

RELATIONS BETWEEN KIRCHHOFF INDEX AND
LAPLACIAN-ENERGY-LIKE INVARIANT

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A b s t r a c t. The Kirchhoff index Kf and the Laplacian-energy-like invariant LEL are two graph invariants defined in terms of the Laplacian eigenvalues. If $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} > \mu_n = 0$ are the Laplacian eigenvalues of a connected n -vertex graph, then $Kf = n \sum_{i=1}^{n-1} 1/\mu_i$ and $LEL = \sum_{i=1}^{n-1} \sqrt{\mu_i}$. We examine the conditions under which $Kf > LEL$. Among other results we show that $Kf > LEL$ holds for all trees, unicyclic, bicyclic, tricyclic, and tetracyclic connected graphs, except for a finite number of graphs. These exceptional graphs are determined.

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Key Words: Laplacian spectrum (of graph), Laplacian eigenvalue, Kirchhoff index, Laplacian-energy-like invariant, LEL

1. Introduction

In this paper we are concerned with simple graph, that is a graph possessing no directed, weighted, or multiple edges, and no self-loops. In addition, we assume that the graphs considered are connected. Let G be

such a graph and let n and m be the number of its vertices and edges, respectively. Let $\mu_1, \mu_2, \dots, \mu_n$ be the Laplacian eigenvalues of G , forming its Laplacian spectrum. For details of Laplacian spectral graph theory see [2, 10, 9]. It is important for us that if the graph G is connected, then $n - 1$ of its Laplacian eigenvalues are real positive numbers, whereas one eigenvalue is equal to zero. In what follows the Laplacian spectrum of the graph G will be denoted by $Spec(G) = \{\mu_1, \mu_2, \dots, \mu_n\}$, assuming that $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} > \mu_n = 0$.

Two graph invariants based on Laplacian eigenvalues have been much studied in last few years. These are the *Kirchhoff index*,

$$Kf = Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i} \quad (0.1)$$

and the *Laplacian-energy-like invariant*,

$$LEL = LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i} . \quad (0.2)$$

Recall that the ordinary distance between two vertices v_i and v_j in a connected graph G is defined as the length (= number of edges) of a shortest path that connects v_i and v_j . Klein and Randić [15] conceived the *resistance distance*, defined in terms of electric resistance in a network corresponding to the considered graph, in which the resistance between any two adjacent nodes is 1 Ohm. The sum of resistance distances between all pairs of vertices of a graph was conceived as a novel graph invariant [15, 1] and – in view of the fact that electric resistances are calculated by means of the Kirchhoff laws – named the “*Kirchhoff index*”. The fact that the Kirchhoff index satisfies the relation (0.1) was independently established in [12] and [23]. Of the numerous investigations on the Kirchhoff index we mention here only a few most recent [4, 6, 8, 20, 21].

Another Laplacian-spectrum-based graph invariant was put conceived by Liu and Liu [17], and defined via Eq. (0.2). Details of the theory of *LEL* and an exhaustive list of references can be found in the recent surveys [11, 16]; for some most recent works on this topic see [22, 13, 14, 19].

2. Relations between **Kf** and **LEL** for graphs with given cyclomatic number

In spite of the intense research done on both *Kf* and *LEL*, the relation between these two closely related Laplacian-spectrum-based graph invari-

ants has not been investigated until quite recently [5]. In [5] the following two results have been established:

Theorem 2.1 *Let G be a connected graph of order n with m edges. If $2m \leq (n-1)n^{2/3}$, then $LEL(G) < Kf(G)$.*

Theorem 2.2 *Let G be a connected graph of order n with m edges. Let δ be the smallest degree of a vertex of G . If $2m \leq (n-2)n^{2/3} + \delta$, then $LEL(G) < Kf(G)$.*

Theorems 2.1 and 2.2 immediately imply:

Corollary 2.3 *Let G be a connected graph of order n . If $Kf(G) < LEL(G)$, then G must have more than $\frac{1}{2}(n-1)n^{2/3}$ edges.*

Corollary 2.4 *Let G be a connected graph of order n . Let δ be the smallest degree of a vertex of G . If $Kf(G) < LEL(G)$, then G must have more than $\frac{1}{2}[(n-2)n^{2/3} + \delta]$ edges.*

In case when the value of δ cannot be specified, we have the following weakened variant of Corollary 2.4:

Corollary 2.5 *Let G be a connected graph of order n . If $Kf(G) < LEL(G)$, then G must have more than $\frac{1}{2}[(n-2)n^{2/3} + 1]$ edges.*

Combining Corollaries 2.3 and 2.5, it is evident that in order that the relation $Kf(G) < LEL(G)$ be obeyed, the graph G must possess more than

$$\frac{1}{2} \min \left\{ (n-1)n^{2/3}, (n-2)n^{2/3} + 1 \right\}$$

edges. It is easy to show that the inequality

$$(n-2)n^{2/3} + 1 < (n-1)n^{2/3}$$

holds for all values of n , $n \geq 3$.

Theorem 2.6 *Let $\mathcal{G}(c)$ be the set of connected graphs with cyclomatic number c . For any fixed value of c , the number of elements of $\mathcal{G}(c)$ for which $Kf < LEL$ holds is finite.*

P r o o f. An n -vertex graph with cyclomatic number c has $n + c - 1$ edges. No matter how large c is, there always will exist some (finite) positive integer $n_0 = n_0(c)$, such that the inequality

$$n + c - 1 < \frac{1}{2} \left[(n - 2) n^{2/3} + 1 \right]$$

be satisfied for all values of $n \geq n_0$. Therefore graphs for which $Kf < LEL$ must possess less than n_0 vertices and, consequently, their number is finite. \square

Remark 2.7 *By direct numerical testing we can verify that n_0 in Theorem 2.6 is equal to 4, 6, 6, 7, 8 for cyclomatic number 0, 1, 2, 3, and 4. This means that for $c = 0, 1, 2, 3, 4$, connected graphs for which the Kirchhoff index is smaller than the Laplacian-energy-like invariant can possess at most 3, 5, 5, 6, and 7 vertices, respectively.*

Remark 2.8 *For the complete graph K_n we have [10, 9] $\text{Spec}(K_n) = \{n, n, \dots, n, 0\}$. Therefore, $Kf(K_n) = n - 1$ and $LEL(K_n) = (n - 1) \sqrt{n}$. Therefore, $Kf(K_n) < LEL(K_n)$ holds for all $n > 1$.*

Corollary 2.9 [5] *The only tree (i. e., a connected graph with $c = 0$) for which $Kf < LEL$ holds is K_2 .*

Corollary 2.10 [5] *The only connected unicyclic graph (i. e., graph with $c = 1$) for which $Kf < LEL$ holds is K_3 .*

P r o o f. In Fig. 1 are depicted all unicyclic graphs with 3, 4, and 5 vertices. Numerical calculation shows that $Kf < LEL$ holds only for the graph H_1 . \square

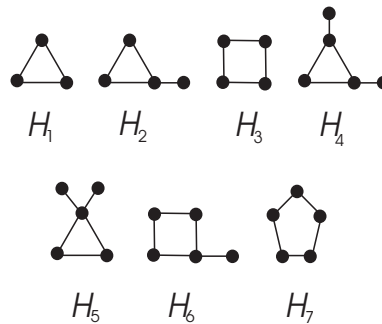


Fig. 1. The connected unicyclic graphs with 3, 4, and 5 vertices.

Corollary 2.11 [5] *The only connected bicyclic graph (i. e., graph with $c = 2$) for which $Kf < LEL$ holds is $K_4 - e$ i. e., the graph H_8 in Fig. 2.*

P r o o f. In Fig. 2 are depicted all bicyclic graphs with 4 and 5 vertices. Numerical calculation shows that $Kf < LEL$ holds only for the graph H_8 .
□

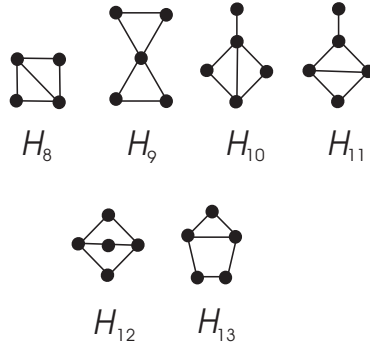


Fig. 2. The connected bicyclic graphs with 4 and 5 vertices.

Corollary 2.12 *The only connected tricyclic graphs (i. e., graphs with $c = 3$) for which $Kf < LEL$ holds are $H_{14} \cong K_4$, H_{16} , H_{17} , and H_{18} , depicted in Fig. 3.*

P r o o f. In Fig. 3 are shown all tricyclic graphs with 4, 5, and 6 vertices. By numerical calculation we obtained the following results:

graph	Kf	LEL	graph	Kf	LEL
H_{14}	3.00	6.00	H_{28}	13.88	8.61
H_{15}	8.50	7.24	H_{29}	13.83	8.61
H_{16}	7.00	7.30	H_{30}	14.52	8.55
H_{17}	6.95	7.33	H_{31}	15.24	8.57
H_{18}	6.42	7.38	H_{32}	14.50	8.63
H_{19}	11.50	8.69	H_{33}	12.70	8.70
H_{20}	14.20	8.51	H_{34}	12.55	8.68
H_{21}	15.20	8.54	H_{35}	11.25	8.75
H_{22}	12.43	8.65	H_{36}	11.34	8.74
H_{23}	11.75	8.70	H_{37}	12.67	8.68
H_{24}	16.50	8.46	H_{38}	12.00	8.72
H_{25}	16.00	8.45	H_{39}	13.50	8.60
H_{26}	19.00	8.51	H_{40}	14.50	8.63
H_{27}	14.14	8.54			

□

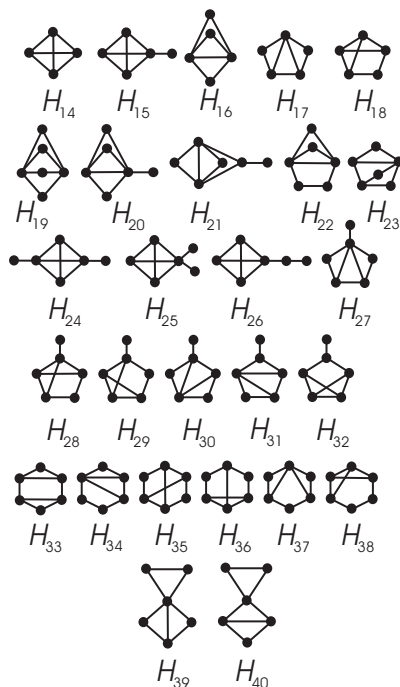


Fig. 3. The connected tricyclic graphs with 4, 5, and 6 vertices.

In a fully analogous manner, by examining all the 154 connected tetracyclic graphs with seven or fewer vertices, we arrive at:

Corollary 2.13 *The only connected tetracyclic graphs (i. e., graphs with $c = 4$) for which $Kf < LEL$ holds are H_{41} , H_{42} , H_{43} , and H_{44} , depicted in Fig. 4.*

Remark 2.14 *There are 2, 20, and 132 connected tetracyclic graphs with 5, 6, and 7 vertices, respectively. Among the 7-vertex species no one satisfies the inequality $Kf < LEL$.*

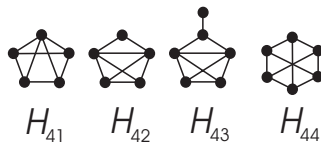


Fig. 4. The only connected tetracyclic graphs for which LEL is greater than the Kirchhoff index.

3. More relations between **Kf** and **LEL**

Theorem 3.15 *Let G be a connected graph and e its edge, such that $G - e$ is also connected. If $Kf(G) > LEL(G)$, then $Kf(G - e) > LEL(G - e)$.*

Proof. Let $Spec(G) = \{\mu_1, \mu_2, \dots, \mu_{n-1}, 0\}$ and $Spec(G - e) = \{\mu'_1, \mu'_2, \dots, \mu'_{n-1}, 0\}$. As well known [10, 9], the Laplacian eigenvalues of $G - e$ interlace the Laplacian eigenvalues of G , i. e.,

$$\mu_1 \geq \mu'_1 \geq \mu_2 \geq \mu'_2 \geq \dots \geq \mu_{n-1} \geq \mu'_{n-1} > \mu_n = \mu'_n = 0 .$$

These inequalities immediately imply

$$\sum_{i=1}^{n-1} \sqrt{\mu_i} \geq \sum_{i=1}^{n-1} \sqrt{\mu'_i} \quad \text{i. e.,} \quad LEL(G) \geq LEL(G - e)$$

and

$$\sum_{i=1}^{n-1} \frac{1}{\mu_i} \leq \sum_{i=1}^{n-1} \frac{1}{\mu'_i} \quad \text{i. e.,} \quad Kf(G) \leq Kf(G - e) .$$

□

Corollary 3.16 *If $Kf(G) > LEL(G)$ and if e_1, e_2, \dots, e_t are edges of G , such that $G - e_1 - e_2 - \dots - e_t$ is connected, then*

$$Kf(G - e_1 - e_2 - \dots - e_t) > LEL(G - e_1 - e_2 - \dots - e_t) .$$

In a fully analogous manner as Theorem 3.15, we can prove also:

Theorem 3.17 *Let $G + e$ be the graph obtained by adding a new edge to the connected graph G . If $Kf(G) < LEL(G)$, then $Kf(G + e) < LEL(G + e)$.*

Corollary 3.18 *If G is a connected graph of order n with cyclomatic number $c \geq 0$, such that $Kf(G) < LEL(G)$, then we can construct a connected graph G^\dagger of order n , with cyclomatic number c^\dagger , $c < c^\dagger \leq (n - 1)(n - 2)/2$, such that $Kf(G^\dagger) < LEL(G^\dagger)$.*

Corollary 3.19 *If $n \geq 4$, then $Kf(K_n - e) < LEL(K_n - e)$ holds.*

Lemma 3.20 [3] *Let G be a connected graph of order n with Laplacian spectrum $Spec(G) = \{\mu_1, \mu_2, \dots, \mu_{n-1}, 0\}$. If G^* is the graph obtained by connecting a new vertex to all vertices of G , then $Spec(G^*) = \{n + 1, \mu_1 + 1, \mu_2 + 1, \dots, \mu_{n-1} + 1, 0\}$.*

The product of G_1 and G_2 is the graph $G_1 \times G_2$ whose vertex set is the Cartesian product $V(G_1) \times V(G_2)$. Suppose $v_1, v_2 \in V(G_1)$ and $u_1, u_2 \in V(G_2)$. Then (v_1, u_1) and (v_2, u_2) are adjacent in $G_1 \times G_2$ if and only if one of the following conditions is satisfied: (i) $v_1 = v_2$ and $\{u_1, u_2\} \in E(G_2)$, or (ii) $\{v_1, v_2\} \in E(G_1)$ and $u_1 = u_2$ [2].

Lemma 3.21 [7, 18] *Let G_1 and G_2 be graphs on n_1 and n_2 vertices, respectively. Then $\text{Spec}(G_1 \times G_2)$ consists of all possible sums $\mu_i(G_1) + \mu_j(G_2)$, $1 \leq i \leq n_1$ and $1 \leq j \leq n_2$.*

Let $H_n = K_p \times K_2$. Then $n = 2p$. In particular, $H_4 = C_4$ for $n = 4$. We have $LEL(C_4) = \sqrt{4} + 2\sqrt{2} < 1 + 2 + 2 = Kf(C_4)$ and $LEL(H_6) = 2\sqrt{5} + 2\sqrt{3} + \sqrt{2} \approx 9.35 < 9.4 = 2.4 + 4 + 3 = Kf(H_6)$. But we have the following:

Theorem 3.22 *Let G be a graph of order $n \geq 8$ (n is even) and let H_n be a subgraph of G . Then $LEL(G) > Kf(G)$.*

P r o o f. We have $n = 2p$. Since $\text{Spec}(K_p) = \{\underbrace{p, p, \dots, p}_{p-1}, 0\}$, from Lemma 3.21 it follows that

$$\text{Spec}(H_n) = \{\underbrace{p+2, p+2, \dots, p+2}_{p-1}, \underbrace{p, p, \dots, p}_{p-1}, 2, 0\}$$

Since H is a subgraph of G , we have $\mu_i(G) \geq \mu_i(H)$, that is,

$$\mu_i(G) \geq p+2 \quad \text{for } i = 1, 2, \dots, p-1;$$

$$\mu_i(G) \geq p \quad \text{for } i = p, p+1, \dots, 2p-2;$$

$$\mu_{2p-1}(G) \geq 2 \quad \text{and} \quad \mu_{2p}(G) = 0.$$

Thus we have

$$\begin{aligned} LEL(G) &= \sum_{i=1}^{n-1} \sqrt{\mu_i(G)} \geq (p-1)\sqrt{p+2} + (p-1)\sqrt{p} + \sqrt{2} \\ &\geq 2(p-1)\sqrt{p} + \sqrt{2} \end{aligned} \quad (3.3)$$

and

$$Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i(G)} \leq (p-1)\frac{2p}{p+2} + (p-1)\frac{2p}{p} + \frac{2p}{2} \leq 5p-4. \quad (3.4)$$

From (3.3) and (3.4),

$$\begin{aligned}
LEL(G) &\geq 3\sqrt{6} + 3\sqrt{4} + \sqrt{2} \approx 14.763 > 14 \\
&= 4 + 6 + 4 \geq Kf(G) \quad \text{for } p = 4 \\
LEL(G) &\geq 4\sqrt{7} + 4\sqrt{5} + \sqrt{2} \approx 20.941 > 18.714 \\
&\approx \frac{40}{7} + 8 + 5 \geq Kf(G) \quad \text{for } p = 5 \\
LEL(G) &\geq 5\sqrt{8} + 5\sqrt{6} + \sqrt{2} \approx 27.804 > 23.5 \\
&= \frac{15}{2} + 10 + 6 \geq Kf(G) \quad \text{for } p = 6 .
\end{aligned}$$

For $p \geq 7$, one can see easily that

$$LEL(G) \geq 2(p-1)\sqrt{p} + \sqrt{2} > 5p - 4 \geq Kf(G) .$$

This completes the proof. \square

Let H'_n be the graph of order n ($n = 2p + 1$) obtained from H_n in such a way that $H'_n = \overline{H_n} \cup K_1$, where $H_n = K_p \times K_2$.

Theorem 3.23 *Let G be a graph of order $n \geq 5$ (n is odd) and let H'_n be a subgraph of G . Then $LEL(G) > Kf(G)$.*

P r o o f. We have $n = 2p + 1$. Since

$$Spec(H_n) = \{\underbrace{p+2, p+2, \dots, p+2}_{p-1}, \underbrace{p, p, \dots, p}_{p-1}, 2, 0\}$$

by Lemma 3.20,

$$Spec(H'_n) = \{n, \underbrace{p+3, p+3, \dots, p+3}_{p-1}, \underbrace{p+1, p+1, \dots, p+1}_{p-1}, 3, 0\} .$$

Since H'_n is a subgraph of G , we have $\mu_i(G) \geq \mu_i(H'_n)$, that is,

$$\begin{aligned}
\mu_1(G) &\geq n \quad ; \quad \mu_i(G) \geq p+3 \quad \text{for } i = 2, 3, \dots, p \quad ; \\
\mu_i(G) &\geq p+1 \quad \text{for } i = p+1, p+2, \dots, 2p-1 \quad ; \\
\mu_{2p}(G) &\geq 3 \quad \text{and} \quad \mu_{2p+1}(G) = 0 .
\end{aligned}$$

Thus we have

$$\begin{aligned} LEL(G) &= \sum_{i=1}^{n-1} \sqrt{\mu_i(G)} \\ &\geq \sqrt{n} + (p-1)\sqrt{p+3} + (p-1)\sqrt{p+1} + \sqrt{3} \\ &> \sqrt{2p+1} + 4.88(p-1) + \sqrt{3} \text{ for } p \geq 4. \end{aligned}$$

and

$$\begin{aligned} Kf(G) &= \sum_{i=1}^{n-1} \frac{n}{\mu_i(G)} \\ &\leq \frac{n}{n} + (p-1)\frac{2p+1}{p+3} + (p-1)\frac{2p+1}{p+1} + \frac{2p+1}{3} \\ &\leq \frac{14}{3}p - \frac{26}{3} + \frac{20}{p+3} + \frac{2}{p+1}. \end{aligned}$$

Now,

$$LEL(G) \geq 2\sqrt{5} + 2\sqrt{3} \approx 7.936 > 5.333 \approx 2 + \frac{10}{3} \geq Kf(G) \quad \text{for } p = 2$$

and

$$\begin{aligned} LEL(G) &\geq \sqrt{7} + 2\sqrt{6} + 4 + \sqrt{3} \approx 13.277 \\ &> 9.166 \approx 1 + \frac{7}{3} + \frac{7}{2} + \frac{7}{3} \geq Kf(G) \quad \text{for } p = 3. \end{aligned}$$

For $p \geq 4$, one can see easily that

$$LEL(G) \geq \sqrt{2p+1} + 4.88(p-1) + \sqrt{3} > \frac{14}{3}p - \frac{26}{3} + \frac{20}{p+3} + \frac{2}{p+1} \geq Kf(G).$$

This completes the proof. \square

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REFERENCES

- [1] D. Bonchev, A. T. Balaban, X. Liu, D. J. Klein, Molecular cyclicity and centrality of polycyclic graphs. I. Cyclicity based on resistance distances or reciprocal distances, *Int. J. Quantum Chem.* **50** (1994) 1–20.
- [2] D. Cvetković, P. Rowlinson, S. Simić, *An Introduction to the Theory of Graph Spectra*, Cambridge Univ. Press, Cambridge, 2010.
- [3] K. C. Das, The Laplacian spectrum of a graph, *Comput. Math. Appl.* **48** (2004) 715–724.
- [4] K. C. Das, A. D. Güngör, A. S. Çevik, On the Kirchhoff index and the resistance–distance energy of a graph, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 541–556.
- [5] K. C. Das, K. Xu, I. Gutman, Comparison between Kirchhoff index and the Laplacian–energy–like invariant, *Lin. Algebra Appl.* **436** (2012) 3661–3671.
- [6] E. Estrada, N. Hatano, Topological atomic displacements, Kirchhoff and Wiener indices of molecules, *Chem. Phys. Lett.* **486** (2010) 166–170.
- [7] M. Fiedler, Algebraic connectivity of graphs, *Czech. Math. J.* **23** (1973) 298–305.
- [8] X. Gao, Y. Luo, W. Liu, Resistance distances and the Kirchhoff index in Cayley graphs, *Discr. Appl. Math.* **159** (2011) 2050–2057.
- [9] R. Grone, R. Merris, The Laplacian spectrum of a graph II, *SIAM J. Discr. Math.* **7** (1994) 221–229.
- [10] R. Grone, R. Merris, V. S. Sunder, The Laplacian spectrum of a graph, *SIAM J. Matrix Anal. Appl.* **11** (1990) 218–238.
- [11] I. Gutman, Comparative studies of graph energies, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.)*, **37** (2012) 1–17. in press.
- [12] I. Gutman, B. Mohar, The quasi-Wiener and the Kirchhoff indices coincide, *J. Chem. Inf. Comput. Sci.* **36** (1996) 982–985.
- [13] I. Gutman, B. Zhou, B. Furtula, The Laplacian–energy like invariant is an energy like invariant, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 85–96.
- [14] A. Ilić, D. Krtinić, M. Ilić, On Laplacian like energy of trees, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 111–122.
- [15] D. J. Klein, M. Randić, Resistance distance, *J. Math. Chem.* **12** (1993) 81–95.
- [16] B. Liu, Y. Huang, Z. You, A survey on the Laplacian–energy–like invariant, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 713–730.
- [17] J. Liu, B. Liu, A Laplacian–energy–like invariant of a graph, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 397–419.
- [18] B. Mohar, The Laplacian spectrum of graphs, in: Y. Alavi, G. Chartrand, O. R. Oellermann, A. J. Schwenk (Eds.), *Graph Theory, Combinatorics, and Applications*, Wiley, New York, 1991, pp. 871–898.
- [19] S. W. Tan, On the Laplacian coefficients and Laplacian–like energy of bicyclic graphs, *Lin. Multilin. Algebra*, in press.

- [20] H. P. Zhang, X. Y. Jiang, Y. J. Yang, Bicyclic graphs with extremal Kirchhoff index, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 697–712.
- [21] H. P. Zhang, Y. J. Yang, C. W. Li, Kirchhoff index of composite graphs, *Discr. Appl. Math.* **107** (2009) 2918–2927.
- [22] B. X. Zhu, The Laplacian–energy like of graphs, *Appl. Math. Lett.* **24** (2011) 1604–1607.
- [23] H. Y. Zhu, D. J. Klein, I. Lukovits, Extensions of the Wiener number, *J. Chem. Inf. Comput. Sci.* **36** (1996) 420–428.

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