

ON EQUIENERGETIC GRAPHS AND MOLECULAR GRAPHS

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(Received March 4, 2007)

ABSTRACT. The energy $E(G)$ of a graph G is the sum of absolute values of the eigenvalues of G . Two graphs G_1 and G_2 are equienergetic if $E(G_1) = E(G_2)$. Since 2004, when the concept of equienergetic graphs was introduced, a large number of results on this matter has been obtained. In this paper we briefly outline these results, and give emphasis on the following. If $L(G) = L^1(G)$ is the line graph of a graph G , then the iterated line graphs of G are defined as $L^k(G) = L(L^{k-1}(G))$ for $k = 2, 3, \dots$. Let \overline{G} denote the complement of the graph G . If G is a regular graph on n vertices, of degree $r \geq 3$, then $E(L^k(G))$ and $E(\overline{L^k(G)})$, $k \geq 2$, depend only on the parameters n and r . This result enables construction of pairs of non-cospectral, equienergetic graphs of same order and of same size.

INTRODUCTION

Let G be a graph of order n . The eigenvalues of the adjacency matrix of G , denoted by $\lambda_1, \lambda_2, \dots, \lambda_n$, are said to be the eigenvalues of G , and they form the spectrum of G . Two nonisomorphic graphs of same order are said to be cospectral if their spectra coincide [1]. The energy of a graph G is defined as

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

This graph–energy–concept was introduced by one of the present authors in 1978 [2], motivated by chemical applications [3–5]. Studies of graph energy are currently very active in both mathematical and chemical literature (see [6–9], the references quoted therein, as well as the references quoted below).

Two graphs G_1 and G_2 are said to be *equienergetic* if $E(G_1) = E(G_2)$. Equienergetic graphs were first time considered in 2004, independently in [10] and [11].

Evidently, if two graphs are cospectral, they are also equienergetic. Therefore, we are always interested in non-cospectral equienergetic graphs.

Constructing non-cospectral equienergetic graphs is extremely simple. If G is any graph with spectrum $\lambda_1, \lambda_2, \dots, \lambda_n$, and G' is the graph obtained by adding to G an isolated vertex, then the spectrum of G' consists of the numbers $\lambda_1, \lambda_2, \dots, \lambda_n, \lambda_{n+1} = 0$. Thus G and G' are not cospectral, but $E(G) = E(G')$.

Also if we additionally require that isolated vertices are not present, equienergetic graphs are easily found. A triple of mutually non-cospectral and mutually equienergetic graphs with not more than 4 vertices is depicted in Fig. 1.

The example shown in Fig. 1 hints towards two further restrictions, namely that the graphs should have equal number of vertices, and be connected. However, pairs of non-cospectral connected graph with equal number of vertices are also not difficult to find. The smallest such pair is shown in Fig. 2.

The graphs in Fig. 2 have different size (different number of edges). Therefore, the next requirement aimed at reducing the triviality of the problem should be that the graphs we are looking for be of equal size. The finding of such graphs is somewhat less easy.

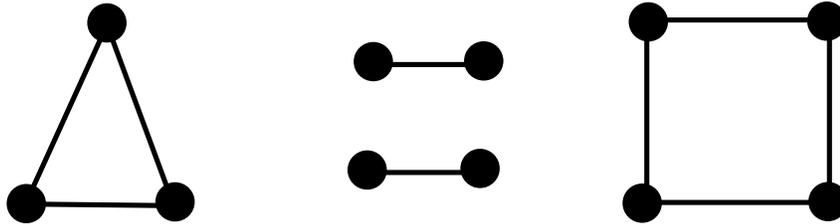


Figure 1. Three graphs with small number of vertices. Their spectra are $\{2, -1, -1\}$, $\{1, 1, -1, -1\}$, and $\{2, 0, 0, -2\}$, respectively. Hence these graphs are mutually non-cospectral and all have energy equal to 4.

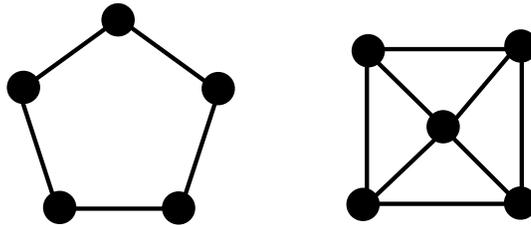


Figure 2. Two connected 5-vertex graphs with different spectra, but equal energy.

From now on we are interested in graphs that are

- non-cospectral
- connected
- with equal number of vertices
- with equal number of edges, and
- equienergetic.

EQUIENERGETIC TREES

Brankov et al. [10] performed a systematic computer-aided search for non-cospectral equienergetic trees. First, by means of numerical calculation, pairs of trees were identified whose spectra differ, but whose E -values coincide on the first few decimal places. This, of course, is not sufficient to establish equienergeticity. In order to complete the proof a detailed examination is needed.

For instance, let T_1 and T_2 be the first two trees, depicted in Fig. 3. By known methods [1,4,5] their characteristic polynomials are computed and found to be of the form:

$$\phi(T_1, \lambda) = \lambda(\lambda^2 - 1)(\lambda^2 - 4)(\lambda^4 - 3\lambda^2 + 1)$$

$$\phi(T_2, \lambda) = \lambda(\lambda^2 - 1)^3(\lambda^2 - 5).$$

The spectra of T_1 and T_2 are now readily obtained:

$$0, 1, 1, 2, -2, \sqrt{\frac{3+\sqrt{5}}{2}}, \sqrt{\frac{3-\sqrt{5}}{2}}, -\sqrt{\frac{3-\sqrt{5}}{2}}, -\sqrt{\frac{3+\sqrt{5}}{2}}$$

and

$$0, 1, 1, 1, -1, -1, -1, \sqrt{5}, -\sqrt{5}$$

respectively. Showing that in both cases the sum of the absolute values of these eigenvalues is equal to $6 + 2\sqrt{5}$ is now an easy exercise from algebra.

The 9-vertex trees T_1 and T_2 happen to be the smallest pair of equienergetic trees. For greater values of n many other equienergetic pairs, triplets, etc. were discovered. Those that are molecular graphs are displayed in Fig. 3. Verifying that these trees are indeed equienergetic (by a procedure explained above on the example of T_1 and T_2) is outstandingly tedious; for $n > 18$ such a verification probably becomes completely infeasible.

It should be noted that until now no systematic method is known for constructing (arbitrarily many) pairs of equienergetic trees.

EQUIENERGETIC GRAPH PRODUCTS

Balakrishnan [11] observed that for any two graphs G_1 and G_2 ,

$$E(G_1 \otimes G_2) = E(G_1) E(G_2) \tag{2}$$

where \otimes denotes the strong product (see [12]). Eventually, the same result was reported also in [13]. The formula (2) is obtained directly from (1) by bearing in mind that the eigenvalues of $G_1 \otimes G_2$ are just the products of the eigenvalues of G_1 and G_2 [1].

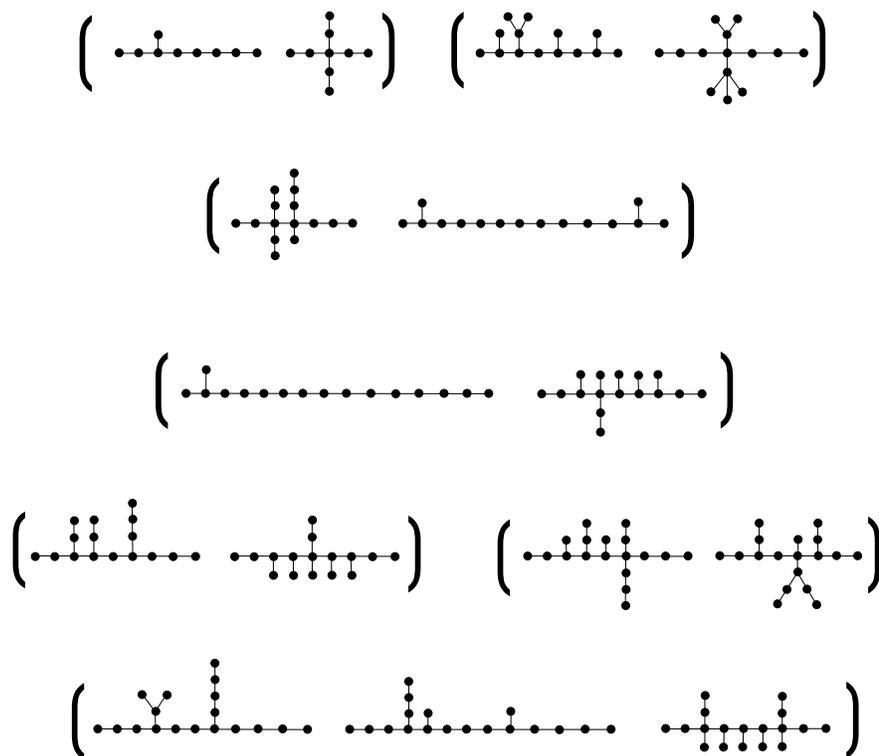


Figure 3. All equienergetic pairs and one triplet of non-cospectral chemical trees with 18 and fewer vertices [10]. The second and third tree in the 18-vertex triplet are cospectral, but have a different spectrum than the first tree.

By means of Eq. (2) one can construct infinitely many pairs of equienergetic graphs. Indeed, if G_a, G_b is such a pair, then for any graph G , also the pair $G_a \otimes G, G_b \otimes G$ is equienergetic.

Another result of this kind was obtained by Indulal and Vijayakumar [14]:

Let $G_1 \odot G_2$ denote the Cartesian product of the graphs G_1 and G_2 (see [12]). Let ℓ and k be positive integers, such that $\ell \geq 2k$. Let K_ℓ be the complete graph on ℓ vertices. Let G be an n -vertex graph whose spectrum lies in the interval $[-k, +k]$. Then

$$E\left((K_\ell)^k \odot G\right) = 2nk(\ell - 1)^k. \quad (3)$$

Because the right-hand side of Eq. (3) depends only on the parameters n, k, ℓ , for any equienergetic G_a, G_b , and for any k, ℓ , satisfying the above stated requirements, also the pairs $(K_\ell)^k \odot G_a, (K_\ell)^k \odot G_b$ are equienergetic.

Two of the present authors [15] proved that

$$E(G_1 \nabla G_2) = E(G_1) + E(G_2) + \sqrt{(r_1 + r_2)^2 + 4(n_1 n_2 - r_1 r_2)} - (r_1 + r_2) \quad (4)$$

where $G_1 \nabla G_2$ denotes the complete product of the graphs G_1 and G_2 (see [12]). Formula (4) holds if for $i = 1, 2$, the graph G_i is regular of degree r_i and has n_i vertices. A special case of this result (for $r_2 = 0$) was recently independently obtained by Liu and Liu [16].

By means of Eq. (4) one can construct (in the above described manner) pairs of n -vertex equienergetic graphs for all $n \geq 9$.

EQUIENERGETIC LINE GRAPHS

In this section we outline in a systematic and somewhat simplified manner our own results, first communicated in [17–21].

Let, as usual, $L(G)$ denote the line graph of the graph G . For $k = 1, 2, \dots$, the k -th iterated line graph of G is defined as $L^k(G) = L(L^{k-1}(G))$, where $L^0(G) = G$ and $L^1(G) = L(G)$.

The line graph of a regular graph G of order n_0 and of degree r_0 is a regular graph of order $n_1 = (n_0 r_0)/2$ and of degree $r_1 = 2r_0 - 2$. Consequently, the order and degree of $L^k(G)$ are [22,23]:

$$n_k = \frac{1}{2} r_{k-1} n_{k-1} \quad \text{and} \quad r_k = 2r_{k-1} - 2$$

where n_i and r_i stand for the order and degree of $L^i(G)$, $i = 0, 1, 2, \dots$. Therefore,

$$r_k = 2^k r_0 - 2^{k+1} + 2 \quad (5)$$

$$n_k = \frac{n_0}{2^k} \prod_{i=0}^{k-1} r_i = \frac{n_0}{2^k} \prod_{i=0}^{k-1} (2^i r_0 - 2^{i+1} + 2) . \quad (6)$$

If $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of a regular graph G of order n and of degree r , then the eigenvalues of $L(G)$ are

$$\left. \begin{array}{ll} \lambda_i + r - 2 & i = 1, 2, \dots, n \\ -2 & n(r - 2)/2 \text{ times} \end{array} \right\} \text{ and } \quad (7)$$

Formula (7) was first reported by Sachs [24]. In view of the fact that $L(G)$ is also a regular graph of order $nr/2$ and of degree $2r - 2$, from (7) the eigenvalues of $L^2(G)$ are easily calculated as:

$$\left. \begin{array}{lll} \lambda_i + 3r - 6 & i = 1, 2, \dots, n & \text{and} \\ 2r - 6 & n(r - 2)/2 \text{ times} & \text{and} \\ -2 & nr(r - 2)/2 \text{ times} & \end{array} \right\} . \quad (8)$$

If G is a regular graph of order n and of degree r , and if $\lambda_1 = r, \lambda_2, \dots, \lambda_n$ are its eigenvalues, then the eigenvalues of \overline{G} , the complement of G , are

$$\left. \begin{array}{lll} -\lambda_i - 1 & i = 2, 3, \dots, n & \text{and} \\ n - r - 1 & & \end{array} \right\} . \quad (9)$$

Formula (9) was also obtained by Sachs [25].

Now, if G is regular of order n and of degree r , then $L^2(G)$ is a regular graph of order $nr(r - 1)/2$ and of degree $4r - 6$. Therefore, from (8) and (9) we get the eigenvalues of $\overline{L^2(G)}$ as follows:

$$\left. \begin{array}{lll} -\lambda_i - 3r + 5 & i = 2, 3, \dots, n & \text{and} \\ -2r + 5 & n(r - 2)/2 \text{ times} & \text{and} \\ 1 & nr(r - 2)/2 \text{ times} & \text{and} \\ nr(r - 1)/2 - 4r + 5 & & \end{array} \right\} . \quad (10)$$

Theorem 1. *If G is a regular graph of order n and of degree $r \geq 3$, then among the positive eigenvalues of $\overline{L^2(G)}$ one is equal to the degree of $\overline{L^2(G)}$, whereas all other are equal to 1.*

Proof. All eigenvalues of a regular graph of degree r satisfy the condition $-r \leq \lambda_i \leq r$, $i = 1, 2, \dots, n$ [1]. Therefore if $r \geq 3$, then $-\lambda_i - 3r + 5 < 0$ and $-2r + 5 < 0$. Theorem 1 follows from (10).

Corollary 1.1. *If G is a regular graph of degree $r \geq 3$, then for $k \geq 2$, among the positive eigenvalues of $\overline{L^k(G)}$, one is equal to the degree of $\overline{L^k(G)}$, whereas all other are equal to 1.*

Theorem 2. *If G is a regular graph of order n and of degree $r \geq 3$, then*

$$E(\overline{L^2(G)}) = (nr - 4)(2r - 3) - 2 . \quad (11)$$

Proof. It is easy to see that $E(G) = 2 \sum_{+} \lambda_i$, where \sum_{+} indicates summation over positive eigenvalues. Then from Theorem 1 and (10),

$$\begin{aligned} E(\overline{L^2(G)}) &= 2 \left[\left(\frac{nr(r-1)}{2} - 4r + 5 \right) + \frac{nr(r-2)}{2} \times 1 \right] \\ &= 2nr^2 - 3nr - 8r + 10 \end{aligned}$$

which straightforwardly leads to Eq. (11).

Corollary 2.1. *Let G be a regular graph of order n_0 and of degree $r_0 \geq 3$. Let n_k and r_k be the order and degree, respectively, of the k -th iterated line graph $L^k(G)$, $k \geq 2$. Then*

$$\begin{aligned} E(\overline{L^k(G)}) &= (n_{k-2} r_{k-2} - 4)(2r_{k-2} - 3) - 2 \\ &= (2n_{k-1} - 4)(r_{k-1} - 1) - 2. \end{aligned}$$

Corollary 2.2. *If G is a regular graph of order n_0 and of degree $r_0 \geq 3$, then in the notation specified in Corollary 2.1, for any $k \geq 2$,*

$$E(\overline{L^k(G)}) = \frac{4n_k r_k}{2 + r_k} - 2(r_k + 1).$$

Corollary 2.3. *If G is a regular graph of order n_0 and of degree $r_0 \geq 3$, then in the notation specified in Corollary 2.1, for any $k \geq 2$,*

$$E(\overline{L^k(G)}) = \left[\frac{n_0}{2^{k-2}} \prod_{i=0}^{k-2} (2^i r_0 - 2^{i+1} + 2) - 4 \right] (2^{k-1} r_0 - 2^k + 1) - 2.$$

From Corollary 2.3 we see that the energy of the complement of any second and higher iterated line graph of a regular graph G of degree greater than two, is fully determined by the order n_0 and degree r_0 of G .

Lemma 3. *Let G_1 and G_2 be two regular graphs of the same order and of the same degree. Then for any $k \geq 1$, the following holds: (a) $L^k(G_1)$ and $L^k(G_2)$ are of the same order and of the same size. (b) $L^k(G_1)$ and $L^k(G_2)$ are cospectral if and only if G_1 and G_2 are cospectral.*

Proof. Statement (a) follows from Eqs. (5) and (6), and the fact that the number of edges of $L^k(G)$ is equal to the number of vertices of $L^{k+1}(G)$. Statement (b) follows from (7), applied a sufficient number of times.

Combining Lemma 3 with Corollary 2.2 we arrive at:

Theorem 4. *Let G_1 and G_2 be two non-cospectral regular graphs of the same order and of the same degree $r \geq 3$. Then for any $k \geq 2$ the iterated line graphs $L^k(G_1)$ and $L^k(G_2)$ form a pair of non-cospectral equienergetic graphs of equal order and of equal size. If, in addition, G_1 and G_2 are chosen to be connected, then also $L^k(G_1)$ and $L^k(G_2)$ are connected.*

It is now easy to generate large families of equienergetic graphs, satisfying the requirements given in Theorem 4. For instance, there are 2, 5, 19, and 85 connected regular graphs of degree 3 of order 6, 8, 10, and 12, respectively. No two of these are cospectral (see [1], pp. 268–269). Their second and higher iterated line graphs form families consisting of 2, 5, 19, 85, \dots , equienergetic graphs.

MISCELLANEOUS EQUIENERGETIC GRAPHS

In the mathematical and mathematico–chemical literature a number of other constructions of equienergetic graphs has been reported [26–30].

In [26] pairs of equienergetic graphs were constructed for $n = 6, 14, 18$ and $n \geq 20$. As already mentioned, in the meantime a stronger result was obtained, covering all $n \geq 9$ [15]. In [27] Xu and Hou reported a method for obtaining infinitely many pairs of bipartite equienergetic graphs. In [28] López and Rada extended the definition of graph energy to digraphs and constructed equienergetic digraphs. In [30] graphs having equal Laplacian energies [31,32] are designed.

CONCLUDING REMARKS AND OPEN PROBLEMS

Based on the numerous results obtained so far, the problem of equienergetic graphs can be considered as basically solved. It is known that such graphs are relatively easy

to find. Several general methods for constructing infinitely many pairs or multiples of such graphs are elaborated. The equienergetic graphs thus obtained satisfy all additional conditions specified in the introduction.

What is not known?

We already mentioned that it is not known how to construct equienergetic trees. The same applies to other classes of (connected) graphs with relatively small number of edges, such as unicyclic, bicyclic,

The graph energy concept has its origin in theoretical chemistry [3–5,8,9] and therefore it is not without interest to find equienergetic molecular graphs. Except the chemical trees from [10], and a few trivially simple examples, no pairs of equienergetic molecular graphs are known. It would be of particular value to find a method for a systematic construction of equienergetic molecular graphs, preferably infinitely many of them. To recall [4,5], pairs of graphs that would be of chemical interest need to be

- non-cospectral
- connected
- with equal number of vertices
- with equal number of edges
- without vertices of degree greater than four, and
- equienergetic.

Acknowledgement. The authors H.B.W. and S.B.H. are thankful to the Department of Science and Technology, Ministry of Science and Technology, Govt. of India, for support through Grant no. DST/MS/1175/02. This work was also supported by the Serbian Ministry of Science and Environmental Protection, through Grant no. 144015G.

REFERENCES

- [1] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, Academic Press, New York, 1980; 2nd revised ed.: Barth, Heidelberg, 1995.
- [2] I. Gutman, *The energy of a graph*, Ber. Math. Statist. Sect. Forschungsz. Graz **103** (1978) 1–22.
- [3] A. Graovac, I. Gutman, N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer–Verlag, Berlin, 1977.

- [4] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, 1986.
- [5] I. Gutman, *Uvod u hemijsku teoriju grafova (Introduction to Chemical Graph Theory)*, PMF Kragujevac, Kragujevac, 2003.
- [6] 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.
- [7] I. Gutman, *Chemical graph theory – The mathematical connection*, in: J. R. Sabin, E. J. Brändas (Eds.), *Advances in Quantum Chemistry 51*, Elsevier, Amsterdam, 2006, pp. 125–138.
- [8] I. Gutman, *Topology and stability of conjugated hydrocarbons. The dependence of total π -electron energy on molecular topology*, J. Serb. Chem. Soc. **70** (2005) 441–456.
- [9] M. Perić, I. Gutman, J. Radić-Perić, *The Hückel total π -electron energy puzzle*, J. Serb. Chem. Soc. **71** (2006) 771–783.
- [10] V. Brankov, D. Stevanović, I. Gutman, *Equienergetic chemical trees*, J. Serb. Chem. Soc. **69** (2004) 549–553.
- [11] R. Balakrishnan, *The energy of a graph*, Lin. Algebra Appl. **387** (2004) 287–295.
- [12] W. Imrich, S. Klavžar, *Product Graphs – Structure and Recognition*, Wiley, New York, 2000.
- [13] D. Stevanović, *Energy and NEPS of graphs*, Lin. Multilin. Algebra **53** (2005) 67–74.
- [14] G. Indulal, A. Vijayakumar, *Energies of some non-regular graphs*, J. Math. Chem., in press.
- [15] H. S. Ramane, H. B. Walikar, *Construction of equienergetic graphs*, MATCH Commun. Math. Comput. Chem. **57** (2007) 203–210.
- [16] J. Liu, B. Liu, *On a pair of equienergetic graphs*, MATCH Commun. Math. Comput. Chem., in press.
- [17] H. S. Ramane, H. B. Walikar, S. B. Rao, B. D. Acharya, P. R. Hampiholi, S. R. Jog, I. Gutman, *Equienergetic graphs*, Kragujevac J. Math. **26** (2004) 5–13.

- [18] H. S. Ramane, I. Gutman, H. B. Walikar, S. B. Halkarni, *Another class of equienergetic graphs*, Kragujevac J. Math. **26** (2004) 15–18.
- [19] H. S. Ramane, H. B. Walikar, S. B. Rao, B. D. Acharya, P. R. Hampiholi, S. R. Jog, I. Gutman, *Spectra and energies of iterated line graphs of regular graphs*, Appl. Math. Lett. **18** (2005) 679–682.
- [20] H. S. Ramane, I. Gutman, H. B. Walikar, S. B. Halkarni, *Equienergetic complement graphs*, Kragujevac J. Sci. **27** (2005) 67–74.
- [21] H. S. Ramane, H. B. Walikar, S. B. Halkarni, *Generation of equienergetic graphs*, presented at the International Conference on Discrete Mathematics, Bangalore, 2006.
- [22] F. Buckley, *Iterated line graphs*, Congr. Numer. **33** (1981) 390–394.
- [23] F. Buckley, *The size of iterated line graphs*, Graph Theory Notes New York **25** (1993) 33–36.
- [24] H. Sachs, *Über Teiler, Faktoren und charakteristische Polynome von Graphen. Teil II*, Wiss. Z. TH Ilmenau **13** (1967) 405–412.
- [25] H. Sachs, *Über selbtkomplementäre Graphen*, Publ. Math. Debrecen **9** (1962) 270–288.
- [26] G. Indulal, A. Vijayakumar, *On a pair of equienergetic graphs*, MATCH Commun. Math. Comput. Chem. **55** (2006) 83–90.
- [27] L. Xu, Y. Hou, *Equienergetic bipartite graphs*, MATCH Commun. Math. Comput. Chem. **57** (2007) 363–370.
- [28] W. López, J. Rada, *Equienergetic digraphs*, Int. J. Pure Appl. Math., in press.
- [29] A. S. Bonifácio, C. T. M. Vinagre, N. M. M. de Abreu, *Constructing pairs of equienergetic and non-cospectral graphs*, Appl. Math. Lett., in press.
- [30] A. S. Bonifácio, C. T. M. Vinagre, N. M. M. de Abreu, *Graphs of the same order and same Laplacian energy (Laplacian equienergetic graphs)*, preprint.
- [31] I. Gutman, B. Zhou, *Laplacian energy of a graph*, Lin. Algebra Appl. **414** (2006) 29–37.
- [32] B. Zhou, I. Gutman, *On Laplacian energy of graphs*, MATCH Commun. Math. Comput. Chem. **57** (2007) 211–220.