21, 2007)

Abstract

Based on the results of the preceding paper [H. Hua, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 57–73], by means of an appropriate computer search, the bipartite unicyclic n-vertex graphs with greatest, second–greatest, and third–greatest energy are determined for all values of n.

INTRODUCTION

Let G be a graph on n vertices, and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues. Then the *energy* of G is defined as [1, 2]

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

A fundamental (and mathematically most obvious) problem encountered within the study of graph energy is the characterization of the graphs that belong to a given class of graphs having maximal or minimal E-values. Numerous results along these lines have been obtained, the first seems to be the finding of the n-vertex trees with maximal, second–maximal, minimal, and second–minimal energy [3]. More details can be found in the review [2], papers [4–6], and in the references quoted therein. For the most recent research in this area see [7–18].

The maximal–energy bipartite unicyclic graphs were examined by Hou and one of the present authors [19, 20], and recently in [21]. In order to state the results obtained in [19–21] as well as the results of this work, we need to define a few special unicyclic graphs.

Let, as usual, P_n and C_n be the path and the cycle, respectively, on n vertices. The vertices of P_n are assumed to be labelled consecutively by $1, 2, \ldots, n$.

For $n \geq 7$, by B_n is denoted the graph obtained by joining (by means of a new edge) a vertex of C_6 to the vertex 1 of P_{n-6}. For $n \geq 9$, D_n is the graph obtained by joining a vertex of C_6 to the vertex 3 of P_{n-6}. For $n \geq 11$, X_n is the graph obtained by joining a vertex of C_6 to the vertex 5 of P_{n-6}. For $n \geq 12$, by Y_n we denote the graph obtained by joining the terminal vertex of B_{n-5} to the vertex 3 of P_5. The structure of the graphs B_n, D_n, X_n, Y_n, and C_n should be evident from the examples depicted in Fig. 1. All these graphs are unicyclic. For any value of n, B_n, D_n, X_n, and Y_n are bipartite, whereas C_n is bipartite only if n is even.

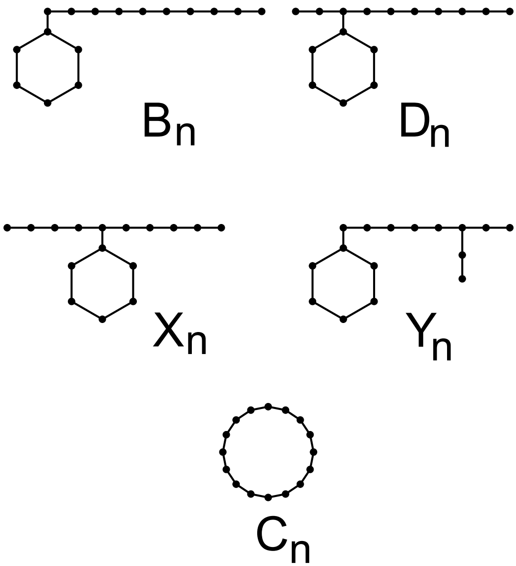

Fig. 1. Examples of the graphs B_n , C_n , D_n , X_n , and Y_n for $n = 16$.

Denote by $\mathcal{BU}_n$ the set of all bipartite unicyclic graphs on n vertices. In the papers [19, 21] the following two results have been proven:

Theorem 1 [19]. If n is odd, $n \geq 7$, then B_n has maximal energy in $\mathcal{BU}_n$. If n is even, $n \geq 8$, then the element of $\mathcal{BU}_n$ that has maximal energy is either B_n or C_n .

Theorem 2 [21]. For $n \geq 13$, the element of $\mathcal{BU}_n \setminus \{B_n, C_n\}$ that has maximal energy is D_n .

In [19] by numerical calculations the following result has also been obtained:

Claim 3. For $n = 10$, the cycle C_n has maximal energy in $\mathcal{BU}_n$. For all other values of n , $n \geq 7$, the element of $\mathcal{BU}_n$ that has maximal energy is B_n .

Although the validity of Claim 3 is out of doubt, a satisfactory proof of it has not been achieved so far. The solution of this seemingly simple problem remains a task for the future and a challenge for mathematicians.

FINDING THE ELEMENTS OF $\mathcal{BU}_n$ WITH SECOND– AND THIRD–MAXIMAL ENERGY

Combining Theorems 1 and 2 and Claim 3 we arrive at the following conclusions, valid for $n \geq 13$:

(a) The n-vertex bipartite unicyclic graph with maximal energy is B_n.

(b) If n is odd, then the n-vertex bipartite unicyclic graph with second–maximal energy is D_n. If n is even, then the n-vertex bipartite unicyclic graph with second–maximal energy is either C_n or D_n.

(c) From the results of the papers [19–21] it cannot be concluded which n-vertex bipartite unicyclic graph has third–maximal energy.

In view of this, we have undertaken a computer–aided search aimed at filling all the missing gaps, and thus determining the n-vertex bipartite unicyclic graphs with maximal, second–maximal, and third–maximal energy for all values of n.

For $n < 4$ there are no bipartite unicyclic graphs, $\mathcal{BU}_n = \emptyset$. For $n = 4$ and $n = 5$, the set $\mathcal{BU}_n$ has just a single element. Only for $n \geq 6$ there are more than three different n-vertex bipartite unicyclic graphs, making our search meaningful. The results obtained for $6 \leq n \leq 12$ are shown in Fig. 2.

For $n \geq 13$, where the results of the work [21] can be applied, the graphs encountered are always some among the above defined B_n, C_n, D_n, X_n, and Y_n. The maximum–energy graph is, of course, B_n. Which graphs have the second–maximal and third–maximal energy is seen from Table 1.

In summary, our results can be formulated as follows:

Claim 4. For all $n \geq 11$, the n-vertex bipartite unicyclic graph with maximal energy is B_n. For all $n \geq 23$, the n-vertex bipartite unicyclic graph with second–maximal energy is D_n. For all $n \geq 27$, the n-vertex bipartite unicyclic graph with third–maximal energy is X_n. For the other (smaller) values of n the graphs with maximal, second–maximal, and third–maximal energies are those specified in Fig. 2 and Table 1.

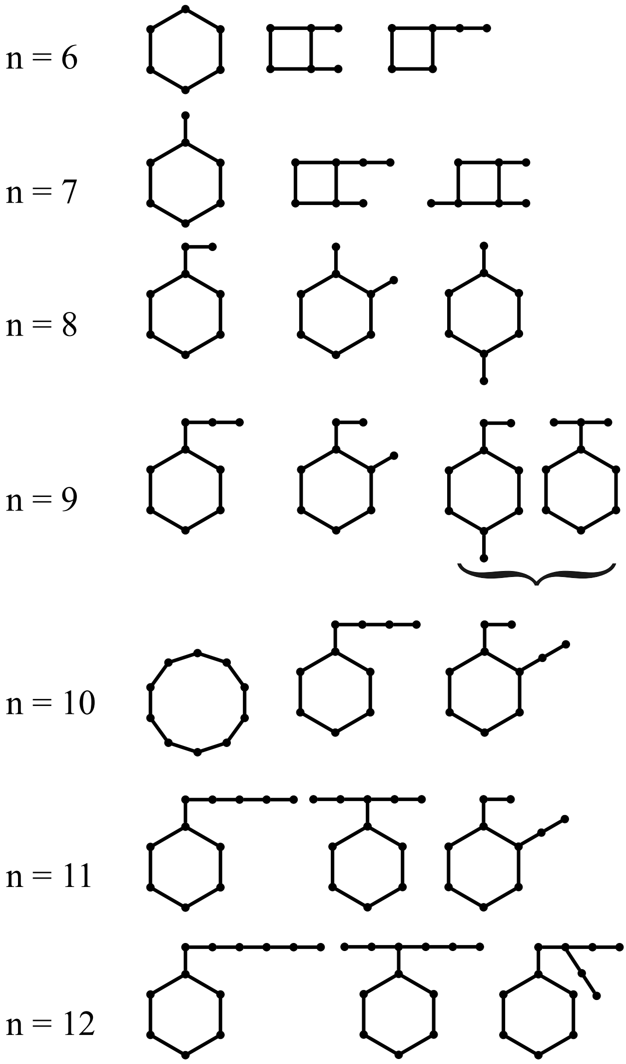

Fig. 2. Bipartite unicyclic graphs on n vertices, $n = 6, 7, \ldots, 12$, with maximal, second–maximal, and third–maximal energies (from left to right). Note that in the case $n = 9$ there are two graphs with third–maximal energy; these graphs are cospectral and, consequently, equienergetic.

n	$\max_1$	E	$\max_2$	E	$\max_3$	E
13	B_n	16.5597	D_n	16.5063	Y_n	16.4987
14	B_n	17.9935	C_n	17.9758	D_n	17.9357
15	B_n	19.1255	D_n	19.0704	X_n	19.0640
16	B_n	20.5319	D_n	20.4750	Y_n	20.4647
17	B_n	21.6855	D_n	21.6299	X_n	21.6216
18	B_n	23.0726	C_n	23.0351	D_n	23.0160
19	B_n	24.2420	D_n	24.1861	X_n	24.1772
20	B_n	25.6147	D_n	25.5582	Y_n	25.5483
21	B_n	26.7963	D_n	26.7402	X_n	26.7310
22	B_n	28.1577	C_n	28.1067	D_n	28.1013
23	B_n	29.3489	D_n	29.2928	X_n	29.2834
24	B_n	30.7014	D_n	30.6451	Y_n	30.6353
25	B_n	31.9004	D_n	31.8442	X_n	31.8347
26	B_n	33.2456	D_n	33.1893	C_n	33.1849
27	B_n	34.4510	D_n	34.3948	X_n	34.3853
28	B_n	35.7902	D_n	35.7339	X_n	35.7242
28	B_n	37.0010	D_n	36.9448	X_n	36.9352
39	B_n	38.3351	D_n	38.2788	X_n	38.2691
31	B_n	39.5504	D_n	39.4942	X_n	39.4846
32	B_n	40.8802	D_n	40.8239	X_n	40.8142
33	B_n	42.0995	D_n	42.0433	X_n	42.0337
34	B_n	43.4254	D_n	43.3692	X_n	43.3595
35	B_n	44.6482	D_n	44.5920	X_n	44.5824

Table 1. The n-vertex bipartite unicyclic graphs, $13 \leq n \leq 35$, with maximal ($\max_1$), second–maximal ($\max_2$), and third–maximal ($\max_3$) energies, and the respective energies.

Those parts of Claim 4 that are new relative to Theorems 1 and 2 are lacking a rigorous mathematical proof. Therefore these should be considered as conjectures, awaiting for a proof or (what we deem to be highly unlikely) refutation.

References

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

[2] 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, pp. 196–211.

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

[4] G. Caporossi, D. Cvetković, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs. 2. Finding graphs with extremal energy, *J. Chem. Inf. Comput. Sci.* **39** (1999) 984–996.

[5] J. Koolen, V. Moulton, Maximal energy graphs, *Adv. Appl. Math.* **26** (2001) 47–52.

[6] J. Koolen, V. Moulton, Maximal energy bipartite graphs, *Graph Combin.* **19** (2003) 131–135.

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

[8] 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.

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

[10] 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.

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

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

[13] 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.

[14] A. Chen, A. Chang, W. C. Shiu, Energy ordering of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 95–102.

[15] 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.

[16] H. Hua, On minimal energy of unicyclic graphs with prescribed girth and pendent vertices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 351–361.

[17] X. Li, J. Zhang, B. Zhou, On unicyclic conjugated molecules with minimal energies, *J. Math. Chem.*, in press.

[18] W. H. Wang, A. Chang, D. Q. Lu, Unicyclic graphs possessing Kekulé structures with minimal energy, *J. Math. Chem.*, in press.

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

[20] Y. Hou, I. Gutman, C. W. Woo, Unicyclic graphs with maximal energy, *Lin. Algebra Appl.* **356** (2002) 27–36.

[21] H. Hua, Bipartite unicyclic graphs with large energy, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 57–73.