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On reciprocal reverse Wiener index

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Abstract We report some properties, especially bounds for the reciprocal reverse Wiener index of a connected (molecular) graph. We find that the reciprocal reverse Wiener index possesses the minimum values for the complete graph in the class of n-vertex connected graphs and for the star in the class of n-vertex trees, and the maximum values for the complete graph with one edge deleted in the class of n-vertex connected graphs and for the tree obtained by attaching a pendant vertex to a pendant vertex of the star on $n-1$ vertices in the class of n-vertex trees. These results are compared with those obtained for the ordinary Wiener index.

Keywords Wiener index · Reciprocal reverse Wiener index · Distance · Diameter · Molecular graph

1 Introduction

We consider simple graphs, i.e., graphs without multiple edges and loops [1]. Let G be a connected (molecular) graph with the vertex-set $V(G) = \{v_1, v_2, \ldots, v_n\}$.

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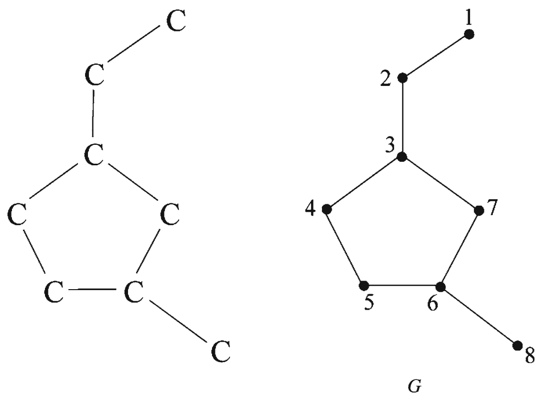


Fig. 1 Carbon skeleton of 1-ethyl-3-methylcyclopentane and the corresponding labeled molecular graph G

The distance matrix **D** of G is an $n \times n$ matrix $\left[d_{ij}\right]$ such that d_{ij} is just the distance (i.e., the number of edges of a shortest path) between the vertices v_i and v_j in G [2,3].

The reverse distance matrix or the reverse Wiener matrix **RW** of the graph G is an $n \times n$ matrix $[r_{ij}]$ such that $r_{ij} = d - d_{ij}$ if $i \neq j$, and 0 otherwise [3,4], where d is the diameter of G [1]. The reciprocal reverse Wiener matrix **RRW** of G is an $n \times n$ matrix $[rr_{ij}]$ such that $rr_{ij} = \frac{1}{r_{ij}} = \frac{1}{d-d_{ij}}$ if $i \neq j$ and $d_{ij} < d$, and 0 otherwise [5].

Parallel to the definitions of the Wiener index [6] $\mathrm{W}(G) = \sum_{i<j} d_{ij}$ using distance matrix and the reverse Wiener index [4] $\Lambda(G) = \sum_{i<j} r_{ij} = \frac{1}{2}n\,(n-1)\,d - \mathrm{W}\,(G)$ using reverse Wiener matrix of the graph G, the reciprocal reverse Wiener index $\mathrm{R}\Lambda(G)$ of the graph G is defined as [5]

$$\mathrm{R}\Lambda(G) = \sum_{i<j} rr_{ij}.$$

This quantity and some other structural descriptors derived from the matrix **RRW** were used to produce QSPR models for the alkane molar heat capacity in [5].

The Wiener index is one of the oldest and the most thoroughly studied topological indices [7–12], and some properties of the reverse Wiener index may also be found [13,14]. We now report some elementary properties, especially bounds for the reciprocal reverse Wiener index of a connected (molecular) graph.

A picture of a simple molecular graph G representing 1-ethyl-3-methylcyclopentane is given in Fig. 1 and we give in Table 1 the distance matrix, the reverse Wiener matrix and the reciprocal reverse Wiener matrix of G, respectively.

2 Preliminaries

Let G be a connected (molecular) graph with $n \geq 2$ vertices. Let $D(G,k)$ be the number of the unordered pairs of vertices of G that are of distance k, for $k = 1, 2, \ldots, d$, where d is the diameter of G. Then

Table 1 Distance matrix **D**, reverse Wiener matrix **RW** and reciprocal reverse Wiener matrix **RRW** of G in Fig. 1

$$\mathbf{D}(G) = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 4 & 3 & 5 \\ 1 & 0 & 1 & 2 & 3 & 3 & 2 & 4 \\ 2 & 1 & 0 & 1 & 2 & 2 & 1 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 & 2 & 3 \\ 4 & 3 & 2 & 1 & 0 & 1 & 2 & 2 \\ 4 & 3 & 2 & 2 & 1 & 0 & 1 & 1 \\ 3 & 2 & 1 & 2 & 2 & 1 & 0 & 2 \\ 5 & 4 & 3 & 3 & 2 & 1 & 2 & 0 \end{bmatrix}$$

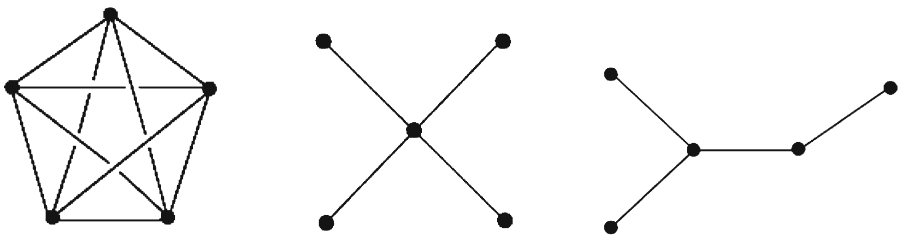
Wiener index = 63

$$\mathbf{RW}(G) = \begin{bmatrix} 0 & 4 & 3 & 2 & 1 & 1 & 2 & 0 \\ 4 & 0 & 4 & 3 & 2 & 2 & 3 & 1 \\ 3 & 4 & 0 & 4 & 3 & 3 & 4 & 2 \\ 2 & 3 & 4 & 0 & 4 & 3 & 3 & 2 \\ 1 & 2 & 3 & 4 & 0 & 4 & 3 & 3 \\ 1 & 2 & 3 & 3 & 4 & 0 & 4 & 4 \\ 2 & 3 & 4 & 3 & 3 & 4 & 0 & 3 \\ 0 & 1 & 2 & 2 & 3 & 4 & 3 & 0 \end{bmatrix}$$

Reverse Wiener index = 77

$$\mathbf{RRW}(G) = \begin{bmatrix} 0 & 1/4 & 1/3 & 1/2 & 1 & 1 & 1/2 & 0 \\ 1/4 & 0 & 1/4 & 1/3 & 1/2 & 1/2 & 1/3 & 1 \\ 1/3 & 1/4 & 0 & 1/4 & 1/3 & 1/3 & 1/4 & 1/2 \\ 1/2 & 1/3 & 1/4 & 0 & 1/4 & 1/3 & 1/3 & 1/2 \\ 1 & 1/2 & 1/3 & 1/4 & 0 & 1/4 & 1/3 & 1/3 \\ 1 & 1/2 & 1/3 & 1/3 & 1/4 & 0 & 1/4 & 1/4 \\ 1/2 & 1/3 & 1/4 & 1/3 & 1/3 & 1/4 & 0 & 1/3 \\ 0 & 1 & 1/2 & 1/2 & 1/3 & 1/4 & 1/3 & 0 \end{bmatrix}$$

Reciprocal reverse Wiener index $= 34/3$



K_5 S_5 Y_5

Fig. 2 Three graphs with 5 vertices: complete graph K_5, star S_5 and tree Y_5

$$\mathrm{R}\Lambda(G) = \sum_{k=1}^{d-1} \frac{D(G,k)}{d-k} \quad \text{if } d \geq 2.$$

Let K_n and S_n respectively be the complete graph and the star with n vertices [1]. Let Y_n be the tree formed by attaching a pendant vertex to a pendant vertex of the star S_{n-1}. Examples of these graphs on five vertices are given in Fig. 2.

3 Properties of reciprocal reverse Wiener index

Now we give some lower and upper bounds for RΛ in terms of the number of vertices and the number of edges. Let $K_n - e$ be the graph obtained from the complete graph K_n by deleting an edge.

Proposition 1 *Let G be a connected graph with $n \geq 3$ vertices. Then*

$$0 \leq R\Lambda(G) \leq \frac{n(n-1)}{2} - 1$$

with left (right, respectively) equality if and only if $G = K_n$ ($G = K_n - e$, respectively).

Proof Since $rr_{ij} \geq 0$, we have $\mathrm{R}\Lambda(G) \geq 0$ with equality if and only if $d = d_{ij} = 1$ for all $i, j = 1, 2, \ldots, n$ with $i \neq j$, i.e., $G = K_n$.

On the other hand, note that $rr_{ij} \leq 1$ with equality if and only if $d_{ij} = d - 1$ and $i \neq j$, and that there is at least one pair of i, j with $i \neq j$ such that $d_{ij} = d$ and then $rr_{ij} = 0$. Thus, $\mathrm{R}\Lambda(G) \leq \frac{n(n-1)}{2} - 1$ with equality if and only if there is exactly one pair of i, j with $i \neq j$ such that $d_{ij} = d$ and for any other pair of i, j with $i \neq j, d_{ij} = d - 1 = 1$, i.e., there is exactly one pair of i, j with $i \neq j$ such that $d_{ij} = 2$ and for any other pair of i, j with $i \neq j, d_{ij} = 1$, which is evidently equivalent to $G = K_n - e$. □

Proposition 2 *Let G be a connected graph with $n \geq 3$ vertices and m edges. Then*

$$R\Lambda(G) \leq \begin{cases} m & \text{if } m \geq \frac{(n+1)(n-2)}{3} \\ \frac{n(n-1)}{2} - \frac{m}{2} - 1 & \text{if } m \leq \frac{(n+1)(n-2)}{3} \end{cases}$$

with equality if and only if G has diameter 2 for $m > \frac{(n+1)(n-2)}{3}$, G has diameter 3 and $D(G,3) = 1$ for $m < \frac{(n+1)(n-2)}{3}$, and either G has diameter 2 or G has diameter 3 and $D(G,3) = 1$ for $m = \frac{(n+1)(n-2)}{3}$.

Proof Let d be the diameter of G. If $d = 1$, then $G = K_n$ and thus $\mathrm{R}\Lambda(G) = 0$. If $d = 2$, then by the definition of reciprocal reverse Wiener index, $\mathrm{R}\Lambda(G) = m$. If $d \geq 3$, then

$$\begin{aligned}
\mathrm{R}\Lambda(G) &= \sum_{k=1}^{d-1} \frac{D(G,k)}{d-k} \leq \frac{D(G,1)}{2} + \sum_{k=2}^{d-1} D(G,k) \\
&= \frac{D(G,1)}{2} + \frac{n(n-1)}{2} - D(G,1) - D(G,d) \\
&= \frac{n(n-1)}{2} - \frac{m}{2} - D(G,d) \\
&\leq \frac{n(n-1)}{2} - \frac{m}{2} - 1
\end{aligned}$$

with equality if and only if G has diameter 3 and $D(G,3) = 1$. It follows that $\mathrm{R}\Lambda(G) \le \max\left\{m, \frac{n(n-1)}{2} - \frac{m}{2} - 1\right\}$ and then the result follows easily. □

A simple example G in Proposition, 2 when $m = \frac{(n+1)(n-2)}{3}$, the diameter is 3 and $D(G,3) = 1$ is the graph formed from $K_4 - e$ by attaching a pendant vertex to a vertex of degree two.

For $v_i \in V(G)$, $\Gamma(v_i)$ denotes the set of its (first) neighbors in G and the degree of v_i is $\delta_i = |\Gamma(v_i)|$. The term $\sum_{i=1}^{n} \delta_i^2$ is known as the first Zagreb index of G, denoted by $\mathrm{M}_1(G)$ [15–20].

Proposition 3 *Let G be a triangle- and quadrangle-free connected graph with n vertices, m edges and diameter $d \ge 3$. Then*

$$\mathrm{R}\Lambda(G) \le \frac{n(n-1)}{2} - \frac{(d-2)m}{d-1} - \frac{d-3}{d-2}\left[\frac{1}{2}\mathrm{M}_1(G) - m\right] - D(G,d)$$

with equality if and only if $d = 3, 4$.

Proof Since G is triangle- and quadrangle-free, we have $D(G,2) = \sum_{v_i \in V(G)} \binom{\delta_i}{2} = \frac{1}{2}\mathrm{M}_1(G) - m$. Then it is easily seen that

$$\begin{aligned}\mathrm{R}\Lambda(G) &= \sum_{k=1}^{d-1} \frac{D(G,k)}{d-k} \le \frac{D(G,1)}{d-1} + \frac{D(G,2)}{d-2} + \sum_{k=3}^{d-1} D(G,k)\\ &= \frac{D(G,1)}{d-1} + \frac{D(G,2)}{d-2} + \frac{n(n-1)}{2} - D(G,1) - D(G,2) - D(G,d)\\ &= \frac{n(n-1)}{2} - \frac{(d-2)m}{d-1} - \frac{d-3}{d-2}\left[\frac{1}{2}\mathrm{M}_1(G) - m\right] - D(G,d)\end{aligned}$$

with equality if and only if $d = 3, 4$. □

Now we consider trees.

Proposition 4 *Let G be a tree with $n \ge 4$ vertices. Then*

$$n - 1 \le R\Lambda(G) \le \frac{n^2 - 4n + 7}{2}$$

with left (right, respectively) equality if and only if $G = S_n$ ($G = Y_n$, respectively).

Proof Let d be the diameter of G. Then $d \ge 2$. Suppose without loss of generality that $v_1 v_2 \ldots v_{d+1}$ be a diametrical path of G, where $V(G) = \{v_1, v_2, \ldots, v_n\}$.

It is easily seen that

$$\sum_{i=1}^{(d+1)-1} rr_{i,d+1} = \sum_{i=2}^{d} rr_{i,d+1} = \sum_{i=2}^{d} \frac{1}{d - d_{i,d+1}} = \sum_{i=2}^{d} \frac{1}{i-1} = \sum_{i=1}^{d-1} \frac{1}{i},$$

and for $2 \le j \le d$, we have

$$\sum_{i=1}^{j-1} rr_{ij} = \sum_{i=1}^{j-1} \frac{1}{d - d_{ij}} = \sum_{i=1}^{j-1} \frac{1}{d-(j-i)} = \sum_{i=1}^{j-1} \frac{1}{d-i}.$$

Thus

$$\begin{aligned}\sum_{j=2}^{d+1}\sum_{i=1}^{j-1} rr_{ij} &= \sum_{j=2}^{d}\sum_{i=1}^{j-1} rr_{ij} + \sum_{i=1}^{d} rr_{i,d+1}\\ &= \sum_{j=2}^{d}\sum_{i=1}^{j-1} \frac{1}{d-i} + \sum_{i=1}^{d-1}\frac{1}{i}\\ &= d-1+\sum_{i=1}^{d-1}\frac{1}{i} = d + \sum_{i=2}^{d-1}\frac{1}{i} \ge d\end{aligned}$$

with equality if and only if $d = 2$, i.e., $G = S_n$.

For any j with $d+2 \le j \le n$, it is easily seen that $d_{2j}, \ldots, d_{d,j} < d$, $\quad rr_{2j}, \ldots, rr_{d,j} \ge \frac{1}{d-1}$, and then

$$\sum_{i=1}^{d+1} rr_{ij} \ge (d+1-2)\cdot\frac{1}{d-1} = 1$$

with equality if and only if $d_{1j} = d_{d+1,j} = d$ and $d_{2j} = \cdots = d_{dj} = 1$ or equivalently $G = S_n$, because G is acyclic. Thus

$$\sum_{j=d+2}^{n}\sum_{i=1}^{d+1} rr_{ij} \ge \sum_{j=d+2}^{n} 1 = n-d-1$$

with equality if and only if $G = S_n$.

Obviously, $\sum_{j=d+3}^{n}\sum_{i=d+2}^{j-1} rr_{ij} \ge 0$ with equality if and only if $d_{ij} = d$ for any i, j with $d+2 \le i < j \le n$,which holds if $G = S_n$.

It follows that

$$\begin{aligned}\mathrm{R}\Lambda(G) &= \sum_{j=2}^{d+1}\sum_{i=1}^{j-1} rr_{ij} + \sum_{j=d+2}^{n}\sum_{i=1}^{d+1} rr_{ij}\\ &\quad + \sum_{j=d+3}^{n}\sum_{i=d+2}^{j-1} rr_{ij} \ge d + (n-d-1) + 0 = n-1\end{aligned}$$

with equality if and only if $G = S_n$.

Now suppose that $d \geq 3$ and $j \geq d + 2$. Obviously, $\sum_{i=d+2}^{j-1} rr_{ij} \leq j - d - 2$ with equality if and only if $d_{ij} = d - 1$ for $j > i \geq d + 2$, and then $\sum_{i=1}^{j-1} rr_{ij} \leq j - d - 2 + \sum_{i=1}^{d+1} rr_{ij}$. If $d = 3$, then $\sum_{i=1}^{j-1} rr_{ij} \leq j - 3 + 0 + \frac{1}{2} = j - \frac{5}{2}$ with equality if and only if $d_{ij} = 2$ for $j > i \geq d + 2$ with $i \neq j$, i.e., $G = Y_n$. Suppose that $d \geq 4$. If $d_{1j} = d$ or $d_{d+1,j} = d$, then $d_{3j} \leq d - 2$, i.e., $rr_{3j} \leq \frac{1}{2}$, and thus $\sum_{i=1}^{j-1} rr_{ij} \leq j - 3 + 0 + \frac{1}{2} = j - \frac{5}{2}$. If $d_{1j} \neq d$ and $d_{d+1,j} \neq d$, then $d_{1j}, d_{2j}, \ldots, d_{d+1,j} \leq d-1$, and thus $d_{2j}, d_{3j}, d_{4j} \leq d-2$, i.e., $rr_{2j}, rr_{3j}, rr_{4j} \leq \frac{1}{2}$, implying that $\sum_{i=1}^{j-1} rr_{ij} \leq j - 4 + \frac{1}{2} \times 3 = j - \frac{5}{2}$. So for $d \geq 3$, we have

$$\sum_{j=d+2}^{n} \sum_{i=1}^{j-1} rr_{ij} \leq \sum_{j=d+2}^{n} \left(j - \frac{5}{2}\right) = \frac{(n + d - 3)(n - d - 1)}{2}$$

with equality when $d = 3$ if and only if $G = Y_n$. It follows that for $d \geq 3$,

$$\begin{aligned}
\mathrm{R}\Lambda(G) &= \sum_{j=2}^{d+1} \sum_{i=1}^{j-1} rr_{ij} + \sum_{j=d+2}^{n} \sum_{i=1}^{j-1} rr_{ij} \\
&\leq d + \sum_{i=2}^{d-1} \frac{1}{i} + \frac{(n + d - 3)(n - d - 1)}{2} \\
&\leq d + \frac{d - 2}{2} + \frac{(n + d - 3)(n - d - 1)}{2} \\
&= \frac{(n - 3)(n - 1)}{2} - \frac{d^2 - 5d + 2}{2} \\
&\leq \frac{(n - 3)(n - 1)}{2} + 2 \\
&= \frac{n^2 - 4n + 7}{2},
\end{aligned}$$

and if the bound $\frac{n^2-4n+7}{2}$ is attained then $d = 3$, and $\sum_{j=d+2}^{n} \sum_{i=1}^{j-1} rr_{ij} = \frac{(n+d-3)(n-d-1)}{2}$, implying that $G = Y_n$. Conversely, if $G = Y_n$ then the bound is obtained. □

Remark 5 Let G be a connected graph on $n \geq 4$ vertices with a connected complement $\overline{G}$ [1]. For $n = 4$, there is exactly one such pair of graphs P_4 and $\overline{P_4} = P_4$, for which $\mathrm{R}\Lambda(P_4) + \mathrm{R}\Lambda\left(\overline{P_4}\right) = 7$. Suppose that $n \geq 5$. Let m and $\overline{m}$ be respectively the number of edges of G and $\overline{G}$. If one of m and $\overline{m}$ is at least $\frac{(n+1)(n-2)}{3}$, say $m \geq \frac{(n+1)(n-2)}{3}$, then as $\overline{m} \leq \frac{n(n-1)}{2} - \frac{(n+1)(n-2)}{3} = \frac{n^2-n+4}{6} < \frac{(n+1)(n-2)}{3}$, we have by Proposition 2 that

$$\mathrm{R}\Lambda(G) + \mathrm{R}\Lambda\left(\overline{G}\right) \leq m + \left[\frac{n(n - 1)}{2} - \frac{\overline{m}}{2} - 1\right] = n(n - 1) - 1 - \frac{3\overline{m}}{2}$$

and thus $\mathrm{R}\Lambda\left(G\right)+\mathrm{R}\Lambda\left(\overline{G}\right) \leq n\left(n-1\right)-1-\frac{3(n-1)}{2}=\frac{2n^2-5n+1}{2}$ with equality if and only if G has diameter 2, $\overline{G}$ is a tree with diameter 3 and $D\left(\overline{G},3\right)=1$, which is impossible, implying that $\mathrm{R}\Lambda\left(G\right)+\mathrm{R}\Lambda\left(\overline{G}\right)<\frac{2n^2-5n+1}{2}$. If $m,\overline{m}<\frac{(n+1)(n-2)}{3}$, then by Proposition 2,

$$\mathrm{R}\Lambda\left(G\right)+\mathrm{R}\Lambda\left(\overline{G}\right) \leq \frac{n\left(n-1\right)}{2}-\frac{m}{2}-1+\frac{n\left(n-1\right)}{2}-\frac{\overline{m}}{2}-1=\frac{3n^2-3n-8}{4}$$

with equality if and only if both G and $\overline{G}$ have diameter 3 and $D\left(G,3\right)=D\left(\overline{G},3\right)=1$. Thus, $\mathrm{R}\Lambda\left(G\right) \leq \max\left\{\frac{2n^2-5n+1}{2},\frac{3n^2-3n-8}{4}\right\}$. Note that $\frac{3n^2-3n-8}{4} \leq \frac{2n^2-5n+1}{2}$ with equality if and only if $n=5$. Now we have:

(a) $\mathrm{R}\Lambda\left(G\right)+\mathrm{R}\Lambda\left(\overline{G}\right) \leq \frac{2n^2-5n+1}{2}$ with equality if and only if G is the graph formed from the path on 5 vertices by adding an edge between the two neighbors of its center;
(b) If G and $\overline{G}$ have at most $\frac{(n+1)(n-2)}{3}$ edges, then $\mathrm{R}\Lambda\left(G\right)+\mathrm{R}\Lambda\left(\overline{G}\right) \leq \frac{3n^2-3n-8}{4}$.

4 Conclusions

In this report, we establish some basic properties for the reciprocal reverse Wiener index. We find that both the reciprocal reverse Wiener index and the ordinary Wiener index possess the minimum values for the complete graph K_n in the class of n-vertex connected graphs, and the minimum values for the star S_n in the class of n-vertex trees. However, the reciprocal reverse Wiener index behaves quite differently from the ordinary Wiener index for the maximum values: the reciprocal reverse Wiener index and the ordinary Wiener index are at maximum for the complete graph with one edge deleted K_n-e and the path P_n respectively in the class of n-vertex connected graphs, and at maximum for the tree Y_n (obtained by attaching a pendant vertex to a pendant vertex of the star S_{n-1}) and the path P_n respectively in the class of n-vertex trees. Our study echoes the statement found by QSPR models in [5]: the reciprocal reverse Wiener matrix reflects some structural features that are absent from the distance matrix.

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