On Wiener Index of Common Neighborhood Graphs

Martin Knor,[a] Borut Lužar,[b] Riste Škrekovski,[b] Ivan Gutman[c]

[a]*Department of Mathematics, Faculty of Engineering, Slovak University of Technology in Bratislava, Radlinskeho 11, 81368 Bratislava, Slovakia*
`knor@math.sk`

[b]*Institute of Mathematics, Physics and Mechanics Jadranska 19, 1000 Ljubljana, Slovenia & Faculty of Information Studies, Sevno 13, 8000 Novo mesto, Slovenia*
`borut.luzar@gmail.com`, `skrekovski@gmail.com`

[c]*Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia & Chemistry Department, Faculty of Science, King Abdulaziz University, Jeddah 21589, Saudi Arabia*
`gutman@kg.ac.rs`

Received July ??, 2013

If G is a simple graph, then con(G), the common neighborhood graph of G, has the same vertex set as G, and two vertices of con(G) are adjacent if they have a common neighbor in G. We show that for any bipartite graph G the Wiener index (i.e., sum of distances between all pairs of vertices) of con(G) is always smaller than the Wiener index of G. For general graphs, however, the Wiener index of common neighbor graphs can be greater. This fact is surprising, since we also show that the diameter of con(G) is at most the diameter of G. We present constructions of two infinite classes of graphs, chemical and unicyclic graphs, which have this property.

KEY WORDS: distance (in graph), common neighborhood graph, Wiener index, chemical graph

1 Introduction

Let G be a simple graph with vertex set $V(G)$. The *common neighborhood graph* (or, shorter: *congraph*) of G, denoted by $\mathrm{con}(G)$, is the graph with $V(\mathrm{con}(G)) = V(G)$, in which two vertices are adjacent if they have a common neighbor in G. The motivation for the consideration of congraphs came from the theory of graph energy [2, 11]. In [1, 3] some basic properties of congraphs have been established. Furthermore, common neighbor graphs are implictly used in the graph coloring theory. Namely, an injective coloring of a graph G is precisely a proper vertex coloring of $\mathrm{con}(G)$ (see e.g. [5, 8, 10, 12] for some results on this topic).

One of the obvious questions that can be asked in connection with congraphs is the following: If $Inv(G)$ is a numerical invariant of the graph G, what can be said about $Inv(\mathrm{con}(G))$? In particular, how $Inv(G)$ and $Inv(\mathrm{con}(G))$ are related?

In this paper, we focus our attention to the Wiener index. For reasons outlined in the subsequent section, it looks plausible (or even, "self-evident") state the following:

Conjecture 1. *Let G be a graph. Then*

$$W(\mathrm{con}(G)) \leq W(G)\,.$$

and the equality holds if and only if $\mathrm{con}(G)$ *is isomorphic to G.*

In what follows, we show that this conjecture is false. Moreover, for every integer d we construct infinite families of graphs, such that the relation $W(\mathrm{con}(G)) - W(G) = d$ holds. Furthermore, we also found a construction of an infinite family of chemical graphs for which the common neighborhood graphs have greater value than the original graphs.

At this point we need to slightly re-define the Wiener index.

Let G be a connected graph and $x, y \in V(G)$. The *distance* between the vertices x and y, denoted by $d(x, y|G)$, is defined as the length of (= number of edges in) a shortest path connecting x and y [4]. Then, the *Wiener index* is defined as [6, 7, 9]

$$W = W(G) = \sum_{\{x,y\} \in V(G)} d(x, y|G)\,. \tag{1}$$

For evident reasons, this definition cannot be applied to non-connected graphs.

Let $d(G,k)$ be the number of vertex pairs of the graph G whose distance is equal to k. Then the Wiener index satisfies the relation

$$W = W(G) = \sum_{k \geq 1} k\, d(G,k) \ . \tag{2}$$

However, contrary to formula (1), the right–hand side of formula (2) is applicable also to non-connected graphs. Furthermore, if the Wiener index is defined via Eq. (2), and if the graph G consists of disconnected components G_1 and G_2, then

$$W(G) = W(G_1) + W(G_2) \ .$$

In what follows we understand that the Wiener index of a disconnected graph is calculated according to Eq. (2). When speaking of the Wiener indices of congraphs, this is important, because of the following result:

Theorem 1. [1] *Let G be a connected bipartite graph, so that its vertex set is partitioned as $V(G) = V_a \cup V_b$. Then $\mathrm{con}(G)$ consists of two disconnected components G_a and G_b, whose vertex sets are V_a and V_b, respectively. Both graphs G_a and G_b are connected.*

By means of Eq. (2), we now have:

Corollary 2. *Using the same notation as in Theorem 1,*

$$W(\mathrm{con}(G)) = W(G_a) + W(G_b) \ .$$

2 On Wiener Index of Common Neighborhood Graphs of Bipartite Graphs

Throughout this section we assume that G is a connected bipartite graph, and that the notation used in Theorem 1 is applicable.

Lemma 3. *If $x,y \in V_a$, then $d(x,y|G_a) = 2\, d(x,y|G)$. Analogously, if $x,y \in V_b$, then $d(x,y|G_b) = 2\, d(x,y|G)$.*

Proof. Suppose that $x, y \in V_a$. Let a shortest path between the vertices x and y in the graph G embraces the vertices $x, u_1, v_1, u_2, v_2, \ldots, u_{k-1}, v_{k-1}, u_k, y$ (in that order). Then, evidently, $v_1, v_2, \ldots, v_{k-1} \in V_a$ and $u_1, u_2, \ldots, u_k \in V_b$, and $d(x, y|G) = 2k$.

Now, according the way in which the common neighborhood graphs are constructed, $x, v_1, v_2, \ldots, v_{k-1}, y$ is a shortest path between the vertices x and y in $\mathrm{con}(G)$. Consequently, $d(x, y|\mathrm{con}(G)) = k$. $\square$

Lemma 3 implies the following:

Theorem 4. *Using the same notation as in Theorem 1, the Wiener indices of a bipartite graph and its congraph are related as:*

$$W(G) = 2\,W(\mathrm{con}(G)) + \sum_{x \in V_a\,;\, y \in V_b} d(x, y|G)\ . \tag{3}$$

Proof.

$$\begin{aligned} W(G) &= \left[\sum_{\{x,y\} \in V_a} + \sum_{\{x,y\} \in V_b} + \sum_{x \in V_a\,;\, y \in V_b} \right] d(x, y|G) \\ &= 2 \sum_{\{x,y\} \in V_a} d(x, y|G_a) + 2 \sum_{\{x,y\} \in V_b} d(x, y|G_b) + \sum_{x \in V_a\,;\, y \in V_b} d(x, y|G) \\ &= 2W(G_a) + 2W(G_b) + \sum_{x \in V_a\,;\, y \in V_b} d(x, y|G) \end{aligned}$$

and Eq. (3) follows from Corollary 2. $\square$

Bearing in mind that

$$\sum_{x \in V_a\,;\, y \in V_b} d(x, y|G) \geq |V_a|\,|V_b|$$

we obtain:

Corollary 5. *If G is a connected bipartite graph with bipartition $V(G) = V_a \cup V_b$, then*

$$W(G) \geq 2\,W(\mathrm{con}(G)) + |V_a|\,|V_b|$$

with equality if and only if G is the complete bipartite graph $K_{a,b}$.

Corollary 6. *If G is a bipartite (not necessarily connected) graph with m edges, then*

$$W(G) \geq 2\,W(\mathrm{con}(G)) + m$$

with equality if and only if every component of G is a complete bipartite graph (which can also be an isolated vertex).

3 On Wiener Index of Common Neighborhood Graphs of Non-bipartite Graphs

From the results in the preceding section, we see that in the case of bipartite graphs, the Wiener index of the congraph is necessarily (much) smaller than the Wiener index of original graph. There are non-bipartite graphs for which $G \cong \mathrm{con}(G)$, namely the complete graphs and the odd cycles [1]. For these graphs, $W(G) = W(\mathrm{con}(G))$. Bearing this in mind, it appears to be plausible to expect that Conjecture 1 holds. This expectation is further corroborated by Corollary 8.

The fact that the conjecture is false is surprising, since we now show that the diameter of G, denoted by $\mathrm{diam}(G)$, is always at least the diameter of $\mathrm{con}(G)$. By $d_e(u,v)$ we denote the length of a shortest walk of even length between the vertices u and v. Notice that $d_e(u,v)$ in G is precisely $d(u,v)$ in $\mathrm{con}(G)$.

Lemma 7. *Let G be a connected non-bipartite graph. Then, for every pair of vertices $u, v \in V(G)$ we have*

$$d_e(u,v) \leq 2\,\mathrm{diam}(G)\,.$$

Proof. Let $u, v \in V(G)$ and let $u = a_0, a_1, \ldots, a_k = v$ be the shortest walk of even length between u and v (since G is connected and not bipartite such a walk always exists). If $d(u,v)$ is even, then $d_e(u,v) = d(u,v) \leq \mathrm{diam}(G)$. Thus, suppose that $d(u,v) < d_e(u,v) = k$. Let j be the smallest index such that $d(u,a_j) < j$. If $d(u,a_j) \leq j-3$, then $d(u,a_{j-1}) \leq j-2$, which contradicts the choice of j. On the other hand, if $d(u,a_j) = j-2$ then there is an even walk from u to v via a_j of length $k-2$, a contradiction. Hence, $d(u,a_j) = j-1$.

Now, let i be the biggest index such that $d(a_i,v) < k-i$. By analogous argument we obtain that $d(a_i,v) = k-i-1$. In case when $j \leq i$ then there is an even walk from

u to v of length $k-2$, a contradiction. Hence, $i < j$. Therefore, $d(u,a_j) = j-1$ and $d(a_j,v) = k-j$, which means that $d_e(u,v) = d(u,a_j)+1+d(a_j,v) \leq 2\text{diam}(G)+1$. However, since $d_e(u,v)$ is even, we infer that $d_e(u,v) \leq 2\text{diam}(G)$. $\square$

Observe that if $u = a_0, a_1, \ldots, a_k = v$ is a shortest walk of even length, then for every even i the triple a_i, a_{i+1}, a_{i+2} forms a path of length 2. This, together with Lemma 7, gives the following.

Corollary 8. *Let G be a connected non-bipartite graph. Then*

$$\text{diam}(\text{con}(G)) \leq \text{diam}(G)\,.$$

Let G be a connected non-bipartite graph. By Corollary 8, we have that the diameter of $\text{con}(G)$ is at most equal to the diameter of G. Moreover, $\text{con}(G)$ has at least as many edges as G. Therefore, one would expect that $W(\text{con}(G)) \leq W(G)$.

In many cases, this inequality is true, but there are also exceptional graphs violating it. In the sequel we describe a class of chemical graphs (i.e., graphs with maximum degree at most 4) $\{G_k\}_{k=0}^{\infty}$, for which $\lim_{k\to\infty}[W(G_k) - W(\text{con}(G_k))] = -\infty$.

Let $k \geq 0$. Take a graph consisting of a triangle, to which there is attached (by one of its endpoints) a path of length $k+2$. This graph has exactly one vertex of degree 3, one vertex of degree 1, and all the other vertices have degree 2. Attach to each vertex of degree 2, with the exception of the three neighbors of the vertex of degree 3, two pendent edges, and denote the resulting graph by G_k, see Fig. 1.

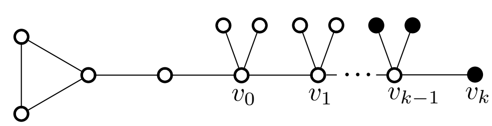

Figure 1: The graph G_k.

Finally, denote $\Delta_k = W(G_k) - W(\text{con}(G_k))$. Then we have:

Theorem 9. *For every integer $i \geq 0$ it holds*

$$\Delta_{2i} = -3i^2 + 9i + 2 \quad \textit{and} \quad \Delta_{2i+1} = -3i^2 + 6i + 11\,.$$

Proof. It is easy to compute that $W(G_0) = 17$ and $W(\text{con}(G_0)) = 15$ (in Fig. 2 for every vertex the sum of distances to all other vertices is determined), and so $\Delta_0 = 2$.

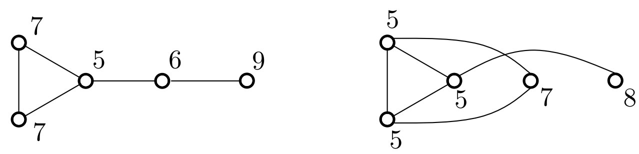

Figure 2: The graphs G_0 and $\mathrm{con}(G_0)$ together with the sums of all distances for every vertex.

Now, we construct G_k from G_{k-1} by attaching three new vertices to the vertex v_{k-1}. These new vertices are depicted black in Fig. 1. For every other (i.e., white) vertex we compute its contribution to the difference $\Delta_k - \Delta_{k-1}$ for every black vertex. Since this contribution is the same for every black vertex, we denote it in Fig. 3. For

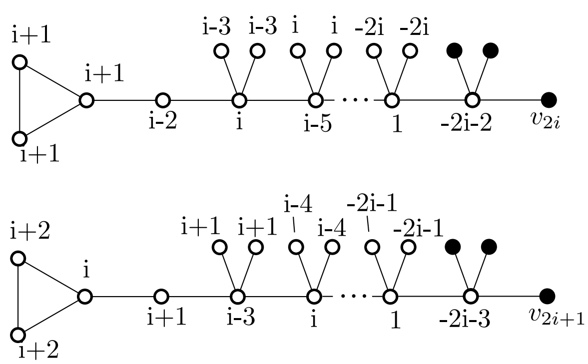

Figure 3: The contributions of the vertices to the difference for every black vertex in graphs G_{2i} and G_{2i+1}.

instance, in G_1 the vertex of degree 4 has distance 1 to a black vertex in G_1 and 4 to a black vertex in $\mathrm{con}(G_1)$, so its contribution to $\Delta_1 - \Delta_0$ is -3 for every black vertex.

Denote by δ_k the sum of the contributions of all white vertices to a black vertex and let $\Delta'_k = \Delta_k - \Delta_{k-1}$. Then, $\Delta'_k = 3\delta_k + 3$, since there are three black vertices in G_k and each pair of them contributes additional 1 to Δ'_k.

In what follows, we compute δ_k. First, we add the contributions of the vertices of the triangle and the contributions of the vertices of degree at least 2 at even distance from a black vertex. Then, we add the contributions of the remaining vertices of degree at least 2 and finally the contributions of the pendent vertices. Hence,

$$\delta_{2i} \;=\; 3(i+1) + \sum_{j=1}^{i} j + \sum_{j=0}^{i} \big(1 + 2j - (2(i+1) + 1 - j)\big)$$

$$+ \quad 2\left(\sum_{j=2}^{i} j + \sum_{j=1}^{i}(2j+1-(2i+4-j))\right) = -i-1$$

and

$$\begin{aligned}\delta_{2i+1} &= 3i+4+\sum_{j=1}^{i+1} j + \sum_{j=0}^{i}(1+2j-(2i+4-j)) \\ &+ \quad 2\left(\sum_{j=2}^{i+1} j + \sum_{j=1}^{i}(2j+1-(2i+5-j))\right) = -i+2\ .\end{aligned}$$

Therefore $\Delta'_{2i} = 3\delta_{2i}+3 = -3i$ and $\Delta'_{2i+1} = 3\delta_{2i+1}+3 = -3i+9$. Thus we infer

$$\Delta_{2i} = 2+\sum_{j=0}^{i-1}(-3j+9)+\sum_{j=1}^{i}(-3j) = -3i^2+9i+2$$

and

$$\Delta_{2i+1} = 2+\sum_{j=0}^{i}(-3j+9)+\sum_{j=1}^{i}(-3j) = -3i^2+6i+11\ .$$

□

For non-chemical graphs we can prove even more. In particular, for every integer Δ, we show that there are infinitely many graphs G such that $W(G)-W(\mathrm{con}(G)) = \Delta$.

Denote by G the graph consisting of one triangle to which a path of length 4 is attached (by one of its endvertices). Denote the three vertices of degree 2 of the attached path by a, b, and c, respectively. Now attach to a, b, and c exactly q, r, and s pendent edges, respectively, and denote the resulting graph by $G_{q,r,s}$.

Let $\Delta_{q,r,s} = W(G_{q,r,s}) - W(\mathrm{con}(G_{q,r,s}))$. In the following theorem we show that for every integer Δ there is infinitely many graphs $G_{q,r,s}$ such that $\Delta_{q,r,s} = \Delta$.

Theorem 10. *For every integer Δ, there are infinitely many graphs $G_{q,r,s}$ such that $\Delta_{q,r,s} = \Delta$. In particular, for every $\ell = 3z-\Delta$ such that $s = 4\ell$, $r = 4\ell^2-2-(5\ell+\Delta)/3$, and $q = r-s+2\ell$ are all positive, we have $\Delta_{q,r,s} = \Delta$.*

Proof. It is easy to compute that $W(G_{0,0,0}) = 51$ and $W(\mathrm{con}(G_{0,0,0})) = 45$, and so $\Delta_{0,0,0} = 6$. Now we construct $G_{q,r,s}$ from $G_{0,0,0}$ by attaching q pendent vertices to a, r pendent vertices to b, and finally s pendent vertices to c.

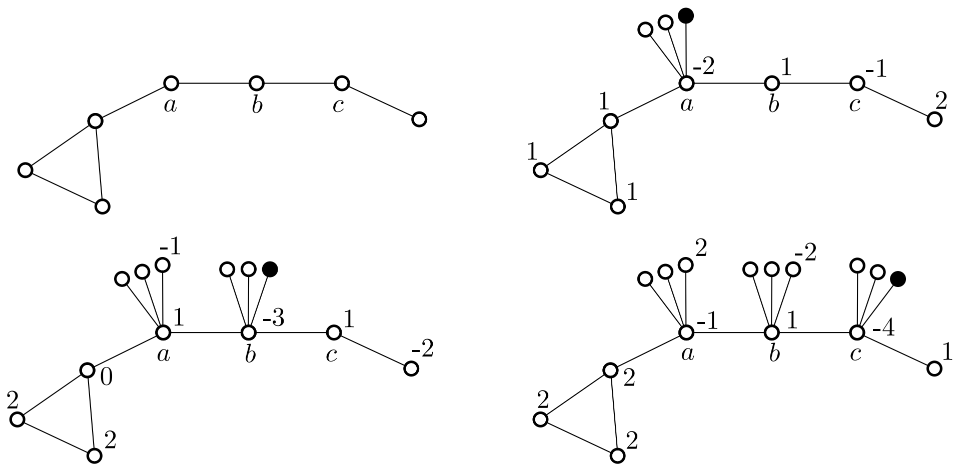

Figure 4: The graphs $G_{0,0,0}$, $G_{3,0,0}$, $G_{3,3,0}$, and $G_{3,3,3}$.

Analogously as in the previous proof, we compute the contribution of the vertices to $\Delta_{q,r,s}$ for every added vertex, in particular, we compute it for the vertices of the same type, e.g. all pendent vertices at vertex a are of the same type, and then multiply the values with the number of the vertices of that type. The contributions (for each of the black vertices) are depicted in Fig. 4.

Since the sums of contributions when attaching pendent vertices to a, b, and c are 3, $1-q$, and $3+2q-2r$, respectively, and since each pair of attached vertices contributes by 1 (observe that the distance between them is 2), we have that

$$\begin{aligned}\Delta_{q,r,s} &= 6+3q+\binom{q}{2}+(1-q)r+\binom{r}{2}+(3+2q-2r)s+\binom{s}{2}\\ &= \frac{1}{2}\left(q^2+5q+r^2+r+s^2+5s-2qr+4qs-4rs+12\right).\end{aligned}$$

Our aim is to find infinitely many solutions of $\Delta_{q,r,s}=\Delta$, i.e.,

$$q^2+5q+r^2+r+s^2+5s-2qr+4qs-4rs+12-2\Delta=0\ . \tag{4}$$

After multiplying by 4, Eq. (4) can be rewritten in the form

$$(2q-2r+4s+5)^2-(2s+5)^2=8s^2-24r-48+8\Delta$$

that is $x^2-y^2=a$. We choose the solution $x+y=(8s^2-24r-48+8\Delta)/2k$ and $x-y=2k$. Obviously, for such a choice it holds that $2k|(8s^2-24r-48+8\Delta)$. Then

$$x=\frac{2s^2-6r-12+2\Delta+k^2}{k} \qquad \text{and} \qquad y=\frac{2s^2-6r-12+2\Delta-k^2}{k}\ .$$

By(5) $y = 2s + 5$, so we obtain

$$r = \frac{2s^2 - 12 + 2\Delta - k^2 - 2sk - 5k}{6} \tag{5}$$

and since $x = 2q - 2r + 4s + 5$, we have that $\frac{2s^2-6r-12+2\Delta+k^2}{k} = 2q - 2r + 4s + 5$. After a substitution for r from Eq. (5), we obtain $\frac{2k^2+2sk+5k}{k} = 2q - 2r + 4s + 5$, and so $q = r - s + k$.

Now we return our attention back to r. Let k be even, say $k = 2\ell$. Then

$$r = \frac{2s^2 - 12 + 2\Delta - 4\ell^2 - 4s\ell - 10\ell}{6} = \frac{(s-\ell)^2 - 3\ell^2 - 5\ell + \Delta - 6}{3}.$$

Choosing $s = 4\ell$, we infer that $r = 3\ell^2 - \ell^2 - 2 - \frac{5\ell-\Delta}{3}$. Hence, by setting $\ell = 3z - \Delta$, then q, r, and s are integers. Obviously, if z is big enough, then q, r, and s are non-negative. □

4 Discussion

Throughout the article we have discussed the Wiener index of the common neighborhood graphs. We have shown that the diameter of the common neighborhood graph is at most the diameter of the original graph, however, the difference between the Wiener indices of these two graphs may be arbitrarily large. In fact we have shown that even in the case of chemical graphs the difference is grows arbitrarily. Moreover, for any integer Δ there is an infinite family of graphs such that $W(\text{con}(G)) - W(G) = \Delta$ for every graph of the family. We believe that the following conjecture is true.

Conjecture 2. *There is an absolute constant C such that for every graph G it holds that*

$$W(\text{con}(G)) \leq C \cdot W(G).$$

Nevertheless, it is not completely clear how the difference grows in terms of the number of the vertices in the graphs. Let $G*$ be a graph on n vertices constructed from a path of length $n/3$ that has attached roughly $n/3$ on the first and on the second vertex and one triangle on the last vertex. We have observed that the difference $W(\text{con}(G^*)) - W(G^*) \in \Theta(n^3)$, more precisely the leading coefficient is $n^3/27$.

Regarding this, it could be interesting to determine the extremal graphs for which the considered difference is maximal.

Acknowledgement. The first author acknowledges the support from VEGA Research Grants 1/0781/11 and 1/0065/13, the APVV Research Grant 0223-10 and APVV support as part of the EUROCORES Programme EUROGIGA Project GREGAS ESF-EC-0009-10 financed by the European Science Foundation. The first three authors thank the ARRS Program P1-0383 and Creative Core - FISNM - 3330-13-500033 for partial support of this work.

References

[1] A. Alwardi, B. Arsić, I. Gutman, N. D. Soner, The common neighborhood graph and its energy, *Iran. J. Math. Sci. Inf.* **7**(2) (2012) 1–8.

[2] A. Alwardi, N. D. Soner, I. Gutman, On the common–neighborhood energy of a graph, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math.* **143** (2011) 49–59.

[3] A. S. Bonifácio, R. R. Rosa, I. Gutman, N. M. M. de Abreu, Complete common neighborhood graphs, *Proceedings of Congreso Latino–Iberoamericano de Investigación Operativa & Simpósio Brasileiro de Pesquisa Operacional* (2012) 4026–4032.

[4] F. Buckley, F. Harary, *Distance in Graphs*, Addison–Wesley, Redwood, 1990.

[5] M. Chen, G. Hahn, A. Raspaud, W. Wang, Some results on the injective chromatic number of graphs, *J. Comb. Optim.* **24** (2012) 299–318.

[6] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[7] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.* **72** (2002) 247–294.

[8] A. Doyon, G. Hahn, A. Raspaud, Some bounds on the injective chromatic number of graphs, *Discrete Math.* **310** (2010) 585–590.

[9] R. C. Entringer, D. E. Jackson, D. A. Snyder, Distance in graphs, *Czech. Math. J.* **26** (1976) 283–296.

[10] G. Hahn, J. Kratochvíl, J. Širáň, D. Sotteau, On the injective chromatic number of graphs, *Discrete Math.* **256** (2002) 179–192.

[11] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.

[12] B. Lužar, R. Škrekovski, M. Tancer, Injective colorings of planar graphs with few colors, *Discrete Math.* **309** (2009) 5636–5649.