MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **75** (2016) 71-80

ISSN 0340 - 6253

On Wiener Inverse Interval Problem

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(Received June 25, 2015)

Abstract

The well studied Wiener index $W(G)$ of a graph G is equal to the sum of distances between all pairs of vertices of G. Denote by $W[\mathcal{G}_n]$ the set of all values of the Wiener index over all connected graphs on n vertices, and let the largest interval which is fully contained in $W[\mathcal{G}_n]$ be denoted by W_n^{int}. In the paper, we show that both W_n^{int} and $W[\mathcal{G}_n]$ are of cardinality $\frac{1}{6}n^3+O\left(n^2\right)$. For $n \geq 25$ we show that W_n^{int} starts at $\binom{n}{2}$ and is uniquely defined. In other words, most of integers between the smallest value $\binom{n}{2}$ and the largest value $\binom{n+1}{3}$ are contained in W_n^{int}, and consequently in $W[\mathcal{G}_n]$. We also discuss some other properties of $W[\mathcal{G}_n]$ and W_n^{int}, and state some open problems.

1 Introduction

The Wiener index $W(G)$, introduced by Wiener [16], is a graph index defined for connected graph G as the sum of the lengths of shortest paths between all pairs of vertices in G, formally

$$W(G) = \sum_{u,v \in V(G)} d_G(u,v) \ .$$

It is the oldest topological index related to molecular branching and based on its success, many other topological indices correlated to distance matrix of chemical graphs have been developed subsequently to Wiener's work. The Wiener index was at first used for predicting the boiling points of paraffins [16], but later a strong correlation between Wiener index and other chemical or physical properties of compounds were found, such as critical points in general [13], the density, the surface tension, and viscosity of compounds liquid phase [12] and the van der Waals surface area of the molecule [4].

There are some recent papers on the Wiener index of trees [6], common neighborhood graphs [3,7] and line graphs [8–10,17]. Finding graph extremals for the Wiener index and its derivatives is nicely summarized in a recent survey by Gutman et. al. [18]. It is easy to determine the minimal and maximal values of the Wiener index in the class of trees or graphs on n vertices. Those and many other bounds for the Wiener index are presented in [18].

For a given integer k, the inverse Wiener index problem is a problem of finding a graph G, such that $W(G) = k$. The problem was proposed in 1995 by Gutman and Yeh [5], where they posed the following conjecture.

Conjecture 1. *For all but finitely many integers w, there exist trees with Wiener index w.*

The conjecture was first checked for integers up to 1206 [11], where authors found 49 integers without Wiener inverse. This result was further extended to integers up to 10^8, see [1]. The conjecture was finally solved in 2006, see [14] and [15]. Furthermore, Fink et al. [2] showed that every sufficiently large integer has sub-exponentially many Wiener inverses in the family of trees. A related question to ask is the following:

Problem 2. *What value of the Wiener index can a graph (or a tree) on n vertices have?*

In relation to this one can also ask how many such values exist, how are they distributed along the related interval or how many of them are contiguous. We call this problem the *Wiener inverse interval problem.*

For integers a and b, the notion $[a, b]$ stands for the set containing a, b and all consecutive integers between them. We now define the core notation for the Wiener inverse interval problem.

Definition 3. For a fixed n, we define $W\left[\mathcal{G}_n\right]$ to be the image of W under $\mathcal{G}_n$, i.e.

$$i \in W\left[\mathcal{G}_n\right] \quad \Leftrightarrow \quad \text{there is a graph } G \in \mathcal{G}_n \text{ such that } W\left(G\right) = i.$$

Also, let W_n^{int} be the largest interval of contiguous integers such that $W_n^{\text{int}} \subseteq W[\mathcal{G}_n]$. Finally, define a relation $\sim \in \mathcal{G}_n^2$, such that for $G, H \in \mathcal{G}_n$, we have

$$G \sim H \quad \Longleftrightarrow \quad [W(G), W(H)] \subseteq W[\mathcal{G}_n],$$

and observe that $\sim$ is an equivalent relation.

The extremals of the set $W[\mathcal{G}_n]$ are well-known, see [18].

Proposition 4. *For the family $\mathcal{G}_n$, it holds that* $\min(W[\mathcal{G}_n]) = \binom{n}{2}$ *and* $\max(W[\mathcal{G}_n]) = \binom{n+1}{3}$, *which are achieved at K_n and P_n, respectively.*

We now define some classes of graphs that we use throughout the paper. *A star* graph S_{n-1} is a graph on n vertices, consisted of some vertex, connected to $n-1$ leaves, i.e. $S_{n-1} \simeq K_{1,n-1}$. Let $D(n,l)$ be the *Dandelion* graph on n vertices, consisted of a copy of the star S_{n-l} and a copy of a path P_l on vertices $p_0, p_1, \ldots, p_{l-1}$, where p_0 is identified with a star center. An example of $D(17,8)$ is shown in Fig. 1. The family of *comet* graphs

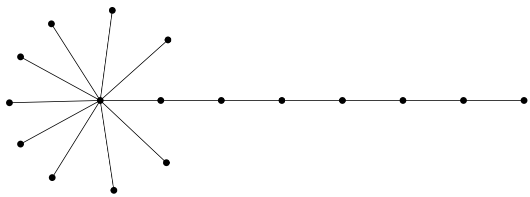

Figure 1: Dandelion graph $D(17,8)$.

looks similar as the family of Dandelion graphs. For a positive integer $l \leq n$ let $C(n,l)$ be the *comet* graph on n vertices, consisted of a copy of the complete graph K_{n-l+1} and a copy of the path P_l, on vertices $p_0, p_1, \ldots, p_{l-1}$, where p_0 is identified with a vertex from K_{n-l+1}. For non-negative integers $a_1, \ldots, a_k$ with $k \geq 1$, let $P(a_1, \ldots, a_k)$ be the graph constructed from a copy of P_k, with additional α_i leaves added to i-th vertex of a path.

A nice example is set $W[\mathcal{G}_4]$, which does not miss any value between $\binom{4}{2}$ and $\binom{5}{3}$.

Example 5. Let $n = 4$ and let K_4^- be a graph isomorphic to complete graph K_4 without one edge, and observe that

$$\mathcal{G}_4 = \left\{P_4, S_3, C_4, C(4,2), K_4^-, K_4\right\}.$$

In Table 1 the values of Wiener index for each graph from $\mathcal{G}_4$ is calculated. From Table 1 we deduce that $W[\mathcal{G}_4] = \{6, 7, 8, 9, 10\}$.

Graph $G \in \mathcal{G}_4$	P_4	S_3	C_4	$C(4,2)$	K_4^-	K_4
$W(G)$	10	9	8	8	7	6

Table 1: Values of the Wiener index of the members of $\mathcal{G}_4$.

For the graphs with induced star, observe the following.

Observation 6. *Let $G \in \mathcal{G}_n$ be a graph that contains k leaves adjacent to the same vertex. Then*

$$\left[W(G) - \binom{k}{2}, W(G)\right] \subseteq W\left[\mathcal{G}_n\right].$$

Proof. Let v be the common neighbor and label its adjacent leaves with $v_1, \ldots, v_k$. Now, iteratively add $\binom{k}{2}$ additional edges between the leaves $v_1, v_2, \ldots, v_k$ to G, each time decreasing the Wiener index of G by one. This concludes the proof of the observation.

■

The Wiener index for the family of Dandelion graphs is determined in the next lemma.

Lemma 7. *For a fixed positive integer n let a and b be two positive integers that sum up to n. The Wiener index of the Dandelion graph $D(n,b)$ can be expressed as follows*

$$W\left(D\left(n,b\right)\right) = \binom{b+1}{3} + \left(\binom{b+1}{2} - 1\right) \cdot a + a^2.$$

Proof. We partition all the pairs of vertices of the graph $D(n,b)$ into three parts. First consider the pairs that belong to the path P_b. They sum up to the Wiener index of a path, i.e. $\binom{b+1}{3}$. Now consider all the pairs from the star S_a (note that this is a tree on $a+1$ nodes and a leaves). One can deduce that

$$W(S_a) = 1 \cdot a + 2 \cdot \binom{a}{2} = a^2.$$

Finally, all the remaining pairs are of type (u,v), where u is one of the leaves of the star, and v is one of the path-vertices, excluding the center of the star. One can easily conclude that for each of a admissible leaves of the star such distances sum up to $\binom{b+1}{2} - 1$. ■

Let us again mention the values of Wiener index for some relevant graph families. For the family of stars, we have $W\left(S_{n-1}\right) = (n-1)^2$, for the family of cliques, we have $W\left(K_n\right) = \binom{n}{2}$, while for the family of paths, we have $W\left(P_n\right) = \binom{n+1}{3}$. For families of comets and Dandelion graphs, we have:

$$\begin{aligned} W\left(C\left(n,b\right)\right) &= \binom{b+1}{3} + \left(\binom{b+1}{2} - 1\right) \cdot (n-b) + \binom{n-b+1}{2} \\ W\left(D\left(n,b\right)\right) &= \binom{b+1}{3} + \left(\binom{b+1}{2} - 1\right) \cdot (n-b) + (n-b)^2 . \end{aligned}$$

In the next section, we show that W_n^{int} is of length $\frac{1}{6}n^3 + O\left(n^2\right)$ and that it starts at $\binom{n}{2}$. Consequently, the same holds for and $W\left[\mathcal{G}_n\right]$. In the concluding section, we discuss some other properties of $W\left[\mathcal{G}_n\right]$ and W_n^{int} and state some open problems.

2 The cardinality of W_n^{int} and $W\left[\mathcal{G}_n\right]$

By Proposition 4, the Wiener index of every graph on n vertices falls inside the interval $\left[\binom{n}{2}, \binom{n+1}{3}\right]$. Since $\binom{n+1}{3} - \binom{n}{2} + 1 = \frac{1}{6} \cdot n^3 - \frac{1}{2} \cdot n^2 + \frac{1}{3} \cdot n + 1$, it is easy to conclude the following upper-bound for $\left|W_n^{\text{int}}\right|$.

Corollary 8. *For the family $\mathcal{G}_n$ it holds that*

$$\left|W_n^{\text{int}}\right| \leq \left|W\left[\mathcal{G}_n\right]\right| \ \leq \ \frac{1}{6} \cdot n^3 - \frac{1}{2} \cdot n^2 + \frac{1}{3} \cdot n + 1.$$

In lemmas that follow, we proceed by defining some intervals that are fully contained in $W\left[\mathcal{G}_n\right]$. We then try to tile these intervals so that their union form a bigger interval. The core part of estimating the length of W_n^{int} is the following lemma.

Lemma 9. *Fix positive integers $n \geq 7$ and $a_1, a_2 \ldots, a_k$ such that $P(a_1, a_2, \ldots, a_k)$ has n vertices and $a_1 + a_2 \geq 2\sqrt{n}$. Then*

$$P\left(a_1, a_2, \ldots, a_k\right) \sim P\left(a_1 + 1, a_2 - 1, \ldots, a_k\right).$$

Proof. For easier notation denote

$$G = P\left(a_1, a_2, \ldots, a_k\right) \quad \text{and} \quad H = P\left(a_1 + 1, a_2 - 1, \ldots, a_k\right)$$

and observe that

$$W\left(H\right) - W\left(G\right) = n - 2a_1 - 3.$$

Depending on which of both graphs H and G had smaller Wiener index we consider the following two cases. In both cases, we fill the space between $W\left(H\right)$ and $W\left(G\right)$ by adding at least $|n - 2a_1 - 3|$ additional edges to one of the graphs G or H that have bigger Wiener index, as described in Observation 6.

Case 1: $a_1 \geq \frac{n}{2} - \frac{3}{2}$. It holds that $W(H) \leq W(G)$, hence we fill the space between $W(H)$ and $W(G)$ by adding at least $|n - 2a_1 - 3|$ additional edges to G. It is therefore enough to show that $\binom{a_1}{2} \geq -(n - 2a_1 - 3)$. Indeed, since $n \geq 7$, we have

$$\binom{a_1}{2} + n - 2a_1 - 3 \quad = \quad \frac{\left(a_1 - \frac{5}{2}\right)^2}{2} - \frac{49}{8} + n \geq n - \frac{49}{8} > 0.$$

Case 2: $a_1 < \frac{n}{2} - \frac{3}{2}$. Now notice $W(H) > W(G)$, hence we fill the space between $W(H)$ and $W(G)$ by adding at least $|n - 2a_1 - 3|$ additional edges to H. From the fact that $a_1 + a_2 \geq 2\sqrt{n} > \sqrt{1 + 4n} - 1$, it is clear that

$$\left(a_1 + \frac{5}{2}\right)^2 + \left(a_2 - \frac{3}{2}\right)^2 \geq \frac{(a_1 + a_2 + 1)^2}{2} > \frac{1}{2} + 2n. \tag{1}$$

Similarly as in the previous case, we are able to use Observation 6 on graph H at least $\binom{a_1+1}{2} + \binom{a_2-1}{2}$ times. It is therefore enough to show that $\binom{a_1+1}{2} + \binom{a_2-1}{2} \geq n - 2a_1 - 3$. By inequality (1) and since $a_1 \geq 0$, $n \geq 8$, we conclude

$$\binom{a_1 + 1}{2} + \binom{a_2 - 1}{2} - (n - 2a_1 - 3) \quad = \quad \frac{\left(a_1 + \frac{5}{2}\right)^2 + \left(a_2 - \frac{3}{2}\right)^2}{2} - \frac{1}{4} - n \geq 0.$$

■

By the transitivity of $\sim$, we have the following corollary.

Corollary 10. *Let $i \in [1, \lfloor n - 2\sqrt{n} - 1 \rfloor]$. Then*

$$D(n, i) \sim D(n, i + 1).$$

In particular, $S_{n-1} \sim D(n, \lfloor n - 2\sqrt{n} - 1 \rfloor)$.

Proof. Let $G = P(0, n - i - 1, 0, 0, \dots)$ and $H = P(n - i - 1, 0, 0, \dots)$ be members of $\mathcal{G}_n$ and note that they are isomorphic to $D(n, i)$ and $D(n, i + 1)$, respectively. Indeed, it follows (by iteratively using Lemma 9 $n - i - 1$ times) that $G \sim H$. Hence, it is enough to verify that $0 + n - i - 1 \geq 2\sqrt{n}$. Indeed

$$n - i - 1 \geq n - \left\lfloor n - 2\sqrt{n} - 1 \right\rfloor - 1 = \left\lceil 2\sqrt{n} \right\rceil \geq 2\sqrt{n},$$

which concludes the proof of the claim. ■

Now recall the Lemma 7 and define a function $f : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ such that

$$\begin{aligned} f(n,b) &= \binom{b+1}{3} + \left[\binom{b+1}{2} - 1\right] \cdot (n-b) + (n-b)^2 \\ &= \frac{1}{2}b^2 n - \frac{1}{3}b^3 + \frac{1}{2}b^2 - \frac{3}{2}bn + \frac{5}{6}b + n^2 - n \,. \end{aligned}$$

Consider the following bound.

Lemma 11. *It holds that*

$$W\left(D\left(n, \lfloor n - 2\sqrt{n} - 1 \rfloor\right)\right) \geq \frac{1}{6}\, n^3 - 2\, n^2 - \frac{1}{3}\, n^{\frac{3}{2}} + \frac{35}{6}\, n + \frac{7}{3}\, \sqrt{n}.$$

Proof. Let $p \in (0,1]$ be a real number, such that $\lfloor n - 2\sqrt{n} - 1 \rfloor = n - 2\sqrt{n} - 2 + p$. By substituting b with $n - 2\sqrt{n} - 2 + p$ in $f(n,b)$, we get

$$\begin{aligned} f\,(n,b) &= \frac{1}{6}\, n^3 - 2\, n^2 + \left(2p - \frac{1}{3}\right) n^{\frac{3}{2}} + \left(\frac{53}{6} - \frac{1}{2}\, p^2 - \frac{5}{2}\, p\right) n \\ &\quad + \left(\frac{31}{3} + 2p^2 - 10p\right) \sqrt{n} + 3 - \frac{1}{3}\, p^3 + \frac{5}{2}\, p^2 - \frac{31}{6}\, p \\ &\geq \frac{1}{6}\, n^3 - 2\, n^2 - \frac{1}{3}\, n^{\frac{3}{2}} + \frac{35}{6}\, n + \frac{7}{3}\, \sqrt{n}, \end{aligned}$$

as claimed. ∎

We are now ready to state the main result.

Theorem 12. *Let $\left[\binom{n}{2}, a\right]$ be an interval of contiguous integers, such that $\left[\binom{n}{2}, a\right] \subseteq W\left[\mathcal{G}_n\right]$. Then*

$$a \;\geq\; \frac{1}{6}n^3 - \frac{5}{2}n^2 + O\left(n^{3/2}\right).$$

In particular, $\left|W_n^{\mathrm{int}}\right| = \frac{1}{6}n^3 + O\left(n^2\right)$.

Proof. We prove the theorem by considering both ends of the interval W_n^{int} separately.

First, consider the left end of the interval. By iteratively adding the edges to the star $S_{n-1} \simeq D(n,1)$, we can easily conclude that $S_{n-1} \sim K_n$. Since by Claim 4, $\binom{n}{2}$ is the minimum of $W\left[\mathcal{G}_n\right]$, we cannot improve the lower-bound of this interval any further.

Now, consider the right part of the interval. By Corollary 10, we have $S_{n-1} \sim D(n, \lfloor n - 2\sqrt{n} - 1 \rfloor)$, Let us now calculate the lower bound of $W\left(D(n, \lfloor n - 2\sqrt{n} - 1 \rfloor)\right)$. Using Lemmas 7 and 11, we have

$$W\left(D\left(n, \lfloor n - 2\sqrt{n} - 1 \rfloor\right)\right) \;\geq\; \frac{1}{6}\, n^3 - 2\, n^2 - \frac{1}{3}\, n^{\frac{3}{2}} + \frac{35}{6}\, n + \frac{7}{3}\, \sqrt{n}.$$

From this, we subtract the left-end of the interval, and obtain a lower-bound on the cardinality of W_n^{int}, i.e.

$$\begin{aligned} \left|W_n^{\text{int}}\right| &\geq \frac{1}{6}n^3 - 2n^2 - \frac{1}{3}n^{\frac{3}{2}} + \frac{35}{6}n + \frac{7}{3}\sqrt{n} - \binom{n}{2} \\ &= \frac{1}{6}n^3 - \frac{5}{2}n^2 - \frac{1}{3}n^{\frac{3}{2}} + \frac{19}{3}n + \frac{7}{3}\sqrt{n}, \end{aligned} \tag{2}$$

which concludes the proof of our theorem. ■

The following corollary clearly follows.

Corollary 13. *Let $W[\mathcal{G}_n]$ be an image of a Wiener index function on the set $\mathcal{G}_n$. Then*

$$|W[\mathcal{G}_n]| = \frac{1}{6}n^3 + O\left(n^2\right).$$

Let us also note that whenever $n \geq 25$ the lower bound from (2) is always greater than a half of our trivial upper-bound form Corollary 8, which also implies uniqueness of the observed interval for $n \geq 25$.

3 Concluding remarks and further work

From Example 5, we observed that $W[\mathcal{G}_4] = W_4^{\text{int}} = \left[\binom{4}{2}, \binom{5}{3}\right]$. Similarly, one can easily check that also for $n \leq 4$ it holds that $W[\mathcal{G}_n] = W_n^{\text{int}} = \left[\binom{n}{2}, \binom{n+1}{3}\right]$. When estimating the cardinality of W_n^{int}, one could improve the final result from (2) by precisely calculating the gap that we made with an inequality from (1). Also, one could improve the cardinality of $W[\mathcal{G}_n]$ by addressing the fact that the intervals of type $\left[W(D(n,i)) - \binom{n-i}{2}, W(D(n,i))\right] \in W[\mathcal{G}_n]$ are disjoint whenever $\left(a_1 + \frac{5}{2}\right)^2 + \left(a_2 - \frac{3}{2}\right)^2 < \frac{1}{2} + 2n$. We suspect that summing these would increase the lower bound of cardinality of $W[\mathcal{G}_n]$ by $O(n^2)$. These optimizations may imply the proof of uniqueness also for $n \leq 24$, which would imply that interval W_n^{int} is unique and starts at $\binom{n}{2}$, for all positive integers n.

The complementary question we are interested in is also the cardinality of $\left[\binom{n}{2}, \binom{n+1}{3}\right] \setminus W[\mathcal{G}_n]$. Notice, that the cardinality of $\left[\binom{n}{2}, \binom{n+1}{3}\right] \setminus W[\mathcal{G}_n]$ is at least linear, since the gap between the two graphs in $\mathcal{G}_n$ with highest Wiener index equals $n-4$ (for $n \geq 4$). We believe that the number of values $W[\mathcal{G}_n]$ misses is linear, hence the following conjecture.

Conjecture 14. *The cardinality of $W[\mathcal{G}_n]$ is of order $\frac{1}{6}n^3 - \frac{1}{2}n^2 + \Theta(n)$.*

Among other generalizations one could also answer similar questions on the family of all trees on n vertices. For a fixed n, we define $W[\mathcal{T}_n]$ to be the image of W under $\mathcal{T}_n$, i.e.

$$i \in W[\mathcal{T}_n] \Leftrightarrow \text{ there is a graph } G \in \mathcal{T}_n \text{ such that } W(G) = i.$$

We conjecture the following.

Conjecture 15. *The cardinality of* $W[\mathcal{T}_n]$ *equals* $\frac{1}{6}n^3 + \Theta(n^2)$.

Conjecture 16. *In the family of* $\mathcal{T}_n$*, the cardinality of* W_n^{int} *equals* $\Theta(n^3)$.

Acknowledgement: The authors would like to thank anonymous referees for fruitful comments and to J.-S. Sereni for careful reading that led to a simplification of Lemma 11. The second author was partially supported by ARRS Program P1-00383 and Creative Core–FISNM–3330-13-500033.

References

[1] Y. E. A. Ban, S. Bespamyatnikh, N. H. Mustafa, On a conjecture on Wiener indices in combinatorial chemistry, in: T. Warnow, B. Zhu (Eds.), *Computing and Combinatorics*, Springer, Berlin, 2003, pp. 509–518.

[2] J. Fink, B. Lužar, R. Škrekovski, Some remarks on inverse Wiener index problem, *Discr. Appl. Math.* **160** (2012) 1851–1858.

[3] C. M. da Fonseca, M. Ghebleh, A. Kanso, D. Stevanović, Counterexamples to a conjecture on Wiener index of common neighborhood graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 333–338.

[4] I. Gutman, T. Kortvelyesi, Wiener indices and molecular surfaces, *Z. Naturforsch.* **50a** (1995) 669–671.

[5] I. Gutman, Y. N. Yeh, The sum of all distances in bipartite graphs, *Math. Slovaca* **45** (1995) 327–334.

[6] K. Hrinakova, M. Knor, R. Škrekovski, A. Tepeh, A congruence relation for the Wiener index of graphs with a tree–like structure, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 791–806.

[7] M. Knor, B. Lužar, R. Škrekovski, I. Gutman, On Wiener index of common neighborhood graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 321–332.

[8] M. Knor, M. Mačaj, P. Potočnik, R. Škrekovski, Complete solution of equation $W(L^3(T)) = W(T)$ for the Wiener index of iterated line graphs of trees, *Discr. Appl. Math.* **171** (2014) 90–103.

[9] M. Knor, M. Mačaj, P. Potočnik, R. Škrekovski, Trees T satisfying $W(L^3(T) = W(T)$, *Filomat* **28** (2014) 551–556.

[10] M. Knor, R. Škrekovski, Wiener index of generalized 4-stars and of their quadratic line graphs, *Australas. J. Comb.* **58** (2014) 119–126.

[11] M. Lepović, I. Gutman, A collective property of trees and chemical trees, *J. Chem. Inf. Comput. Sci.* **38** (1998) 823–826.

[12] D. H. Rouvray, B. C. Crafford, The dependence of physical–chemical properties on topological factors, *South Africa J. Sci.* **72** (1976) 47–51.

[13] L. I. Stiel, G. Thodos, The normal boiling points and critical constants of saturated aliphatic hydrocarbons, *Am. Inst. Chem. Engin.* **8** (1962) 527–529.

[14] S. G. Wagner, A class of trees and its Wiener index, *Acta Appl. Math.* **91** (2006) 119–132.

[15] H. Wang, G. Yu, All but 49 numbers are Wiener indices of trees, *Acta Appl. Math.* **92** (2006) 15–20.

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

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

[18] K. Xu, M. Liu, K. C. Das, I. Gutman, B. Furtula, A survey on graphs extremal with respect to distance–based topological indices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 461–508.