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ON THE TERMINAL WIENER INDEX AND ZAGREB INDICES OF KRAGUJEVAC TREES

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Abstract: In this paper we find the extremal values of the terminal Wiener index, Zagreb indices and Zagreb coindices of Kragujevac trees. Further, we find the terminal Wiener index of line graphs of Kragujevac trees.

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1. Introduction

Let $G = (V, E)$ be a graph. The number of vertices of G we denote by n and the

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number of edges we denote by m, thus $|V(G)| = n$ and $|E(G)| = m$. The degree of a vertex v, denoted by $deg_G(v)$. If $deg_G(v) = 1$ then v is called a pendent vertex. An edge $e = uv$ of a graph G is called a pendent edge if $deg_G(u) = 1$ or $deg_G(v) = 1$. The distance between the vertices v_i and v_j, $v_i, v_j \in V(G)$, is equal to the length (= number of edges) of the shortest path starting at v_i and ending at v_j (or vice versa) and will be denoted by $d(v_i, v_j \setminus G)$. The line graph $L(G)$ of a graph is the graph derived from G in such a way that the edges in G are replaced by vertices in $L(G)$ and two vertices in $L(G)$ are connected whenever the corresponding edges in G are adjacent [16].

The oldest molecular structure is the one put forward in 1947 by H. Wiener [34], nowadays referred to as the Wiener index and denoted by W. It is defined as the sum of distance between all pairs of vertices of a graph.

$$W(G) = \sum_{\{u,v \subseteq V(G)\}} d(u, v \setminus G) = \sum_{1 \leq i < j \leq n} d(u, v \setminus G) \tag{1}$$

For details on its chemical applications and mathematical properties one may refer to [7, 8, 9, 12, 22, 28] and the references cited therein.

If G has k-pendent vertices labeled by $v_1, v_2 \cdots v_k$, then its terminal distance matrix is the square matrix of order k whose (i, j)-th entry is $d(v_i, v_j \setminus G)$. Terminal distance matrices were used for modeling amino acid sequences of proteins and of the genetic code [18, 26, 27].

The terminal Wiener index $TW(G)$ of a connected graph G is defined as the sum of the distances between all pairs of its pendent vertices.
Thus if $V_T = \{v_1, v_2, \cdots , v_k\}$ is the set of all pendent vertices of G, then

$$TW(G) = \sum_{\{u,v \subseteq V_T(G)\}} d(u, v \setminus G) = \sum_{1 \leq i < j \leq k} d(u, v \setminus G) \tag{2}$$

This distancebased molecular structure descriptor was recently put forward by Gutman et.al.,[11]. For more details on terminal wiener index refer to [17, 18, 25, 35].

The Zagreb indices were first introduced by Gutman and Trinajstić [13]. They are important molecular descriptors and have been closely correlated with many chemical properties[29]. There was a vast research concerning the mathematical properties and bounds for Zagreb indices and their various variants [3, 5, 6, 15, 19, 21, 23, 24, 30, 31, 32, 33, 36].

$$M_1(G) = \sum_{u \in V(G)} deg_G(u)^2 \qquad \text{and} \tag{3}$$

$$M_2(G) \quad = \sum_{uv \in E(G)} deg_G(u)\, deg_G(v). \tag{4}$$

Noticing that contribution of nonadjacent vertex pairs should be taken into account when computing the weighted Wiener polynomials of certain composite graphs (see [7]) defined first Zagreb coindex and second Zagreb coindex as

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} \left[deg_G(u) + deg_G(v)\right] \tag{5}$$

and $$\overline{M_2}(G) = \sum_{uv \notin E(G)} deg_G(u)\, deg_G(v). \tag{6}$$

For more information on Zagreb coindices see [1, 2].

Kragujevac trees

The formal definition of a Kragujevac tree was introduced in [10].

Definition 1. [10] Let P_3 be the 3-vertex tree, rooted at one of its terminal vertices. For $k = 2, 3, \cdots$, construct the rooted tree B_k by identifying the roots of k copies of P_3. The vertex obtained by identifying the roots P_3-trees is the root of B_k.

Examples illustrating the structure of the rooted tree B_k are depicted in Figure 1.

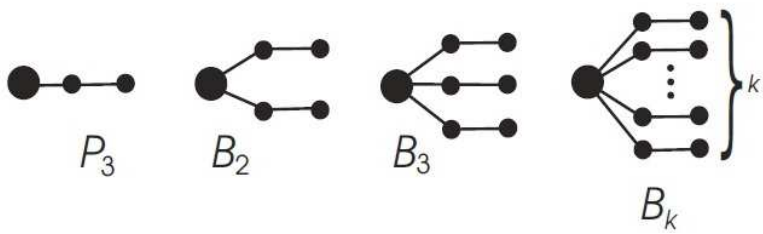

Figure 1

Definition 2. [10] Let $d \geq 2$ be an integer. Let $\beta_1, \beta_2, \cdots, \beta_d$ be rooted trees specified in Definition 1, i. e., $\beta_1, \beta_2, \cdots, \beta_d \in \{B_2, B_3, \cdots\}$. A Kragujevac tree T is a tree possessing a vertex of degree d, adjacent to the roots of $\beta_1, \beta_2, \cdots, \beta_d$. This vertex is said to be the central vertex of T, whereas d is the degree of T. The subgraphs $\beta_1, \beta_2, \cdots, \beta_d$ are the branches of T. Recall that some (or all) branches of T may be mutually isomorphic.

A typical Kragujevac tree is depicted in Figure 2.

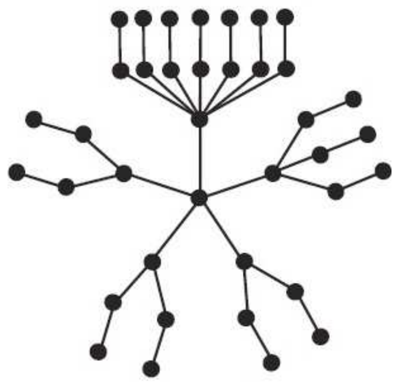

Figure 2

Recent information on Kragujevac trees can be found in [4].

2. Terminal Wiener Index of Kragujevac Trees

By the definition 1, the branch B_{k_i} contains k_i pendant vertices and the vertex set of $B_{k_i} = 2k_i + 1$.

Theorem 1. *Let T be the Kragujevac tree of degree $d \geq 2$ with branches B_{k_i}, $i = 1, 2, \cdots$, then*

$$TW(T) = 4\sum_{i=1}^{n} \frac{k_i(k_i-1)}{2} + 6\sum_{1\leq i<j\leq n} k_ik_j \tag{7}$$

Proof. By the definition of Kragujevac tree of degree $d \geq 2$ contains branches B_{k_i}, $i = 1, 2, \cdots$. Consider first the branch B_{k_i} which contains k_i pendant vertices. Each of these are at distance 4, and therefore their contribution to $TW(T)$ is $\frac{k_i(k_i-1)}{2} \times 4$. This lead to the first term on the right-hand side of (3).

Consider the branches B_{k_i} and B_{k_j}, $i \neq j$ with k_i and k_j pendant vertices. Each of these are at distance 6. Since there are $k_j \times k_j$ pairs of pendant vertices of this kind, their contribution to $TW(T)$ is equal to $6k_ik_j$. This leads to the second term on the right-hand side of (3). □

Before going to prove our next results, we have the following observations.

Observation 2. *The order and size of the Kragujevac tree are $n = 1 + \sum_{i=1}^{d}(2k_i + 1)$ and $m = \sum_{i=1}^{d}(2k_i + 1)$ respectively.*

Observation 3. *Let $e = uv$ be an edge of Kragujevac tree such that $deg_T(u) = 1$ and $deg_T(v) = 2$. Then $deg_{L(T)}(e) = deg_T(u) + deg_T(v) - 2 = 1$. Therefore, e is a pendant vertex of $L(T)$.*

We define $D_2(T)$ as

$$D_2(T) = \{v \setminus deg_T(v) = 2 \text{and one neighbour of v is pendent}\}$$

Now we are at a position to establish our next result.

Theorem 4. *Let T be a Kragujevac tree with $d \geq 2$ and let $D_2(T) = \{v_1, v_2, \cdots, v_k\}$. Then*

$$TW(L(T)) = \sum_{1 \leq i < j \leq m} d(v_i, v_j \setminus T) + \frac{m(m-1)}{2}. \tag{8}$$

Proof. Bearing in mind Observation 2 and 3. The proof of (8) follows from the same lines of the proof of Theorem 2.1 in [25]. □

3. Zagreb Indices of Kragujevac Trees

We begin with the following straightforward, previously known, auxiliary result.

Lemma 1. [1] *Let G be any nontrivial graph of order n and size m. Then*

$$M_1(G) + \overline{M_1}(G) = 2m(n-1).$$

Lemma 2. [1] *Let G be any nontrivial graph of order n and size m. Then*

$$\overline{M_2}(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G).$$

Theorem 5. *Let T be the Kragujevac tree of degree $d \geq 2$ with branches B_{k_i}, $i = 1, 2, \cdots,$ then*

$$M_1(T) \quad = \quad d^2 + \sum_{i=1}^{n} [(k_i + 1)^2 + 5k_i]. \tag{9}$$

Proof. We obtain formula (9) by applying Eq. (3). First consider the branch B_k, by Definition 1, it is clear that the degree of a root u is k and the degree of vertices which are adjacent to u is 2 i.e., $deg_{B_k}(N(u)) = 2$, finally, the degree of remaining vertices are one. Hence,

$$\begin{aligned} M_1(B_k) &= \sum_{i=1}^{n} deg_{B_k}(v_i)^2 \\ &= k^2 + k4 + k \\ &= k^2 + 5k. \end{aligned}$$

Note that, $deg_T(u_i) = (k_i+1)$, $i = 1, 2, \cdots$. With this background by employing Eq. (3) to the Kragujevac tree T, we have

$$\begin{aligned} M_1(T) &= \sum_{i=1}^{n} deg_T(v_i)^2 \\ &= d^2 + \sum_{i=1}^{n}[(k_i + 1)^2 + 5k_i]. \end{aligned}$$

This leads to the right-hand side of (9). $\square$

Corollary 6. *Let T be the Kragujevac tree of degree $d \geq 2$ with branches B_{k_i}, $i = 1, 2, \cdots$, then*

$$\overline{M_1}(T) = 2\sum_{i=1}^{n}(2k_i + 1)^2 - d^2 - \sum_{i=1}^{n}[(k_i + 1)^2 + 5k_i]. \tag{10}$$

Proof. Apply Lemma 1 and Theorem 5, bearing in mind that $n = 1 + \sum_{i=1}^{d}(2k_i + 1)$ and $m = \sum_{i=1}^{d}(2k_i + 1)$. $\square$

Theorem 7. *Let T be the Kragujevac tree of degree $d \geq 2$ with branches B_{k_i}, $i = 1, 2, \cdots$, then*

$$M_2(T) = d^2\sum_{i=1}^{n}(k_i + 1) + 2\sum_{i=1}^{n} k_i(k_i + 2). \tag{11}$$

Proof. We obtain formula (11) by applying Eq. (4). First consider the branch B_k, by Definition 1, it is clear that the degree of a root u is k and the degree of vertices which are adjacent to u is 2 i.e., $deg_{B_k}(N(u)) = 2$, finally, the degree of remaining vertices are one. Hence,

$$M_2(B_k) = \sum_{v_i,v_j \in E(B_k)} deg_{B_k}(v_i)deg_{B_k}(v_j)$$

$$= \quad 2k^2 + 2k$$

Note that, $deg_T(u_i) = (k_i+1)$, $i = 1, 2, \cdots$. With this background by employing Eq. (4) to the Kragujevac tree T, we have

$$\begin{aligned} M_2(T) &= \sum_{i=1}^{n} deg_T(v_i)^2 \\ &= d^2 + \sum_{v_i, v_j \in E(T)} d \sum_{i=1}^{n} (k_i + 1)d + \sum_{i=1}^{n} 2k_i(k_{i+2}) \\ &= d^2 \sum_{i=1}^{n} (k_i + 1) + 2 \sum_{i=1}^{n} k_i(k_i + 2). \end{aligned}$$

This leads to the right-hand side of (11). □

Corollary 8. *Let T be the Kragujevac tree of degree $d \geq 2$ with branches B_{k_i}, $i = 1, 2, \cdots$, then*

$$\begin{aligned} \overline{M_2}(T) &= 2 \sum_{i=1}^{n} (2k_i + 1)^2 - d^2 \sum_{i=1}^{n} (k_i + 1) - 2 \sum_{i=1}^{n} k_i(k_i + 2) \\ &- \frac{1}{2} \big[d^2 + \sum_{i=1}^{n} [(k_i + 1)^2 + 5k_i] \big]. \end{aligned}$$

Proof. Apply Lemma 2 and Theorem 7, bearing in mind that $n = 1 + \sum_{i=1}^{d} (2k_i + 1)$ and $m = \sum_{i=1}^{d} (2k_i + 1)$. □

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References

[1] A. R. Ashrafi, T. Došlić, A. Hamzeh, The Zagreb coindices of graph operations, *Discrete Applied Mathematics*, **158** (2010), 1571-1578, **doi:** 10.1016/j.dam.2010.05.017.

[2] A. R. Ashrafi, T. Došlić, A. Hamzeh, Extremal graphs with respect to the Zagreb coindices, *MATCH Communications in Mathematical and in Computer Chemistry*, **65** (2011), 85-92.

[3] G. Caporossi, P. Hansen, D. Vukičević, Comparing Zagreb indices of cyclic graphs, *MATCH Communications in Mathematical and in Computer Chemistry*, **63** (2010), 441-451.

[4] R. Cruz, I. Gutman, J. Rada, Topological indices of Kragujevac trees, *Proyecciones Journal of Mathematics*, **33** No. 4 (2014), 471-482, **doi:** 10.4067/S0716-09172014000400008.

[5] K. C. Das, I. Gutman, B. Zhou, New upper bounds on Zagreb indices, *Journal of Mathematical Chemistry*, **46** (2009), 514-521, **doi:** 10.1007/s10910-008-9475-3.

[6] K.C. Das , I. Gutman, Some properties of the second Zagreb index, *MATCH Communications in Mathematical and in Computer Chemistry*, **52** (2004), 103-112.

[7] T. Došlić, Vertex-weighted Wiener polynomials for composite graphs, *Ars Mathematica Contemporanea*, **1** (2008), 66-80.

[8] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Applicandae Mathematicae*, **66** (2001), 211-249, **doi:** 10.1023/A:1010767517079.

[9] L. Feng, A. Ilić, Zagreb, Harary and hyper-Wiener indices of graphs with a given matching number, *Applied Mathematics Letters*, **23** (2010), 943-948, **doi:** 10.1016/j.aml.2010.04.017.

[10] I. Gutman, Kragujevac trees and their energy, *Scientific Publications of the State University of Novi Pazar Series A: Applied Mathematics, Informatics and mechanics*, **6** No. 2 (2014), 71-79, **doi:** 10.5937/SPSUNP1402071G.

[11] I. Gutman, B. Furtula, M. Petrović, Terminal Wiener index, *Journal of Mathematical Chemistry*, **46** (2009), 522-531, **doi:** 10.1007/s10910-008-9476-2.

[12] I. Gutman, Y. N. Yeh, S. L. Lee, Y. L. Luo, Some recent results in the theory of the Wiener number, *Indian Journal of Chemistry*, **32A** (1993), 651-661.

[13] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chemical Physics Letters*, **17** (1972), 535-538, **doi:** 10.1016/0009-2614(72)85099-1.

[14] I. Gutman, Distance in thorny graph, *Publications de l'Institut Mathmatique (Beograd)*, **63** (1998), 31-36.

[15] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Communications in Mathematical and in Computer Chemistry*, **50** (2004), 83-92.

[16] F. Harary, *Graph Theory*, Addison-Wesely, Reading, 1969.

[17] A. Heydari, I. Gutman, On the terminal Wiener index of thorn graphs, *Kragujevac Journal of Science*, **32** (2010), 57-64.

[18] B. Horvat, T. Pisanski, M. Randić, Terminal polynomials and star-like graphs, *MATCH Communications in Mathematical and in Computer Chemistry*, **60** (2008), 493-512.

[19] S. M. Hosamani and I. Gutman, Zagreb indices of transformation graphs and total transformation graphs, *Applied Mathematics and Computation*, **247** (2014), 1156-1160, **doi:** 10.1016/j.amc.2014.09.080.

[20] S. M. Hosamani, B. Basavanagoud, New upper bounds for the first Zagreb index, *MATCH Communications in Mathematical and in Computer Chemistry*, **74** No. 1 (2015), 97-101.

[21] A. Ilić, D. Stevanović, On comparing Zagreb indices, *MATCH Communications in Mathematical and in Computer Chemistry*, **62** (2009), 681-687.

[22] X. Lin, On the Wiener index and circumference, *MATCH Communications in Mathematical and in Computer Chemistry*, **67** (2012), 331-336.

[23] B. Liu, Z. You, A Survey on comparing Zagreb indices, *MATCH Communications in Mathematical and in Computer Chemistry*, **65** (2011), 581-593.

[24] J.B. Liu, Ch. Wang, Sh. Wang, B. Wei, Zagreb Indices and Multiplicative Zagreb Indices of Eulerian graphs, *Bulletin of the Malaysian Mathematical Sciences Society*, (2016), In press.

[25] H. S. Ramane, K. P. Narayankar, S. S. Shirkol, A. B. Ganagi, Terminal Wiener Index of Line Graphs, *MATCH Communications in Mathematical and in Computer Chemistry*, **69** (2013), 775-782.

[26] M. Randić, J. Zupan, Highly compact 2D graphical representation of DNA sequences, *SAR and QSAR in Environmental Research*, **15** (2004), 191-205, **doi:** 10.1080/10629360410001697753.

[27] M. Randić, J. Zupan, D. Vikić-Topić, On representation of proteins by star-like graphs, *Journal of Molecular Graphics and Modelling*, **26** (2007), 290-305, **doi:** 10.1016/j.jmgm.2006.12.006.

[28] N. S. Schmuck, S. G. Wagner, H. Wang, Greedy trees, caterpillars and Wiener-type graph invariants, *MATCH Communications in Mathematical and in Computer Chemistry*, **68** (2012), 273-292.

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

[30] C. Wang, Sh. Wang, B. Wei, Cacti with Extremal PI Index, *Transactions on Combinatorics*, **5** (2016), 1-8.

[31] S. Wang, B. Wei, Multiplicative Zagreb indices of Cacti, *Discrete Mathematics, Algorithms and Applications*, **8** No. 3 (2016), 1650040, **doi:** 10.1142/S1793830916500403.

[32] S. Wang, M.R. Farahani, M.R.R. Kanna, M.K. Jamil, R.P. Kumar. The Wiener Index and the Hosoya Polynomial of the Jahangir Graphs, *Applied and Computational Mathematics*, **5** (2016), 138-141, **doi:** 10.11648/j.acm.20160503.17.

[33] S. Wang, B. Wei, Multiplicative Zagreb indices of k-trees, *Discrete Applied Mathematics*, **180** (2015), 168-175, **doi:** 10.1016/j.dam.2014.08.017.

[34] H. Wiener, Structural determination of paraffin boiling points, *Journal of the American Chemical Society*, **1** No. 69 (1947), 17-20, **doi:** 10.1021/ja01193a005.

[35] M. Zeryouh, M. Marraki, M. Essalih, Wiener and Terminal Wiener Indices of Some Rooted Trees, *Applied Mathematical Sciences*, **8** (2014), 4995-5002, **doi:** 10.12988/ams.2014.46461.

[36] B. Zhou, Remarks on Zagreb indices, *MATCH Communications in Mathematical and in Computer Chemistry*, **57** (2007), 597-616.