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ODD–VERTEX–DEGREE TREES MAXIMIZING WIENER INDEX

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Abstract. Wiener index is the oldest and one among the most investigated topological indices in mathematical chemistry and in related disciplines. Recently, Wiener index of odd–vertex–degree (T^{odd}) trees has been investigated. In this paper, trees with second, third, ..., seventeenth maximal Wiener index are characterized.

1. Introduction

Wiener index is the oldest topological descriptor that found diverse applications in theoretical chemistry [21]. It was introduced in 1947 as a tool for predicting various physico–chemical properties, initially applied on small, simple, and acyclic organic molecules [22] [19] [20]. In the seminal paper [21], the Wiener index is calculated (but not defined!) as:

$$W(T) = \sum_{e \in E(T)} n_1(e) \cdot n_2(e) \tag{1.1}$$

where summation goes over all edges of a tree T. Here $n_1(e)$ and $n_2(e)$ are the numbers of vertices of the subgraphs obtained by deleting the edge e from T.

Until 1970s, this molecular descriptor had not received the deserved attention. However, in seventies of the last century, the Wiener index revived in theoretical (especially mathematical) chemistry as well as in mathematics. It should be mentioned, as an illustration, that in those days, mathematicians (not knowing anything about

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Dedicated to the memory of my father Dragiša Furtula (18th August 1950 – 18th April 2013).

Wiener index) introduced it again naming it as "*distance of a graph*" [4] or "*transmission*" [15]. Eq. (1.1) is valid only for trees. The formal definition of the Wiener index, which can be applied to all graphs, was given by Hosoya in [9]:

$$W(G) = \frac{1}{2} \sum_{u=1}^{n} \sum_{v=1}^{n} d(u,v) \tag{1.2}$$

where $d(u,v)$ is the distance between vertices u and v.

Nowadays, there is a legion of papers dealing with the Wiener index (e.g., see [1] [10] [23] [16] [13] [12] [18] [17] [7] and [6] as the most recent ones, and the references cited therein). It was demonstrated its usability also in other scientific areas such as biology, medicine, sociology, etc.

1.1. **Odd–vertex–degree graphs.** Quite recently, Lin [11] investigated extremal graphs with respect to the Wiener index among odd–vertex–degree graphs. The degree (d_v) of a vertex v of a graph is the number of edges incident to v. Then the definition of the odd–vertex–degree class of graphs is:

Definition 1.1. A graph G belongs to the odd–vertex–degree graphs ($\mathbb{O}_G$) if all degrees of vertices of G are odd numbers. Such a graph is denoted as G^{odd}. These graphs must have an even number of vertices.

In [11], the odd–vertex–degree tree (T^{odd}) with maximal Wiener index is characterized. It is shown in Fig. 1.

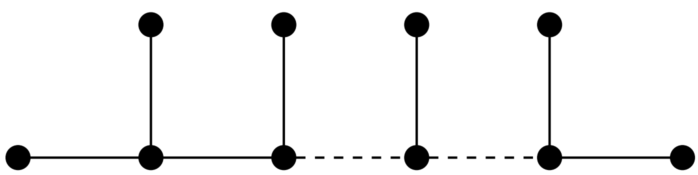

FIGURE 1. The odd–vertex–degree graph with maximal Wiener index.

This result can be anticipated since the tree depicted in Fig. 1 possesses the maximum diameter among all odd–vertex–degree trees (i.e., non-pendent vertices have the smallest possible degree). Following the same way of reasoning, odd–vertex–degree trees with second and third maximal Wiener, as well as trees with minimal, second, and third minimal Wiener index were conjectured [5]. In Fig. 2 are shown these trees.

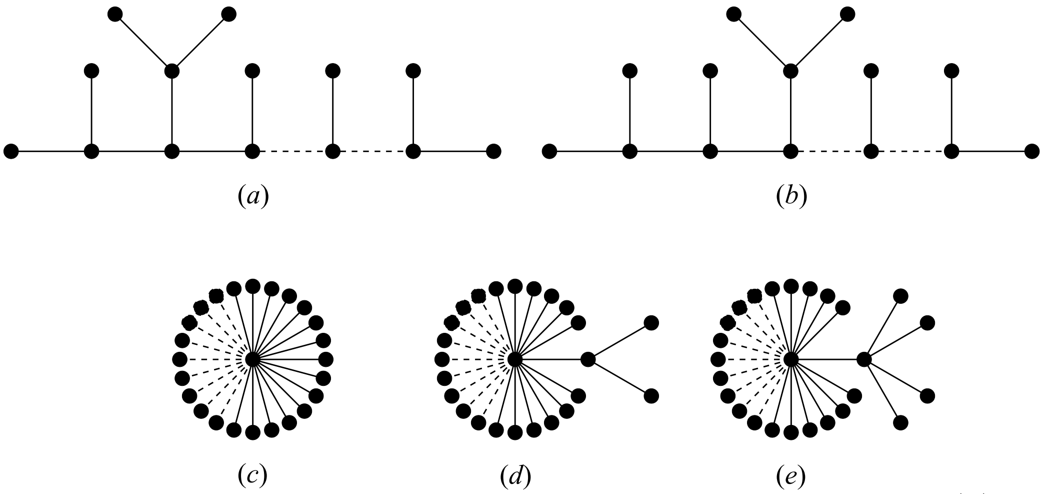

FIGURE 2. Odd–vertex–degree trees with second–maximal W (a), third–maximal W (b), minimal W (c), second–minimal W (d), and third–minimal W (e).

2. CHARACTERIZATION OF ODD–VERTEX–DEGREE TREES WITH SECOND AND THIRD MAXIMAL WIENER INDEX

One of the first mathematical results in graph theory was the following equality:

$$\sum_{d_u>0} n_u \cdot d_u = 2m \quad \text{for } d_u = 1, 2, 3, \ldots \tag{2.1}$$

where d_u and n_u is the degree of vertex u and the number of vertices having degree d_u, respectively. The number of edges of G is denoted by m. Recall that in the case of trees $m = n - 1$.

Let T^{odd} be a tree with n vertices belonging to the set of odd–vertex–degree trees $(\mathbb{O}_T)$. In a such tree, two types of vertices can be distinguished: pendent vertices whose number will be denoted with π, and so–called "inner" vertices whose number will be denoted by ι. Pendent vertices are those whose degree is equal to 1, while the "inner" vertices are those possessing degree greater than 1. It is obvious that

$$\pi + \iota = n \tag{2.2}$$

Using this way of classifying vertices, Eq. (1.1) can be rewritten as:

$$W(T) = (n-1) \cdot \pi + \sum_{e_\iota \in E(T)} n_1 \cdot n_2 \tag{2.3}$$

where π is the number of pendent vertices, and summation goes over all edges e_ι that connect "inner" vertices in a tree T.

Observe that the tree with maximal Wiener index in the set $\mathbb{O}_T$ contains only two types of vertices, pendent and vertices of degree equal to 3 (see Fig. 1). In general, if the degree of "inner" vertices in a tree T^{1,d_ι} is denoted by d_ι, then by combining Eqs. (2.1) and (2.2) it is obtained that $n = (d_\iota - 1)\iota + 2$. Using this equality, the Eq. (2.3) can be further simplified:

$$\begin{aligned} W(T^{1,d_\iota}) &= (n-1)\,\pi + \sum_{e_\iota} [(d_\iota - 1)\,\iota_1 + 1]\,[(d_\iota - 1)\,\iota_2 + 1] \\ &= (n-1)\,\pi + (n-1-\pi)\,(d_\iota - 1)\,\iota + (n-1-\pi) + (d_\iota - 1)^2 \sum_{e_\iota} \iota_1 \cdot \iota_2 \end{aligned}$$

After simple algebraic manipulation with help of Eqs. (2.1) and (2.2), the final equation is obtained

$$W(T^{1,d_\iota}) = (n-1)^2 + (d_\iota - 1)^2 \sum_{e_\iota} \iota_1 \cdot \iota_2 \tag{2.4}$$

where ι_1 and ι_2 are the numbers of "inner" vertices of subtrees obtained by deleting an edge e_ι. Summation goes over all edges that connect "inner" vertices.

For trees with given number of vertices and same degree for "inner" vertices, the value of the Wiener index depends only of the Wiener index of subtree constructed of only "inner" vertices, $W(T_\iota)$. So, Eq. (2.4) can be rewritten as:

$$W(T^{1,d_\iota}) = (n-1)^2 + (d_\iota - 1)^2\, W(T_\iota) \tag{2.5}$$

Eq. (2.5) tells that trees T^{1,d_ι} with given number of vertices are ordered by Wiener index in the same way as subtrees created from the "inner" vertices. This is in a full analogy with the result for the odd–vertex–degree tree with the maximal Wiener index. It is known that among all trees, the path has maximal Wiener index. From Fig. 1, it is obvious that the subtree created from the "inner" vertices is a path.

Applying previously known results on ordering trees by the greatest Wiener index [2] [14] (see Fig. 3) and taking into account that odd–vertex–degree trees that maximize Wiener index must have degree of the "inner" vertices as small as possible, it is evident that the conjecture given in [5] for trees with the second and the third maximal Wiener index for odd–vertex-degree trees is correct (see Fig. 2 (a) and (b)). In other words, odd–vertex–degree trees that have the second and the third maximal Wiener index must have subtrees made of "inner" vertices like those depicted in Fig. 3. Moreover, since in [2] [14] the first seventeen trees with greatest Wiener indices were characterized, it also can be applied to odd–vertex-degree trees. Therefore, this result characterizes the first seventeen odd-vertex–degree trees with greatest Wiener indices.

For odd–vertex–degree trees with the smallest, second and third smallest Wiener index the proof is not needed because the result published in [3] can be used to characterize these trees too.

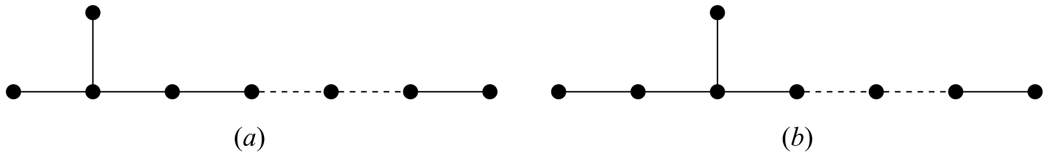

Figure 3. The tree with second maximal Wiener index (a). The tree with the third maximal Wiener index (b).

In addition, Eq. (2.5) gives the relation between so–called plerograms (Pl) and kenograms (Ke) which are different graph–representations of organic molecules.

$$W(Pl) = (n-1)^2 + 9\,W(Ke)$$

where n is the number of vertices of Pl. This relation was already published in [8].

Also, using Eq. (2.5), the nice recurrence equation for calculating the Wiener index of a path (P_n) can be obtained:

$$W(P_n) = (n-1)^2 + W(P_{n-2})$$

This equation is probably known, but the author of this text could not find any source that contains such or similar result.

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