

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

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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 $\lambda_1, \lambda_2, \dots, \lambda_n$ be its eigenvalues. Then the *energy* of G is defined as [1, 2]

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

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 $1, 2, \dots, n$.

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.

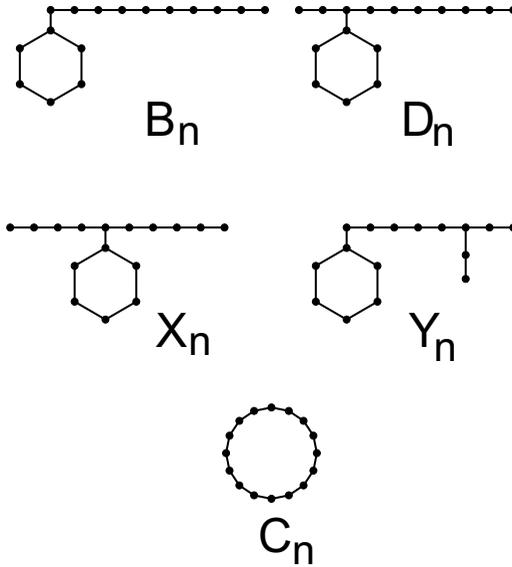


Fig. 1. Examples of the graphs B_n , C_n , D_n , X_n , and Y_n for $n = 16$.

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.

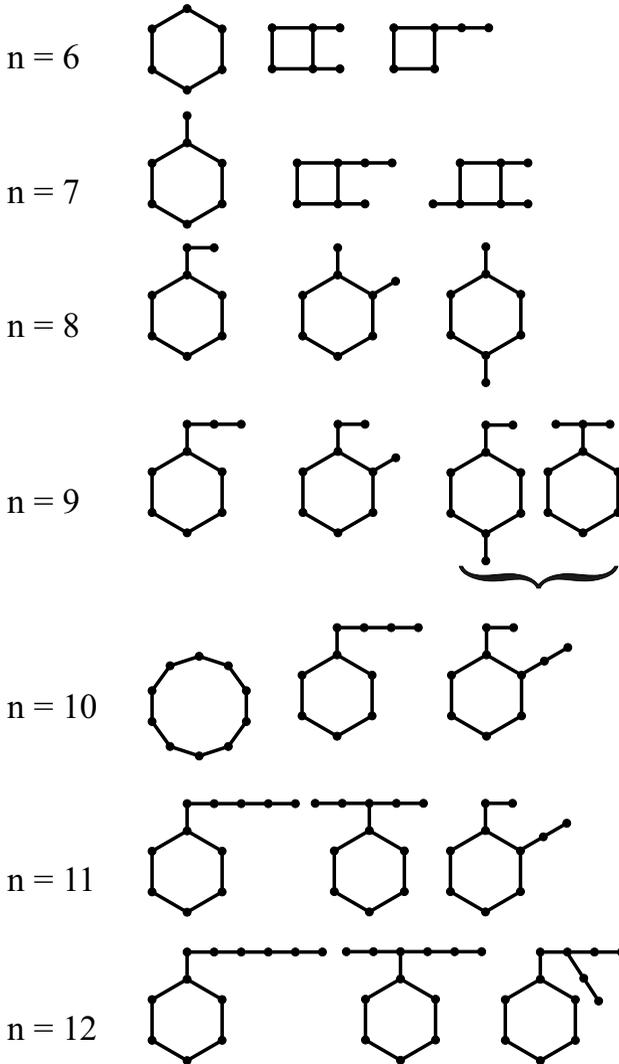


Fig. 2. Bipartite unicyclic graphs on n vertices, $n = 6, 7, \dots, 12$, with maximal, second-maximal, and third-maximal energies (from left to right). Note that in the case $n = 9$ there are two graphs with third-maximal energy; these graphs are cospectral and, consequently, equienergetic.

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
30	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.

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