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On terminal Wiener indices of kenograms and plerograms

I. GUTMAN[a], B. FURTULA[a], J. TOŠOVIĆ[a], M. ESSALIH[b] AND M. EL MARRAKI[b]

[a]*Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia*
[b]*LRIT Associated Unit to CNRST URAC n∘29, Faculty of Sciences, Mohammed V-Agdal University, PO Box 1014, Rabat, Morocco*

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ABSTRACT

Whereas there is an exact linear relation between the Wiener indices of kenograms and plerograms of isomeric alkanes, the respective terminal Wiener indices exhibit a completely different behavior: Correlation between terminal Wiener indices of kenograms and plerograms is absent, but other regularities can be envisaged. In this article, we analyze the basic properties of terminal Wiener indices of kenograms and plerograms.

Keywords: Wiener index, kenogram, plerogram.

1. INTRODUCTION

In his pioneering paper [1], Arthur Cayley conceived the concept of molecular graphs. He introduced two types of such graphs, naming them "*kenograms*" and "*plerograms*". (It is worth noting that in the 1870s, when Cayley wrote his article [1], the word "graph" was still not in use in the mathematical literature.) According to Cayley, if every atom in a molecule is represented by a vertex, then we get a "plerogram". If, as usual, we disregard hydrogen atoms, then the respective mathematical representation of a molecule is called "kenogram". As well known, in the later development of chemical graph theory, the molecular graphs considered are almost exclusively kenograms, and when saying "molecular graph" this fact is usually tacitly understood. In order to avoid any misunderstanding, in Fig. 1 is depicted the plerogram and the kenogram of 2,4,4,6-tetramethylheptane.

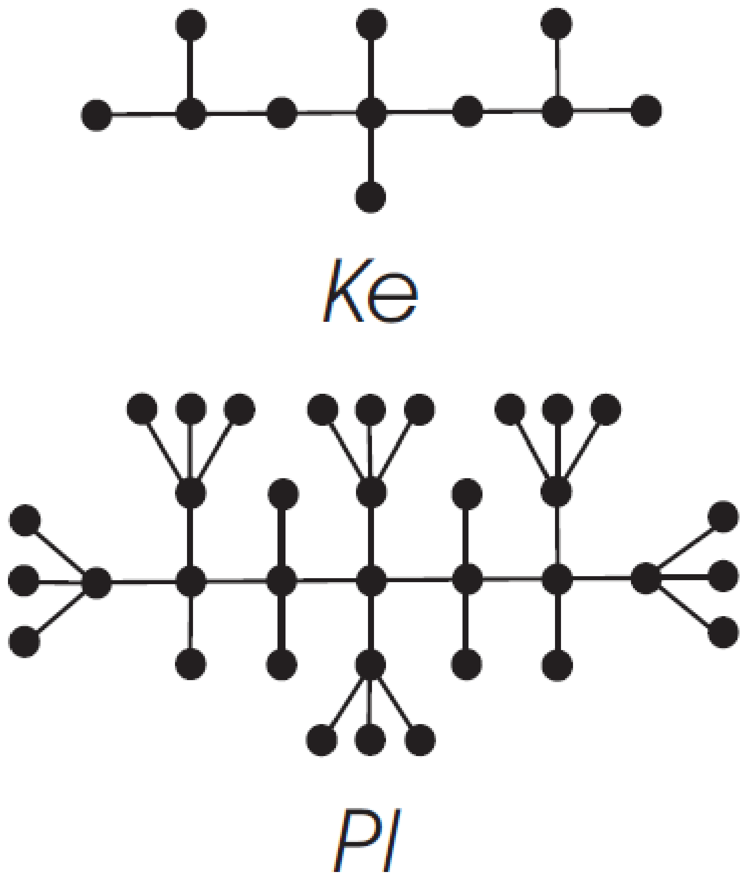

Fig. 1. The kenogram (*Ke*) and the plerogram (*Pl*) of 2,4,4,6-tetramethylheptane.

In [8], a remarkable regularity was discovered. Namely, the Wiener indices of plerograms and kenograms of alkanes are mutually linearly related as shown in Fig. 2.

In the case of isomeric alkanes of formula C_nH_{2n+2} , the relation between the two Wiener indices reads [8]:

$$W(Pl) = 9W(Ke) + 9n^2 + 6n + 1. \tag{1}$$

Recall that the Wiener index $W(G)$ of a connected graph G is equal to the sum of distances between all pairs of vertices of G. More formally,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v). \tag{2}$$

where $V(G)$ is the vertex set of the graph G and $d_G(u,v)$ denotes the distance of the vertices u and v (= number of edges in a shortest path connecting u and v). Details on the Wiener index can be found in the reviews [2, 3, 9, 10, 12].

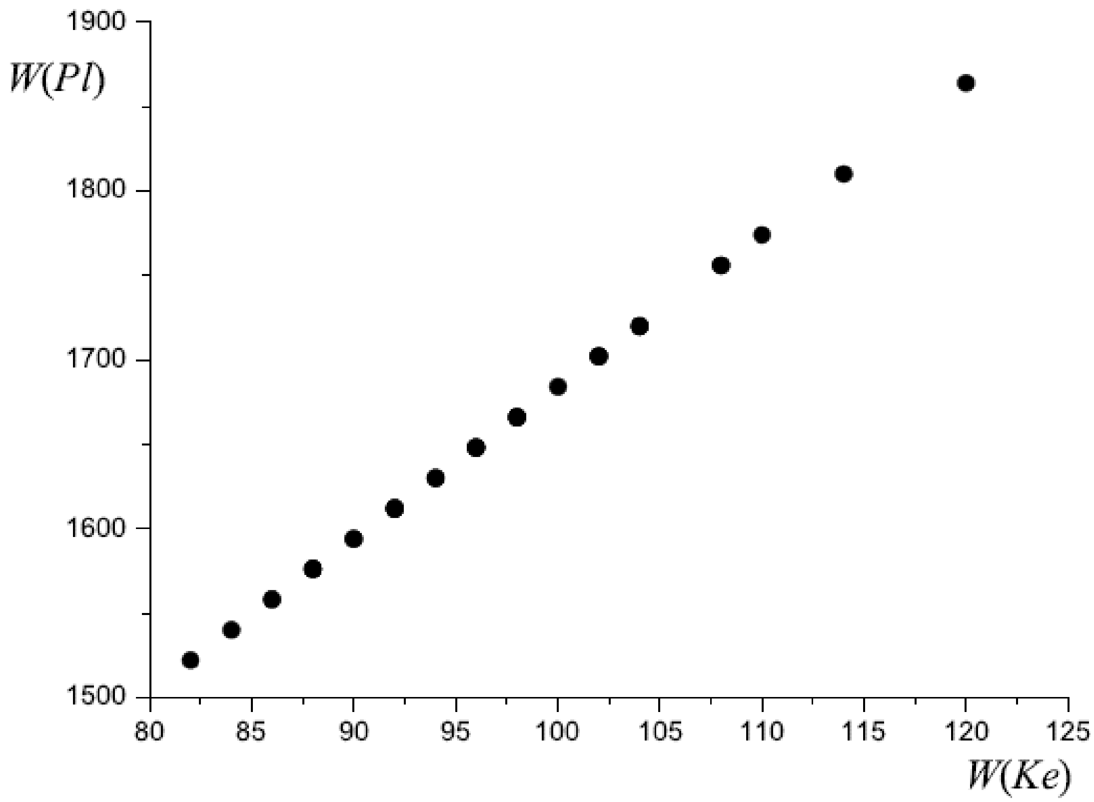

Fig. 2. The (exact) linear relation between the Wiener indices of plerograms and kenograms in the case of isomeric nonanes ($n = 9$), cf. Eq. (1).

In this paper we are considering the so-called terminal Wiener index, defined as the sum of distance between all pairs of pendent vertices of the graph G. (A vertex is said to be pendent if its degree is unity, i.e., if it has just a single neighbor.) The motivation for the introduction of the terminal Wiener index was a theorem by Zaretskii [13], according to which any tree is fully determined by the distances between its pendent vertices.

The concept of terminal Wiener index was put forward by Petrović and two of the present authors [7]. Somewhat later, but independently, Székely, Wang, and Wu arrived at the same idea [11]. Let $V_1(G) \subset V(G)$ be the set of pendent vertices of the graph G. Then TW is defined in full analogy with the Wiener index, Eq. (2), as

$$TW(G) = \sum_{\{u,v\} \subseteq V_1(G)} d_G(u,v). \tag{3}$$

For review on terminal Wiener index see [6, 12].

According to Eq. (3), if the graph G has no pendent vertex, or just one such vertex, then $TW(G) = 0$. The application of this molecular structure descriptor is purposeful only for graphs with many pendent vertices, especially for trees.

If T is a tree, then its terminal Wiener index can be calculated by means of the formula [7]

$$TW(T) = \sum_e p_1(e|T)\, p_2(e|T) \tag{4}$$

where $p_1(e|T)$ and $p_2(e|T)$ are the number of pendent vertices of T, lying on the two sides of the edge e. Summation in (4) goes over all edges of the tree T. Recall that if the tree T possesses a total of p pendent vertices, then for for any edge e,

$$p_1(e\,|T) + p_2(e\,|T) = p.$$

The terminal Wiener index may be viewed as a simplified version of the ordinary Wiener index. Indeed, in the case of trees and chemical trees, there exists a reasonably good correlation between W and TW, as seen from the example shown in Fig. 3.

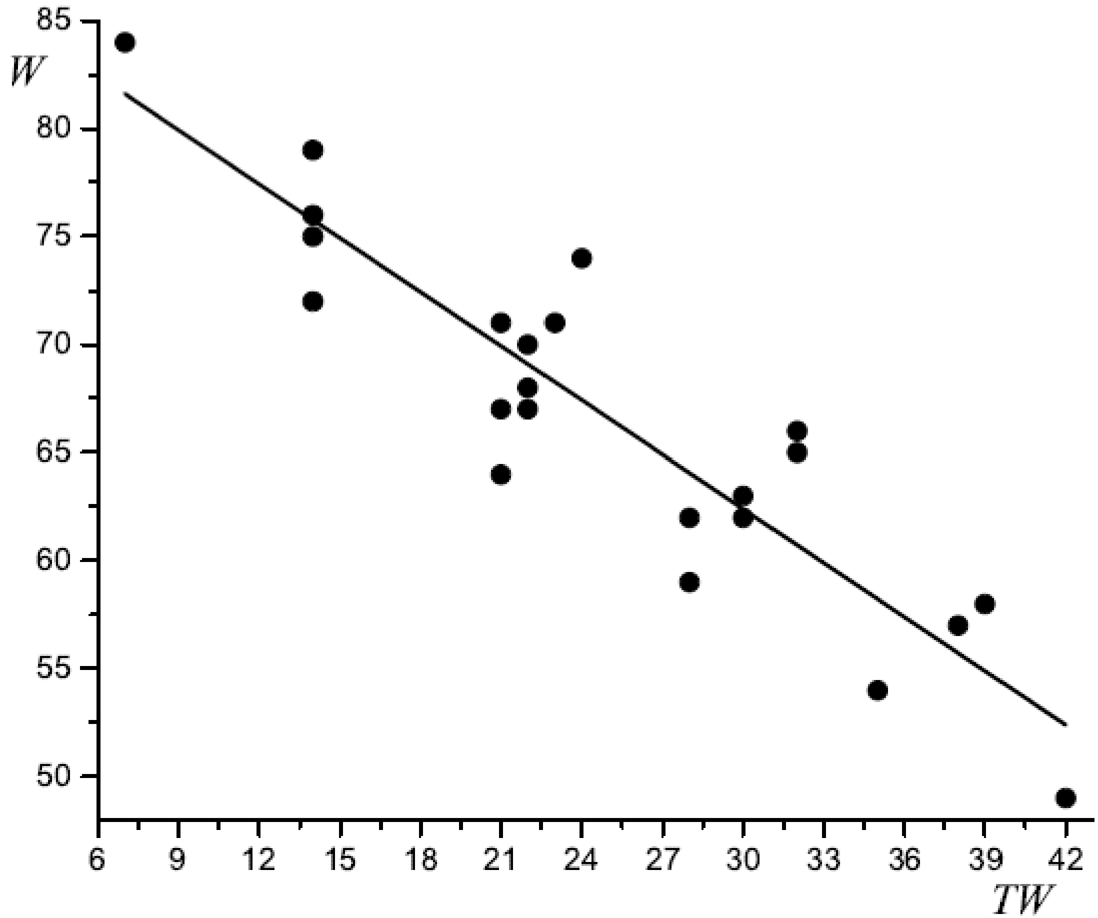

Fig. 3. Correlation between Wiener index (W) and terminal Wiener index (TW) of trees of order 8. Correlation coefficient: -0.91.

At this point we mention that recently it was shown [5] that, in addition to Eq. (1), also the terminal Wiener index of a plerogram linearly depends on the Wiener index of the kenogram:

$$TW(Pl) = 4W(Ke) + 6n^2 + 5n + 1 \,. \tag{5}$$

In view of the linear correlation between W and TW (cf. Fig. 3), and the exact linear relations between $W(Pl)$ and $W(Ke)$ as well as between $TW(Pl)$ and $W(Ke)$ (cf. Eqs. (1) and (5)), one would expect that also $TW(Pl)$ and $TW(Ke)$ are linearly (or, at least, somehow) correlated. Surprisingly, however, this is not the case, as seen from the example shown in Fig. 4.

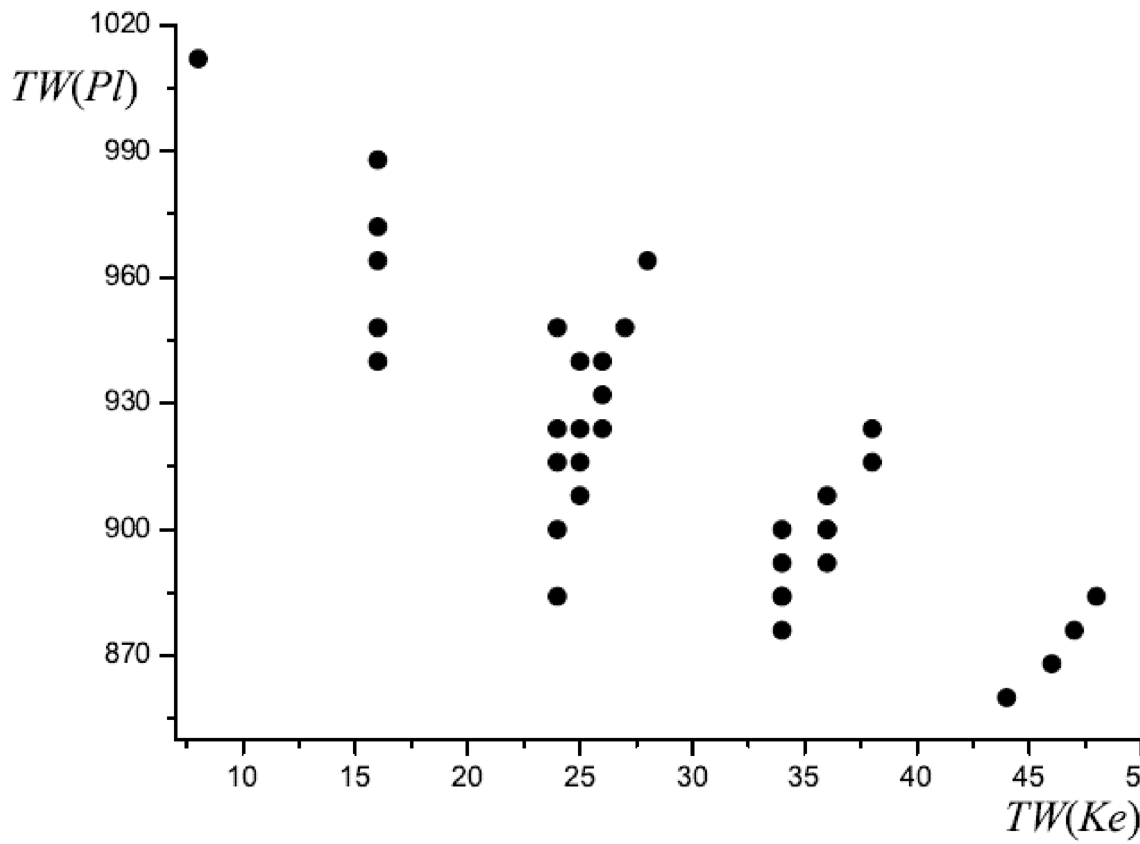

Fig. 4. The terminal Wiener indices of the plerograms of isomeric nonanes (n = 9) plotted versus the terminal Wiener indices of the respective kenograms. The five disjoint groups of data points pertain to p = 2*;* 3*;* 4*;* 5*;* 6 (from left to right). How much the behavior of terminal Wiener indices differ from that of Wiener indices is evident by comparing Figs. 2 and 4.

The peculiar form of the relation between $TW(Pl)$ and $TW(Ke)$ calls for explanation. Our results obtained along these lines are presented in the subsequent sections.

In what follows, for the sake of simplicity we shall say that an edge of a tree T is of (p_1, p_2)-type, if on its two sides there are p_1 and p_2 pendent vertices.

2. ON STRUCTURE–DEPENDENCY OF *TW*(*Ke*)

In what follows, the kenogram *Ke* is assumed to possess *n* vertices, i.e., that it represents an alkane C_nH_{2n+2} with *n* carbon atoms. The corresponding plerogram *Pl* has thus $3n+2$ vertices, of which $2n + 2$ are pendent.

The kenogram *Ke* with *n* vertices has $n-1$ edges. Its number of pendent vertices will be denoted by *p*.

The first detail that is noticed by inspecting Fig. 4 (as well as the other analogous plots for $n \neq 9$) is that the data–points are grouped into several disjoint clusters. It was not difficult to recognize that each of these clusters is determined by a particular value of *p*.

Indeed, there exists a unique *n*-vertex kenogram with $p = 2$, namely the path (= kenogram of the normal alkane). It corresponds to the single data–point on the most left–hand side of Fig. 4. Since all edges of this kenogram are of (1,1)-type,

$$TW(Ke) = n - 1 \text{ for the unique kenogram with } p = 2,\ n \geq 2\ . \tag{6}$$

If $p = 3$, then each edge of *Ke* is of (1,2)-type. Therefore, each summand on the right–hand side of Eq. (4) is equal to $1 \times 2 = 2$, resulting in $TW(Ke) = 2(n - 1)$, i.e.,

$$TW(Ke) = 2n - 2 \text{ for all kenograms with } p = 3,\ n \geq 4\ . \tag{7}$$

Eq. (7) means that the kenograms of all isomeric alkanes with a single tertiary carbon atom and no quaternary carbon atom have equal terminal Wiener indices, whereas the *TW*-values of their plerograms differ. Consequently, the data–points in the second left–hand side cluster lie on a single vertical line.

If $p = 4$, then the edges of *Ke* are either of (1,3)– or of (2,2)-type. At least 4 of these edges must be of (1,3)-type. Each summand on the right–hand side of Eq. (4) is equal to either $1 \times 3 = 3$ or $2 \times 2 = 4$, implying $3(n - 1) \leq TW(Ke) \leq 3 \cdot 4 + 4(n - 5)$, i.e.,

$$3n - 3 \leq TW(Ke) \leq 4n - 8 \text{ if } p = 4,\ n \geq 5\ . \tag{8}$$

If $p = 5$, then the edges of *Ke* are either of (1,4)– or of (2,3)-type. At least 5 of these edges must be of (1,4)-type and at least one must be of (2,3)-type. Each summand on the right–hand side of Eq. (4) is equal to either $1 \times 4 = 4$ or $2 \times 3 = 6$, implying $4(n - 2) + 6 \leq TW(Ke) \leq 4 \cdot 5 + 6(n - 6)$, i.e.,

$$4n - 2 \leq TW(Ke) \leq 6n - 16 \text{ if } p = 5,\ n \geq 7\ . \tag{9}$$

In an analogous manner we obtain:

$$5n - 1 \leq TW(Ke) \leq 9n - 33 \text{ if } p = 6,\ n \geq 8 \tag{10}$$

$$6n + 6 \leq TW(Ke) \leq 12n - 54 \text{ if } p = 7,\, n \geq 10\,. \tag{11}$$

Eqs. (6)–(11) imply that the clusters of data–points for $p = 2;\ 3;\ 4$ are disjoint for all values of n. On the other hand, for n being sufficiently large, the data–points for $p \geq 5$ overlap. In particular, for $n = 15$ there exist kenograms with $p = 5$ and $p = 6$, having equal TW-values. For $n > 15$ some kenograms with $p = 5$ have greater terminal Wiener indices than some kenograms with $p = 6$. For $n = 13$ there exist kenograms with $p = 6$ and $p = 7$, having equal TW-values. For $n > 13$ some kenograms with $p = 6$ have greater terminal Wiener indices than some kenograms with $p = 7$. Examples are depicted in Figs. 5 and 6.

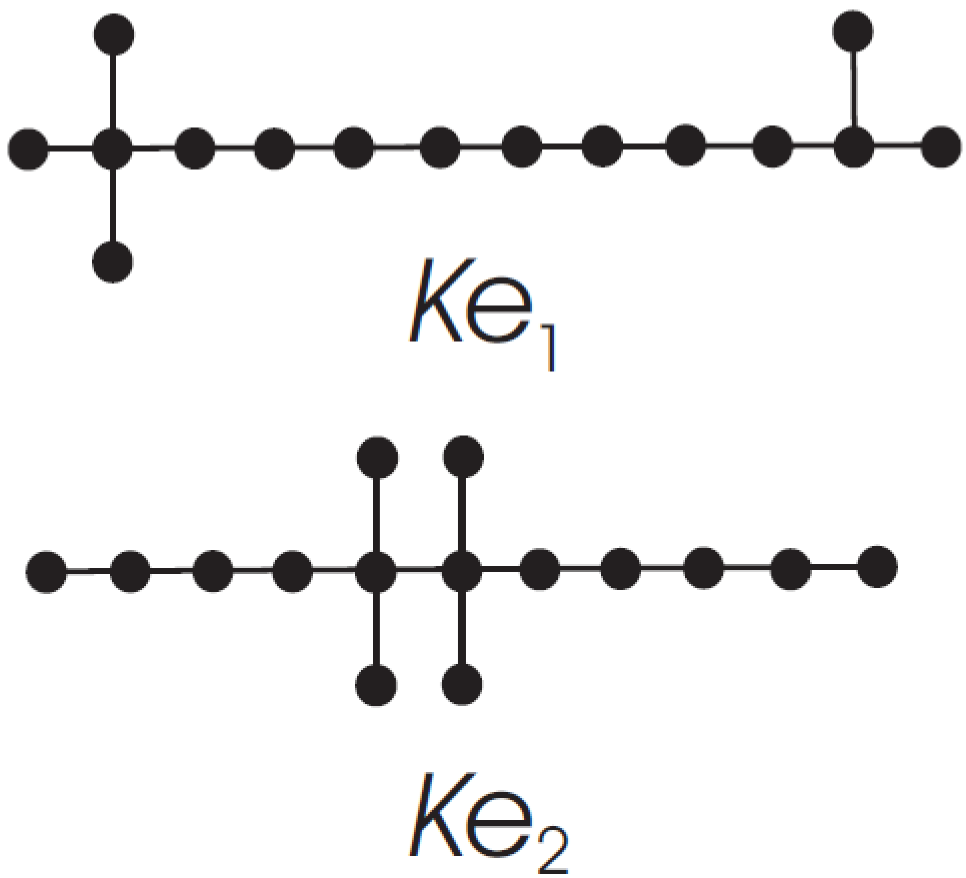

Fig. 5. Two kenograms of order 15 with different number of pendent vertices, but equal terminal Wiener indices: $p(Ke_1) = 5$, $p(Ke_2) = 6$, $TW(Ke_1) = TW(Ke_2) = 74$.

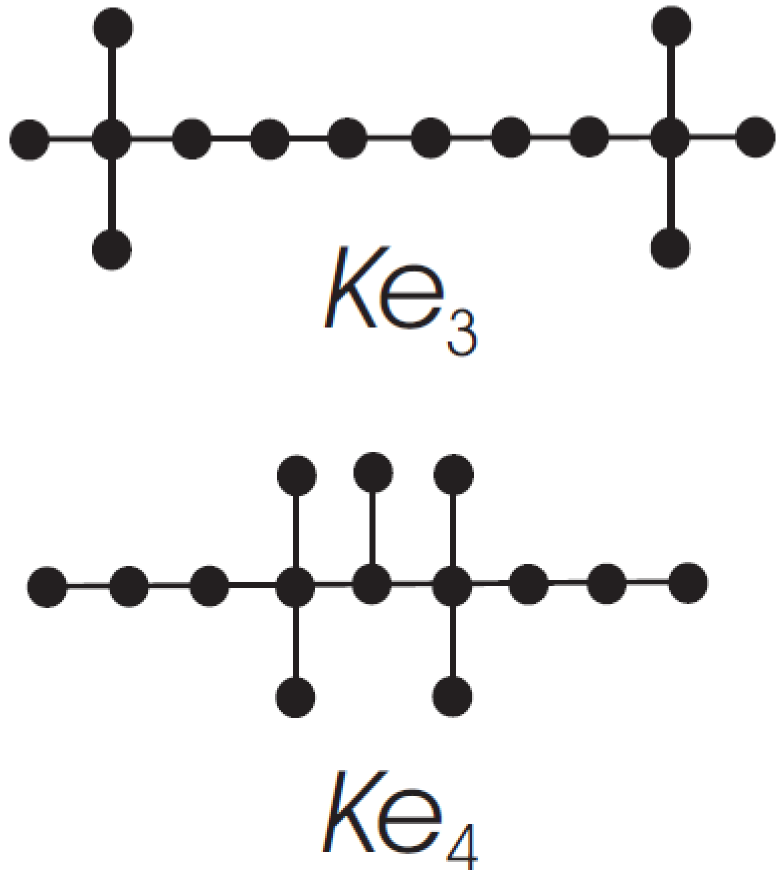

Fig. 6. Two kenograms of order 14 where the species with smaller number of pendent vertices has greater terminal Wiener index: $p(Ke_3) = 6$, $p(Ke_4) = 7$, $TW(Ke_3) = 93$, $TW(Ke_4) = 90$.

The analysis of the cases $p \geq 8$ is analogous, yet somewhat more complicated.

Whereas in the case $p = 3$, all data–points lie on a single vertical line, if $p \geq 4$, from Fig. 4 we see that there exist several such vertical lines. This is caused by the fact that there are only a few possible distributions of (p_1, p_2)-edge types. The following theorem shows what happens when the (p_1, p_2)-type of just one edge is changed.

Theorem 2.1. Let Ke be a kenogram possessing p pendent vertices, whose relevant structural details are indicated in Fig. 7. Perform the transformation $Ke \rightarrow Ke'$ as indicated *in* Fig. 7. Let the edge uv of Ke be of $(q, p - q)$-type. Then

$$TW(Ke') - TW(Ke) = q(p - q) - (p - 1) \,. \tag{12}$$

If $q = 1$, then we have the trivial case $TW(Ke') = TW(Ke)$, whereas if $q \geq 2$, then $TW(Ke') > TE(Ke)$.

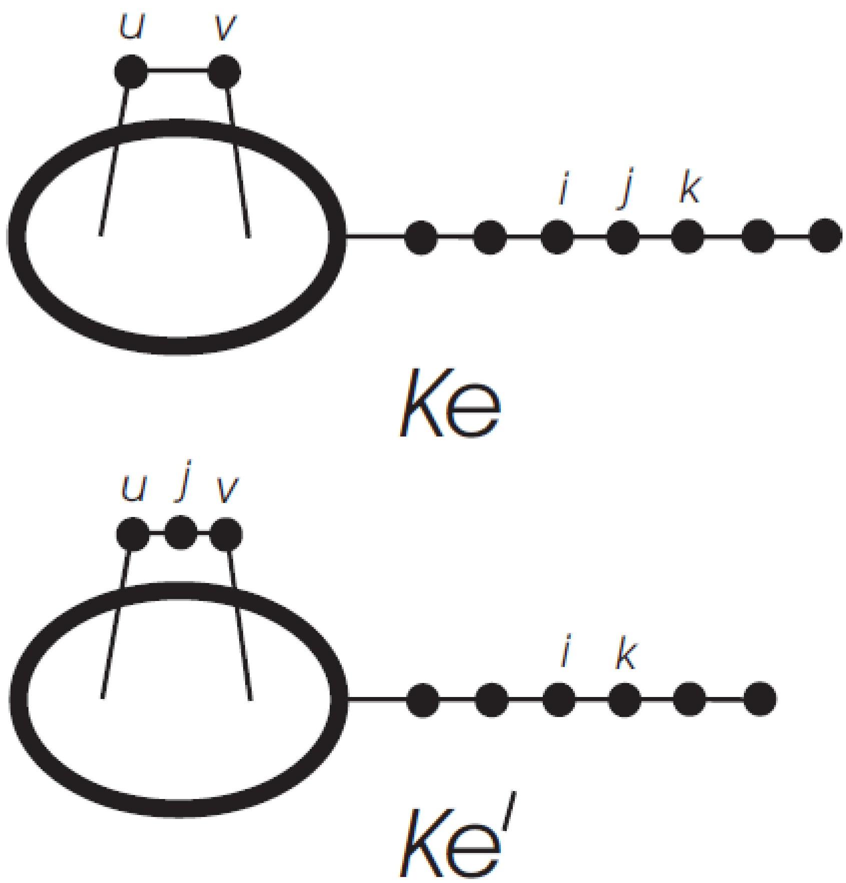

Fig. 7. The kenograms playing role in Theorem 2.1 and the labeling of their relevant structural details.

Proof. In the kenogram *Ke* the edges *uv*, *ij*, and *jk* are of types $(q, p-q)$, $(1, p-1)$, and $(1, p-1)$, respectively. In the kenogram *Ke′* the edges *uj*, *jv*, and *ik* are of types $(q, p-q)$, $(q, p-q)$, and $(1, p-1)$, respectively. Therefore, by Eq. (4),

$$TW(Ke) = q(p-q) + (p-1) + (p-1) + \text{terms same for both } Ke \text{ and } Ke'$$
$$TW(Ke') = q(p-q) + q(p-q) + (p-1) + \text{terms same for both } Ke \text{ and } Ke'$$

from which Eq. (12) follows straightforwardly. □

The below special cases of Theorem 2.1 are worth particular attention.

Corollary 2.1.
(*a*) If $p = 4$, then because $q \le \lfloor p=2 \rfloor = 2$, it must be $q = 2$ and therefore $TW(Ke') - TW(Ke) = 1$.
(*b*) If $p = 5$, then because $q \le \lfloor p=2 \rfloor = 2$, it must be $q = 2$ and therefore $TW(Ke') -$

$TW(Ke) = 2$.

(*c*) If $p = 6$, then either $q = 2$ *or* $q = 3$, resulting in either $TW(Ke') - TW(Ke) = 3$ or $TW(Ke') - TW(Ke) = 4$.

From Fig. 4 we see that the distance between the vertical lines in the $p = 4$ cluster is unity, whereas this distance in the $p = 5$ cluster is two. Corollary 2.1 provides an explanation of these facts. The separation between the vertical lines in the clusters with $p \geq 6$ can be rationalized analogously, but the situation there is somewhat more complicated.

3. ON STRUCTURE–DEPENDENCY OF *TW*(*Pl*)

The dependency of the terminal Wiener index of plerograms on molecular structure appears to be much more complex than in the case of kenograms. In order to gain some information on this dependency, we have analyzed in detail the case $p = 3$. This, of course, is the simplest non-trivial case, in which (as explained in the preceding section), all kenograms have the same *TW*-value.

Denote by $Ke(a_1, a_2, a_3)$ the kenogram with n vertices, having exactly one vertex of degree 3, to which branches with a_1, a_2, and a_3 vertices are attached. Thus, $a_1 + a_2 + a_3 + 1 = n$. By convention, $a_1 \leq a_2 \leq a_3$. The plerogram corresponding to $Ke(a_1, a_2, a_3)$ will be denoted by $Pl(a_1, a_2, a_3)$.

The plerogram $Pl(a_1, a_2, a_3)$ has $p^* = 2n + 2$ pendent vertices. Bearing in mind that therefore it has $p*$ edges of $(1, p^* - 1)$-type, by applying Eq. (4), we get

$$
\begin{aligned}
TW(pl(a_1, a_2, a_3)) &= p^*[(p^* - 1) \times 1] + \sum_{k=1}^{3} \sum_{i=1}^{a_k} (2i+1)[p^* - (2i+1)] \\
&= (2n+2)(2n+1) + \sum_{k=1}^{3} \sum_{i=1}^{a_k} (2i+1)(2n-2i+1).
\end{aligned}
$$

A lengthy calculation leads then to:

$$
TW(Pl(a_1, a_2, a_3)) = 2(n-1) \sum_{k=1}^{3} a_k^2 - \frac{4}{3} \sum_{k=1}^{3} a_k^3 + 8n^2 + \frac{7}{3} n + \frac{5}{3}. \tag{13}
$$

Thus, the actual value of the terminal Wiener index of this plerogram depends on the length of the three branches, namely on the parameters a_1, a_2, and a_3.

From Eq. (13) it is not immediately seen which choice of the parameters a_1, a_2, a_3 corresponds to the greatest and which to the smallest *TW*-values. Nevertheless, we established the following:

Theorem 3.1. Let $n \geq 4$, $a_1 + a_2 + a_3 = n-1$ and $a_1 \leq a_2 \leq a_3$. Among the plerograms $Pl(a_1, a_2, a_3)$, the greatest terminal Wiener index is achieved for $a_1 = a_2 = 1$,$a_3 = n-3$, whereas the smallest if $a_3 - a_1 \leq 1$.

The ordering of plerograms $Pl(a_1, a_2, a_3)$ between the above specified extremal values was found to follow a complicated pattern that depends on the actual value of n.

4. APPENDIX: A GENERALIZATION

Because of chemical reasons, kenograms of alkanes are trees whose maximal vertex degree is at most 4. Therefore, plerograms are trees whose all vertices have degrees 1 or 4. The results obtained earlier [5, 8] for the Wiener and terminal Wiener indices of kenograms and plerograms, namely Eqs. (1) and (5), can be generalized in the following manner (see also [4]).

Let T be an n-vertex tree with maximal vertex degree Δ. Let R be an integer, such that $R \geq \Delta$. Let $v_1, v_2, \ldots, v_n$ be the vertices of T and let the degree of v_i be d_i , $i = 1, 2, \ldots, n$. Construct the tree T^* by attaching $R - d_i$ pendent vertices to the vertex v_i and doing this for all $i = 1, 2, \ldots, n$.

Theorem 4.1. The Wiener indices of the trees $T*$ and T are related as

$$W(T^*) = (R-1)^2 W(T) + (R-1)^2 n^2 + 2(R-1)n + 1. \tag{14}$$

The terminal Wiener index of T^* is related with the Wiener index of T as

$$TW(T^*) = (R-2)^2 W(T) + (R-2)(R-1)n^2 + (2R-3)n + 1. \tag{15}$$

Remark 4.1. If $R = 4$, then the tree T may be viewed as a kenogram, in which case T^* would be the corresponding plerogram. Eq. (1) is the special case of Eq. (14) for $R = 4$. Eq. (5) is the special case of Eq. (15) for $R = 4$.

Proof. The tree T^* consists of pendent vertices and vertices of degree R. The number of vertices of degree R is n. The number of pendent vertices is

$$p(T^*) = \sum_{i=1}^{n} (R - d_i) = nR - \sum_{i=1}^{n} d_i = nR - 2(n-1) = (R-2)n + 2.$$

Therefore $T*$ has a total of $n(T^*) = (R-1)n + 2$ vertices.

The Wiener index of a tree T can be computed by means of the formula [2, 9]

$$W(T) = \sum_e n_1(e|T)\, n_2(e|T) \tag{16}$$

where $n_1(e|T)$ and $n_2(e|T)$ are the number of vertices of T, lying on the two sides of the edge e. Summation in (16) goes over all edges of the tree T. For any edge e,

$$n_1(e|T) + n_2(e|T) = n\ . \tag{17}$$

When applying formula (16) to the tree T^*, we need to take into account the it has $p(T^*)$ edges incident to a pendent vertex, each contributing to $W(T^*)$ by $1\times[n(T^*)-1]$. If e is an edge connecting two vertices of degree R, then its contribution to $W(T^*)$ is $[(R-1)\, n_1(e|T) + 1][(R-1)\, n_2(e|T) + 1]$. Then

$$W(T^*) = p(T^*)[n(T^*)-1] + \sum_e [(R-1)n_1(e|T)+1][(R-1)n_2(e|T)+1]$$

which, by bearing in mind relation (17) and the fact that the summation in the above expression goes over $n-1$ edges e, results in Eq. (14).

For the terminal Wiener index of T^* we have to apply Eq. (4). Using an analogous reasoning as for $W(T^*)$ we get

$$TW(T^*) = p(T^*)[p(T^*)-1] + \sum_e [(R-2)\, n_1(e|T)+1][(R-2)n_2(e|T)+1]$$

which then straightforwardly yields Eq. (15). □

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