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The Szeged and Wiener Indices of Line Graphs*

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Abstract

The Wiener index and Szeged indices are structural descriptors based on distances between vertices of a graph G. The Szeged index appears as generalization of Wiener's formula for acyclic molecules. The concept of line graph, $L(G)$, for a graph G has found various applications in chemical research. Some results for the Szeged index of line graphs are presented. In particular, we are interesting in finding of graphs G with property $Sz(G) = Sz(L(G))$. The obtained results will be compared with the similar properties of the Wiener index.

1 Introduction

Topological indices have been extensively applied for the development of quantitative structure-property relationships in which various physico-chemical properties of molecules are correlated with their chemical structure [1, 8, 10, 28, 36, 37, 39]. The Wiener index is a well-known topological index introduced originally for molecular graphs of alkanes [40]. To calculate this index, the following formula was proposed by H. Wiener:

$$W(T) = \sum_{(u,v)} n_u n_v \,,$$

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where the summation goes over all edges (u, v) in a connected acyclic graph T and n_u is the number of the vertices of T which lie closer to the vertex u than to the vertex v. Analogously, n_v counts the vertices of T which lie closer to v than to u.

The extension of W for general graphs was put forward by H. Hosoya [32]. For an arbitrary graph G with vertex set $V(G)$, the Wiener index is now defined as the sum of distances between all unordered pairs of its vertices:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v),$$

where $d(u, v)$ is the number of edges in a shortest path connecting vertices u and v. Chemical applications and mathematical properties of the Wiener index can be found in books and reviews [12, 15, 17, 23, 24, 27, 33–35].

A generalization of the Wiener formula for cyclo-containing graphs was proposed by Gutman [19]. This topological index is now referred to as the Szeged index and is defined by the following formula:

$$Sz(G) = \sum_{(u,v)} n_u n_v,$$

where the summation goes over all edges (u, v) in of G and $n_u = |\{w \mid d(w, u) < d(w, v)\}|$, $n_v = |\{w \mid d(w, v) < d(w, u)\}|$. The basic properties of the Szeged index and bibliography on Sz are presented in [21].

Line graph, $L(G)$, of a graph G has vertex set $V(L(G)) = E(G)$ and two distinct vertices of $L(G)$ are adjacent if the corresponding edges of G share a common endvertex. The concept of line graph has found various applications in chemical research and applications [2–6, 18, 22, 29–31, 38]. An example of line graph is shown in Fig. 1.

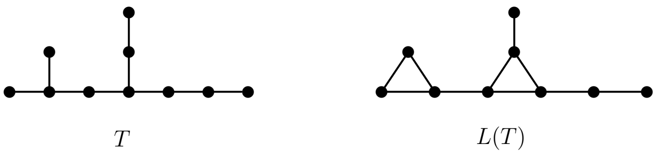

Figure 1. Tree T and its line graph $L(T)$.

In this paper we find graphs having property

$$Sz(G) = Sz(L(G)). \tag{1}$$

The obtained results are compared with the similar property of the Wiener index:

$$W(G) = W(L(G)). \tag{2}$$

Infinite families of graphs satisfying equality (1) are also constructed.

2 Connected acyclic graphs

By definition, the Szeged index coincides with the Wiener index in the case of connected acyclic graphs, that is, trees. There is a simple relation between the Wiener index of a tree and of its line graph [7].

Proposition 1. [7] *Let T be an arbitrary tree on n vertices. Then*

$$W(T) = W(L(T)) + \binom{n}{2}.$$

The problem of relation between Sz and W is basically resolved in [13, 20]. A block of a graph is a subgraph which has no cut vertices and is maximal with respect to this property. Two blocks have one cut vertex in common or have no common vertices. Let $\mathcal{B}$ be the set of all connected graphs, all blocks of which are complete graphs. It is clear that all trees belong to $\mathcal{B}$.

Proposition 2. [13] *For a connected graph G, $Sz(G) = W(G)$ if and only if $G \in \mathcal{B}$.*

Since line graph $L(T)$ of a tree T always belongs to $\mathcal{B}$, Proposition 2 implies that $Sz(L(T)) = W(L(T))$. Then Proposition 1 can be reformulated for the Szeged index.

Proposition 3. *Let T be an arbitrary tree on n vertices. Then*

$$Sz(T) = Sz(L(T)) + \binom{n}{2}.$$

This equality immediately implies that there no exist trees T satisfying equality $Sz(T) = S(L(T))$.

3 Unicyclic graphs

Denote by C_n the simple cycle on n vertices. Cycle C_n is the unique graph for which $L(G) \cong G$. It is known that graphs with property (2) have at least two cycles.

Proposition 4. [20] *If G is a unicyclic n–vertex graph, then $W(L(G)) \leq W(G)$ with equality only if G is the simple cycle C_n.*

By contrast with the Wiener index, there are many unicyclic graphs satisfying property (1). Table 1 contains number N_{Sz} of all such unicyclic graphs with $6 \leq n \leq 18$ vertices (graphs of order $n \leq 5$ are simple cycles). Here N_u is the number of all connected unicyclic n-vertex graphs.

Table 1. Number of unicyclic n-vertex graphs G with $Sz(G) = Sz(L(G))$.

n	6	7	8	9	10	11	12	13	14	15	16	17	18
N_u	13	33	89	240	657	1806	5026	13999	39260	110381	311465	880840	2497405
N_{Sz}	2	3	5	14	29	74	173	419	984	2386	5677	13831	33604

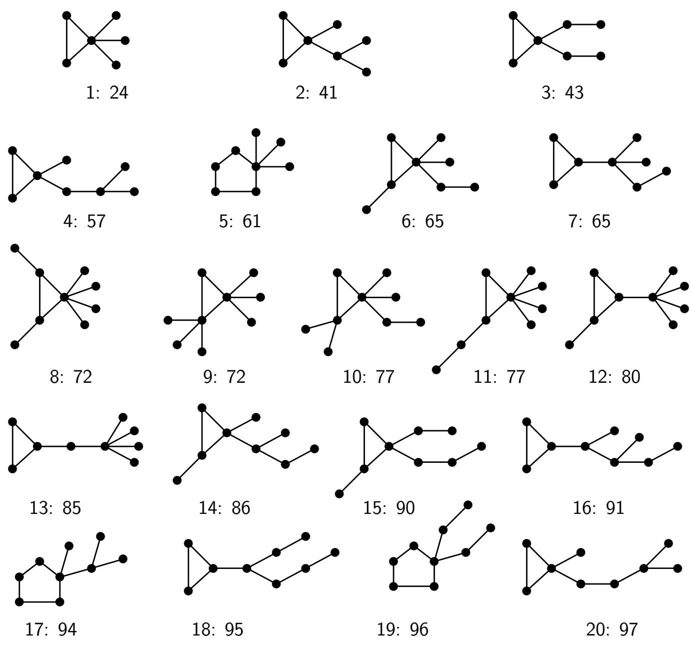

Figure 2. Smallest unicyclic graphs G with $Sz(G) = Sz(L(G))$.

Diagrams of the corresponding graphs of order $n \leq 9$ are shown in Fig. 2 (except simple cycles). The number of every graph and its Szeged index are presented near diagrams.

There are infinite families of unicyclic graphs G having property (1). We construct such a family starting with graphs 1, 2, 4, and 20 of Fig. 2.

Proposition 5. *For every $n \geq 6$, there exists an unicyclic graph G of order n such that $Sz(G) = Sz(L(G))$.*

Proof. Consider graph G_k with $n = k+5$ vertices and $q = k+5$ edges, $k \geq 1$, shown in Fig. 3. In order to obtain the Szeged index, we compute the quantity $n_u n_v$ for every edge (u,v) and add them together. First consider edges of path $P_1 = \{v_1, v_2, \ldots, v_k\}$. Every edge (v_i, v_{i+1}), $i = 1,2,...,k-1$, makes the contribution $(3+i)(k-i+2)$ to Sz. Let $(u,v) \in E(G_k) \setminus P_1$ and vertex u lies closer to path P_1. Then $n_u n_v = 1 \cdot (k+3)$ for edges e_1 and e_2; $n_u n_v = 1 \cdot (k+4)$ for edges e_3, e_4 and e_5; $n_u n_v = 1 \cdot 1$ for edge e_6. Summing contributions for all edges of G_k, we arrive at

$$\begin{aligned} Sz(G_k) &= 1 + 2(k+3) + 3(k+4) + \sum_{i=1}^{k-1} (3+i)(k-i+2) \\ &= \frac{1}{6}\left(k^3 + 15k^2 + 50k + 78\right). \end{aligned}$$

Line graph $L(G_k)$ has $n = k+5$ vertices and $q = k+9$ edges (see Fig. 3). Denote the path $\{u_1, u_2, \ldots, u_{k-1}\}$ by P_2. Every edge (u_i, u_{i+1}), $i = 1,2,...,k-2$, provides the contribution $(4+i)(k-i+1)$ to Sz. Suppose that vertex u lies closer to P_2 for every edge $(u,v) \in E(L(G_k)) \setminus P_2$. Then $n_u n_v = 1 \cdot (k+3)$ for edges e_1, e_2, e_3 and e_4; $n_u n_v = 2 \cdot (k+1)$ for edges e_5 and e_6; $n_u n_v = 1 \cdot (k+1)$ for edge e_7; $n_u n_v = 1 \cdot 2$ for edges e_8 and e_9; $n_u n_v = 1 \cdot 1$ for edges e_{10} and e_{11}. Therefore

$$\begin{aligned} Sz(L(G_k)) &= 6 + 5(k+1) + 4(k+3) + \sum_{i=1}^{k-2} (4+i)(k-i+1) \\ &= \frac{1}{6}\left(k^3 + 15k^2 + 50k + 78\right). \end{aligned}$$

The obtained equalities of $Sz(G_k)$ and $Sz(L(G_k))$ complete the proof. □

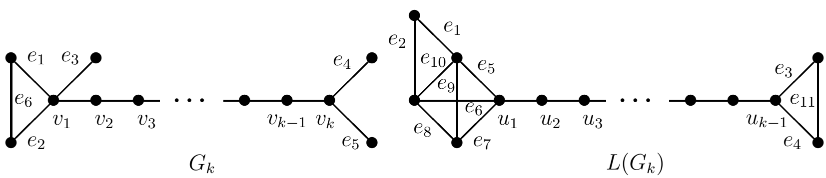

Figure 3. Unicyclic graph G_k having property $Sz(G_k) = Sz(L(G_k))$.

Unicyclic graphs give examples of structures for which properties of indices W and Sz are distinct.

4 Bicyclic graphs

Graphs G with property $W(G) = W(L(G))$ have been found for the first time among bicyclic graphs (see [14, 25, 26]). The basic properties of the Wiener index for bicyclic graphs are collected in the following statement.

Proposition 6. [14, 17] *1) There are no graphs of order* $n \leq 8$ *satisfying property* (2). *2) There exist exactly 26 graphs from* $\mathcal{G}_9$ *satisfying property* (2)*. All graphs are bicyclic. 3) There exist exactly 166 graphs from* $\mathcal{G}_{10}$ *satisfying property* (2)*. All graphs are bicyclic. 4) There exist exactly 503, 1082, and 2282*† *bicyclic graphs from* $\mathcal{G}_{11}$, $\mathcal{G}_{12}$, *and* $\mathcal{G}_{13}$, *respectively, satisfying property* (2).

Here we present new data for the Szeged index as well as for the Wiener index. Table 2 contains numbers N_{Sz} and N_W of bicyclic graphs with up to 18 vertices having properties (1) and (2), respectively. The number of all connected n-vertex bicyclic graphs is denoted by N_b. The smallest graphs with property (1) have 7 vertices while the smallest graphs with property (2) have 9 vertices.

Table 2. Number of bicyclic graphs G with $Sz(G) = Sz(L(G))$.

n	7	8	9	10	11	12	13	14	15	16	17	18
N_b	67	236	797	2678	8833	28908	93569	300748	959374	3042808	9597679	30134509
N_{Sz}	1	2	1	15	45	111	387	1307	3061	9738	32897	93608
N_W	0	0	26	166	503	1082	2282	7825	17705	33514	69760	194352

Diagrams of all graphs with $n \leq 10$ vertices are depicted in Fig. 4. Values of the Szeged index are shown near diagrams. Several examples of graphs with large diameter are shown in Fig. 5. An example of joint degeneracy of the invariants is bicyclic graph 19 of Fig. 4 for which properties (1) and (2) are valid simultaneously. Namely, $Sz(G) = Sz(L(G)) = 218$ and $W(G) = W(L(G)) = 122$.

Infinite families of bicyclic graphs with property (2) have been constructed for the first time in [26].

†Review [17] reports a wrong number of such graphs in $\mathcal{G}_{13}$ (2243).

Proposition 7. [26] *There exist infinitely many bicyclic graphs for which condition* (2) *is satisfied.*

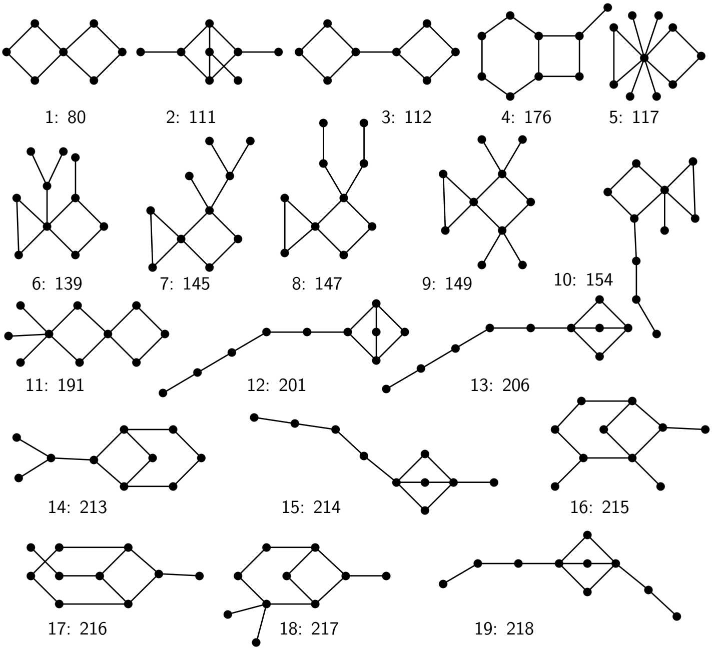

Figure 4. Smallest bicyclic graphs with equality $Sz(G) = Sz(L(G))$.

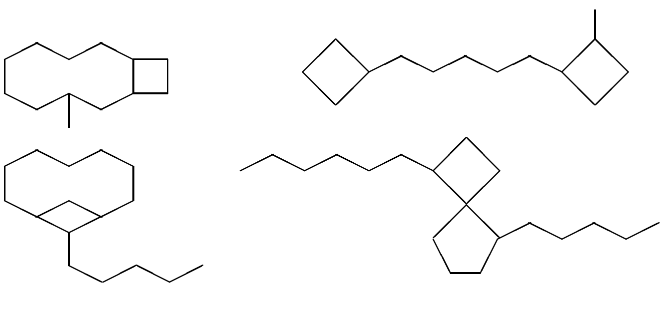

Figure 5. Bicyclic graphs of large order with $Sz(G) = Sz(L(G))$.

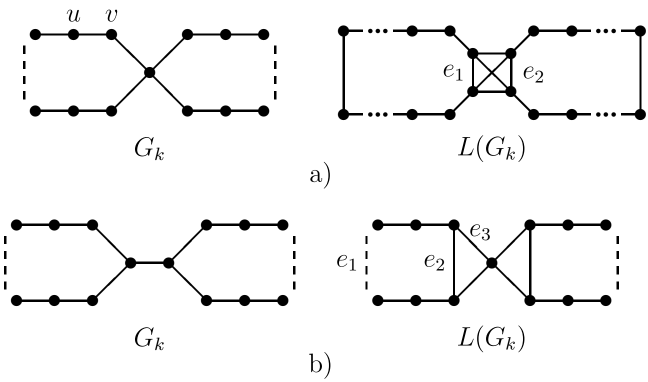

Figure 6. Bicyclic graphs G_k for which $Sz(G_k) = Sz(L(G_k))$.

It seems that a method developed in [26] is suitable for constructing n-vertex bicyclic graphs for every $n \geq 9$ (each family of graphs covers only a subset of all possible n). For the Szeged index, it is sufficient to consider a unique family. The first members of this family are graphs 1 and 3 of Fig. 4.

Proposition 8. *For every $n \geq 7$, there is a bicyclic graph G with n vertices such that $Sz(G) = Sz(L(G))$.*

Proof. First consider graphs having odd number of vertices. Let graph G_k be obtained by identifying a single vertex of two copies of cycle C_k (see Fig. 6a). Graph G_k has $n = 2k - 1$ vertices and $q = 2k$ edges. It easy to see that every edge (u, v) of G_k has the same product $n_u n_v$. Namely, if vertex v lies closer to the central vertex of G_k then $n_u n_v = k/2 \cdot (k/2 + n(C_k) - 1) = k(k/2 + k - 1)/2$. This implies

$$Sz(G_k) = \frac{1}{2}k^2(3k - 2).$$

Line graph $L(G_k)$ consists of a complete graph K_4 and two cycles C_k attached to K_4 by one edge (see Fig. 6a). For this graph, $n = 2k$ and $q = 2k + 4$. The edge set of $L(G_k)$ can be divided into two disjoint subsets. For edges e_1 and e_2 of K_4, $n_u n_v = k/2 \cdot k/2$. Contributions of the other $2(k-2)$ edges are the same, $n_u n_v = k/2 \cdot (k/2 + n(C_k))$. Then

$$Sz(L(G_k)) = 8\frac{k^2}{4} + 2(k - 2)\frac{k}{2}\left(\frac{k}{2} + k\right) = \frac{1}{2}k^2\left(3k - 2\right).$$

Consider now graphs of even order. Let graph G_k be obtained by joining a single vertex of two cycles C_k as depicted in Fig. 6b. By construction, $n = 2k$ and $q = 2k + 1$.

For the central edge of G_k, $n_u n_v = k \cdot k$. The other edges have the same value of $n_u n_v$. If u is closer to the central edge, then $n_u n_v = k/2 \cdot (k/2 + k)$. Hence

$$Sz(G_k) = k^2 + 2k\frac{k}{2}\left(\frac{k}{2} + k\right) = \frac{1}{2}\,k^2\,(3k + 2)\,.$$

Line graph $L(G_k)$ has $n = 2k+1$ and $q = 2k+4$ (see Fig. 6b). Because of symmetry, it is sufficient to examine the left part of $L(G_k)$. For edges e_1 and e_2, $n_u n_v = k/2 \cdot k/2$. Suppose that $(u, v) \in E(L(G_k)) \setminus \{e_1, e_2\}$ and vertex u is closer to the central vertex of $L(G_k)$. Then $n_u n_v = k/2 \cdot (k + 1)$ for edge e_3; $n_u n_v = k/2 \cdot (k/2 + n(C_k) + 1) = k(k/2 + k + 1)/2$ for the other $k - 2$ edges. Summing contributions for all edges, we have

$$Sz(L(G_k)) = k^2 + 4\frac{k}{2}\,(k + 1) + 2(k - 2)\frac{k}{2}\left(\frac{3k}{2} + 1\right) = \frac{1}{2}\,k^2\,(3k + 2)\,.$$

The obtained expressions of $Sz(G_k)$ and $Sz(L(G_k))$ coincide. □

Denote by $\delta(G)$ the minimal vertex degree in G. It was shown that if a graph G has no pendant vertices then $W(L(G))$ is not equal to $W(G)$.

Proposition 9. [9, 41] *Let G be a connected graph with $\delta(G) \geq 2$ and $G \ncong C_n$. Then $W(L(G)) > W(G)$.*

Graphs of Proposition 8 with $\delta(G) = 2$ demonstrate that Proposition 9 does not valid for the Szeged index (see Fig. 6). This is another difference between the considered indices.

5 Tricyclic graphs

To make sure that there exist graphs with the cyclomatic number $\lambda \geq 3$ having property (2), the computer searching has been applied for tricyclic graphs ($\lambda = 3$).

Proposition 10. [17] *1) There are no tricyclic graphs of order $n \leq 11$ with property* (2). *2) There exist exactly 71 and 733 tricyclic graphs from $\mathcal{G}_{12}$ and $\mathcal{G}_{13}$, respectively, satisfying property* (2).

New data of this kind for the Szeged and Wiener indices are presented in Table 3. Here N_{Sz} and N_W are the numbers of tricyclic graphs with up to 16 vertices having properties (1) and (2), respectively (N_t is the number of all connected n-vertex tricyclic graphs). Diagrams of all smallest tricyclic graphs on 10 vertices and their Szeged indices are depicted in Fig. 7.

Table 3. Number of tricyclic graphs G with $Sz(G) = Sz(L(G))$.

n	10	11	12	13	14	15	16
N_t	8548	33851	130365	489387	1799700	6499706	23118465
N_{Sz}	12	40	146	488	2071	6895	23734
N_W	0	0	71	733	3933	30758	143683

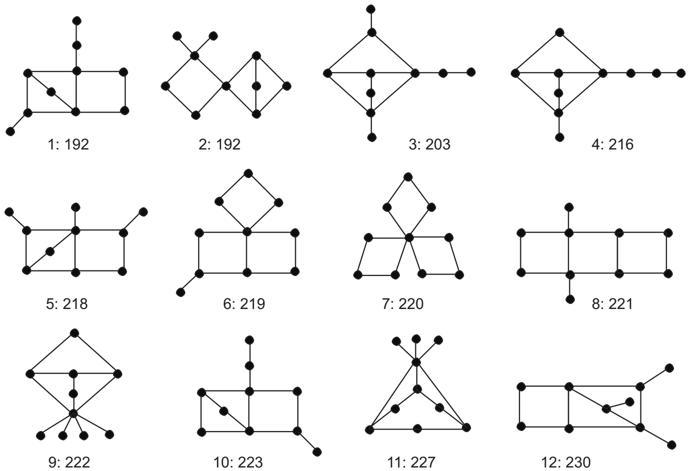

Figure 7. Smallest tricyclic graphs with $Sz(G) = Sz(L(G))$.

Recall that the last bicyclic graph G of Fig. 4 with 10 vertices satisfies the following equations: $Sz(G) = Sz(L(G))$, $W(G) = W(L(G))$ and $Sz(G) \neq W(G)$. Table 4 presents data concerning such joint degeneracy of Sz and W for n-vertex bicyclic and tricyclic graphs. Here N_{bi} and N_{tri} denote the numbers of graphs having this property.

Table 4. Number of bicyclic and tricyclic graphs G with $W(G) = W(L(G))$ and $Sz(G) = Sz(L(G))$.

n	10	11	12	13	14	15	16	17	18
N_{bi}	1	4	10	3	30	82	77	145	566
N_{tri}	0	0	0	3	3	75	274	-	-

Diagrams of the smallest tricyclic graphs and values of the indices are shown in Fig. 8.

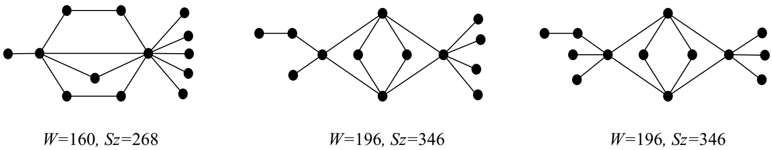

Figure 8. Tricyclic graphs with $Sz(G) = Sz(L(G))$ and $W(G) = W(L(G))$.

6 Graphs with many cycles

Graphs 1 of Fig. 4 and 7 of Fig. 7 give some information about a possible structure of graphs with many cycles satisfying equality (1). The following result shows that there are similar graphs having an arbitrary number of cycles of even length. The girth g of a graph is the length of its shortest cycle.

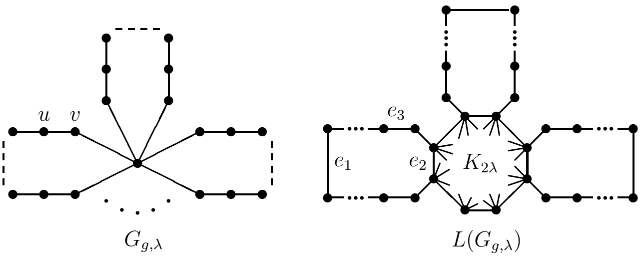

Figure 9. Polycyclic graphs having with $Sz(G) = Sz(L(G))$.

Proposition 11. *For every $\lambda \geq 2$ and even $g \geq 4$, there is a graph G with cyclomatic number λ and girth g such that $Sz(G) = Sz(L(G))$.*

Proof. Let graph $G_{g,\lambda}$ be obtained by identifying a single vertex of λ copies of cycle C_g as depicted in Fig. 9. Graph $G_{g,\lambda}$ has $n = g\lambda - \lambda + 1$ vertices and $q = g\lambda$ edges. We have $n_u n_v = g/2 \cdot (g/2 + n(G_{g,\lambda-1}) - 1)$ for every edge (u, v) of $G_{g,\lambda}$ (vertex u is closer to the central vertex). Then

$$Sz(G_{g,\lambda}) = g\lambda \frac{1}{2} g(g\lambda - \lambda - g/2 + 1) = \frac{1}{4} g^2 \lambda \left(2\lambda(g-1) - g + 2\right).$$

Line graph $L(G_{g,\lambda})$ consists of a complete graph $K_{2\lambda}$ and λ cycles C_g attached to $K_{2\lambda}$ (see Fig. 9). Then $n = g\lambda$ and $q = \lambda(2\lambda + g - 3)$. Consider edges of cycle C_g attached to $K_{2\lambda}$. For edges e_1 and e_2, we have $n_u n_v = g/2 \cdot g/2$. For the other $\lambda(g-2)$ edges of C_g, we can write $n_u n_v = g/2 \cdot (g/2 + p(L(G_{g,\lambda})) - g)$ (vertex v is closer to $K_{2\lambda}$). For every edge of $2\lambda(\lambda-1)$ remaining edges of $K_{2\lambda}$, we have $n_u n_v = g/2 \cdot g/2$. Then

$$\begin{aligned} Sz(L(G_{g,\lambda})) &= 2\lambda\frac{g^2}{4} + \lambda\,(g-2)\,\frac{g}{2}\left(\frac{g}{2} + g\lambda - g\right) + 2\lambda(\lambda-1)\frac{g^2}{4} \\ &= \frac{1}{4}g^2\lambda\,(2\lambda(g-1) - g + 2)\,. \end{aligned}$$

The equality $Sz(G_{g,\lambda}) = Sz(L(G_{g,\lambda}))$ is obtained. □

For the Wiener index, we mention the following results: bicyclic graphs with growing girth $g \geq 5$ satisfying property (2) were presented in [11]; bipartite graphs with growing cyclomatic number $\lambda \geq 2$ and girth $g = 4$ satisfying property (2) were constructed in [16].

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References

[1] A. T. Balaban, I. Motoc, D. Bonchev, O. Mekenyan, Topological indices for structure-activity correlations, *Topics Curr. Chem.* **114** (1983) 21–55.

[2] S. H. Bertz, The bond graph, *J. Chem. Soc. Chem. Commun.* (1981) 818–820.

[3] S. H. Bertz, A mathematical model of molecular complexity, in: R. B. King (Ed.), *Chemical Application of Topology and Graph Theory*, Elsevier, Amsterdam, 1983, pp. 201–206.

[4] S. H. Bertz, Branching in graphs and molecules, *Discr. Appl. Math.* **19** (1988) 65–83.

[5] S. H. Bertz, A mathematical model of molecular complexity, *Stud. Phys. Theor. Chem.* **28** (1993) 206–221.

[6] S. H. Bertz, W. F. Wright, The graph theory approach to synthetic analysis: definition and application of molecular complexity and synthetic complexity, *Graph Theory Notes New York* **35** (1998) 32–48.

[7] F. Buckley, Mean distance in line graphs, *Congr. Num.* **32** (1981) 153–162.

[8] J. Devillers, A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon & Breach, Reading, 2000.

[9] N. Cohen, D. Dimitrov, R. Krakovski, R. Škrekovski, V. Vukašinović, On Wiener index of graphs and their line graphs, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 683–698.

[10] M. V. Diudea (Ed.), *QSPR/QSAR Studies by Molecular Descriptors*, Nova, Huntington, New York, 2001.

[11] A. A. Dobrynin, The Wiener index of graphs of arbitrary girth and their line graphs, *J. Appl. Ind. Math.* **4** (2010) 505–511.

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

[13] A. A. Dobrynin, I. Gutman, Solving a problem connected with distances in graphs, *Graph Theory Notes New York* **28** (1995) 21–23.

[14] A. A. Dobrynin, I. Gutman, V. Jovašević, Bicyclic graphs and their line graphs having the same Wiener index, *Diskr. Anal. Issl. Oper. Ser. 2* **4** (1997) 3–9, in Russian.

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

[16] A. A. Dobrynin, L. S. Mel'nikov, Wiener index, line graphs and the cyclomatic number, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 209–214.

[17] A. A. Dobrynin, L. S. Mel'nikov, Wiener index of line graphs, in: I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs — Theory*, Univ. Kragujevac, Kragujevac, 2012, pp. 85–121.

[18] E. Estrada, I. Gutman, A topological index based on distances of edges of molecular graphs, *J. Chem. Inf. Comput. Sci.* **36** (1996) 850–853.

[19] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes New York* **27** (1994) 9–15.

[20] I. Gutman, Distance of line graphs *Graph Theory Notes New York* **31** (1996) 49–52.

[21] I. Gutman, A. A. Dobrynin, The Szeged index — a success story, *Graph Theory Notes New York* **34** (1998) 37–44.

[22] I. Gutman, E. Estrada, Topological indices based on the line graph of the molecular graph, *J. Chem. Inf. Comput. Sci.* **36** (1996) 541–543.

[23] I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs — Theory*, Univ. Kragujevac, Kragujevac, 2012.

[24] I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs — Applications*, Univ. Kragujevac, Kragujevac, 2012.

[25] I. Gutman, V. Jovašević, A. A. Dobrynin, Smallest graphs for which the distance of the graph is equal to the distance of its line graph, *Graph Theory Notes New York* **33** (1997) 19–19.

[26] I. Gutman, L. Pavlović, More on distance of line graphs, *Graph Theory Notes New York* **33** (1997) 14–18.

[27] I. Gutman, J. H. Potgieter, Wiener index and intermolecular forces, *J. Serb. Chem. Soc.* **62** (1997) 185–192.

[28] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.

[29] I. Gutman, Ž. Tomović, On the application of line graphs in quantitative structure–property studies, *J. Serb. Chem. Soc.* **65** (2000) 577–580.

[30] I. Gutman, Ž. Tomović, More on the line graph model for predicting physico–chemical properties of alkanes, *ACH Models Chem.* **137** (2000) 439–445.

[31] I. Gutman, Ž. Tomović, B. K. Mishra, M. Kuanar, On the use of iterated line graphs in quantitative structure–property studies, *Indian J. Chem.* **40A** (2001) 4–11.

[32] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.* **44** (1971) 2332–2339.

[33] M. Knor, R. Škrekovski, Wiener index of line graphs, in: M. Dehmer, F. Emmert-Streib (Eds.), *Quantitative Graph Theory: Mathematical Foundations and Applications*, Chapman and Hall, 2014, pp. 279–301.

[34] M. Knor, R. Škrekovski, A. Tepeh, Mathematical aspects of Wiener index, *Ars Math. Contemp.* **11** (2016) 327–352.

[35] S. Nikolić, N. Trinajstić, Z. Mihalić, The Wiener index: developments and applications, *Croat. Chem. Acta*, **68** (1995) 105–129.

[36] D. H. Rouvray, The modeling of chemical phenomena using topological indices, *J. Comput. Chem.* **8** (1987) 470–480.

[37] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[38] Ž. Tomović, I. Gutman, Modeling boiling points of cycloalkanes by means of iterated line graph sequences, *J. Chem. Inf. Comput. Sci.* **41** (2001) 1041–1045.

[39] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1983.

[40] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947) 17–20.

[41] B. Wu, Wiener index of line graphs, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 699–706.