Iranian J. Math. Chem. 8 (4) December (2017) 339 − 343

Iranian Journal of Mathematical Chemistry

Journal homepage: www.ijmc.kashanu.ac.ir

Borderenergetic Graphs of Order 12

Boris Furtula• **and Ivan Gutman**

Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia

ARTICLE INFO

Article History:

Received 23 May 2017
Accepted 6 June 2017
Published online 22 July 2017
Academic Editor: Tomislav Došlić

Keywords:

Graph energy
Borderenergetic graph
Spectrum (of graph)

ABSTRACT

A graph G of order n is said to be borderenergetic if its energy is equal to $2n - 2$ and if G differs from the complete graph K_n. The first such graph was discovered in 2001, but their systematic study started only in 2015. Until now, the number of borderenergetic graphs of order n was determined for $n \leq 11$. We now establish that there exist exactly 572 connected borderenergetic graphs of order 12.

1. Introduction

Let G be a simple graph of order n, possessing m edges. Let the eigenvalues of G (i.e., the eigenvalues of the adjacency matrix of G) be $\lambda_1, \lambda_2, \ldots, \lambda_n$ [1] The energy of the graph G is defined as

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

This graph-spectrum-based invariant has been extensively studied. Details of its mathematical theory can be found in the book [2] whereas details of its chemical applications in [3].

The upper bound

$$E \leq \sqrt{2mn}$$

•Corresponding author (Email: furtula@kg.ac.rs)
DOI: 10.22052/ijmc.2017.87093.1290

was established by McClelland in the early 1970s [4]. In the same paper [4], an approximate formula was proposed:

$$E \approx a\sqrt{2mn} \ , \ a \approx 0.9 \tag{1}$$

which was eventually demonstrated to be highly accurate in the case of molecular graphs [5,6]. An additional corroboration of this formula was the analogous lower bound

$$E \geq \sqrt{\frac{16}{27}}\sqrt{2mn}$$

that holds for certain molecular graphs, in particular, for benzenoid systems [7].

According to formula (1), the energy of a graph would be a monotonically increasing function of the number m of edges. If this formula could be applied to all graphs, then among graphs with a fixed number n of vertices, the complete graph K_n would have the greatest energy, equal to $E(K_n) = 2n-2$. Counterexamples for this naive conjecture were soon discovered [8]. Somewhat later [9], the first systematic construction of graphs with the property $E(G) > E(K_n)$ were reported.

Graphs of order n with the property $E(G) > 2n-2$ were named *hyperenergetic* [10]. Numerous classes of hyperenergetic graphs have been recognized; for details see the survey [11]. The search for hyperenergetic graphs became purposeless after Nikiforov proved in 2007 [12] that for almost all n-vertex graphs

$$E = \left(\frac{4}{3\pi} + o(n)\right) n^{3/2}$$

implying that almost all graphs are hyperenergetic.

The question that remained open was if there exist graphs of order n, other than K_n, satisfying the equality

$$E(G) = 2n-2 \, .$$

In 2015, such graphs were named *borderenergetic* [13]. It is understood that the complete graph is not borderenergetic.

The first borderenergetic graph was discovered by Yaoping Hou and one of the present authors already in 2001 [14], but in that time it did not attract much attention. The first systematic research of borderenergetic graphs is reported in the paper [13], which was then continued in [15-19]. By means of computer-aided checking, the following was established.

Theorem 1.

1. There are no borderenergetic graphs of order $n \leq 6$ [13].
2. There exists a unique borderenergetic graph of order 7 [13].
3. For any $n \geq 7$, there exist borderenergetic graphs of order n [13].
4. There are exactly 6 borderenergetic graphs of order 8 [13].

5. There are exactly 17 borderenergetic graphs of order 9 [13].
6. There are exactly 49 borderenergetic graphs of order 10 [15,18].
7. There are exactly 158 borderenergetic graphs of order 11 [18], of which 157 are connected.

We now can extend Theorem 1 by establishing:

Theorem 2. There are exactly 572 connected borderenergetic graphs of order 12.

2. NUMERICAL WORK

Determining computationally the borderenergetic graphs of order 12 is not an easy task to be done. This could be illustrated by the fact that the total number of such graphs is 164059830476. In order to reduce the number of investigated graphs, the fact that the size of the borderenergetic species must be greater than $2n-3$ is incorporated. Such intervention decreased the total number of 12-vertex connected graphs by 343198848.

The *geng* tool from the *nauty* package was employed for the generation of the dataset containing 163716631628 graphs stored in 100000 files [20]. The total size of these files is more than 2 TB. All these files are moved to the cluster having 4 nodes with 32 CPUs per node. A Python program was developed for filtering borderenergetic graphs. Using PySpark for processing large datasets, the jobs were distributed over cluster using in total 80 CPUs simultaneously. The computations took about a month or so and finally, we obtained the result that there were exactly 572 connected twelve-vertex borderenergetic graphs.

Table 1 shows the distribution of 12-vertex borderenergetic graphs by the number of edges. Their size varies from 25 to 58. It should be noted that there are no 12-vertex borderenergetic graphs with 49, 53, and 59-65 edges.

3. CONCLUSION

In this note, we reported the preliminary results on searching for and studying of connected borderenergetic graphs with twelve vertices. There are 572 such species, and these provide a class of equienergetic graphs suitable for examining the structural factors on which graph energy does depend or does not depend. In addition, the distribution of these graphs with regard to the number of edges is presented in Table 1, indicating that equienergetic graphs may significantly differ in their edge counts.

Table 1. The distribution of twelve-vertex borderenergetic graphs by the number of edges.

Number of Edges	Number of Graphs
25	2
26	5
27	1
28	8
29	7
30	42
31	20
32	62
33	58
34	50
35	44
36	43
37	37
38	27
39	25
40	24
41	20
42	26
43	12
44	14
45	14
46	7
47	4
48	7
50	2
51	1
52	4
54	1
55	2
56	1
57	1
58	1

REFERENCES

1. D. Cvetković, P. Rowlinson, S. Simić, *An Introduction to the Theory of Graph Spectra*, Cambridge Univ. Press, Cambridge, 2010.
2. X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.
3. I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.

4. B. J. McClelland, Properties of the latent roots of a matrix: The estimation of π-electron energies, *J. Chem. Phys.* **54** (1971) 640−643.
5. I. Gutman, Total π-electron energy of benzenoid hydrocarbons, *Topics Curr. Chem.* **162** (1992) 29−63.
6. I. Gutman, T. Soldatović, (*n*,*m*)-Type approximations for total π-electron energy of benzenoid hydrocarbons, *MATCH Commun. Math. Comput. Chem*. **44** (2001) 169−182.
7. I. Gutman, McClelland-type lower bound for total π-electron energy, *J. Chem. Soc. Faraday Trans.* **86** (1990) 3373−3375.
8. D. Cvetković, I. Gutman, The computer system GRAPH: A useful tool in chemical graph theory, *J. Comput. Chem*. **7** (1986) 640−644.
9. H. B. Walikar, H. S. Ramane, P. R. Hampiholi, On the energy of a graph, in: R. Balakrishnan, H. M. Mulder, A. Vijayakumar (Eds.), *Graph Connections*, Allied Publishers, New Delhi, 1999, pp. 120−123.
10. I. Gutman, Hyperenergetic molecular graphs, *J. Serb. Chem. Soc*. **64** (1999) 199−205.
11. I. Gutman, Hyperenergetic and hypoenergetic graphs, in: D. Cvetković, I. Gutman (Eds.), *Selected Topics on Applications of Graph Spectra*, Math. Inst., Belgrade, 2011, pp. 113−135.
12. V. Nikiforov, Graphs and matrices with maximal energy, *J. Math. Anal. Appl*. **327** (2007) 735−738.
13. S. Gong, X. Li, G. Xu, I. Gutman, B. Furtula, Borderenergetic graphs, *MATCH Commun. Math. Comput. Chem.***74** (2015) 321−332.
14. Y. Hou, I. Gutman, Hyperenergetic line graphs, *MATCH Commun. Math. Comput. Chem*. **43** (2001) 29−39.
15. X. Li, M. Wei, S. Gong, A computer search for the borderenergetic graphs of order 10, *MATCH Commun. Math. Comput. Chem*. **74** (2015) 333−342.
16. B. Deng, X. Li, I. Gutman, More on borderenergetic graphs, *Lin. Algebra Appl.* **497** (2016) 199−208.
17. Y. Hou, Q. Tao, Borderenergetic threshold graphs, *MATCH Commun. Math. Comput. Chem.* **75** (2016) 253−262.
18. Z. Shao, F. Deng, Correcting the number of borderenergetic graphs of order 10, *MATCH Commun. Math. Comput. Chem*. **75** (2016) 263−265.
19. X. Li, M. Wei, X. Zhu, Borderenergetic graphs with small maximum or large minimum degrees, *MATCH Commun. Math. Comput. Chem*. **77** (2017) 25−36.
20. B. D. McKay, A. Piperno, Practical graph isomorphism II, *J. Symb. Comput.* **60** (2013) 94−112.