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ORIGINAL PAPER

On reciprocal molecular topological index

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Abstract We report some properties of the reciprocal molecular topological index RMTI of a connected graph, and, in particular, its relationship with the first Zagreb index M_1. We also derive the upper bounds for RMTI in terms of the number of vertices and the number of edges for various classes of graphs, including K_{r+1} -free graphs with $r \geq 2$, quadrangle-free graphs, and cacti. Additionally, we consider a Nordhaus-Gaddum-type result for RMTI.

Keywords Molecular topological index · Reciprocal molecular topological index · First Zagreb index · Connected graphs · K_{r+1}-free graphs · Quadrangle free-graphs · Cacti

1 Introduction

The molecular topological index MTI has been introduced by Schultz [1] in 1989 for characterization of alkanes by integer. A year later (1990) Müller et al. [2] produced an expression for computing the MTI and studied its discriminatory properties. The term Schultz index has also been frequently used for MTI [3,4]. Some researchers have termed this molecular descriptor as Schultz molecular topological index [e.g., 5]. There were several directions of the further development of the MTI, e.g., Schultz

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and Schultz [6] introduced the reciprocal MTI, Klein et al. [7] showed that the MTI is strongly correlated with the Wiener index, Gutman reported several properties of the MTI [8], Zhou established some lower and upper bounds for the MTI in terms of selected graph invariants [9] and an even attempt has been made to extend the use of the MTI to heterosystems [10]. The MTI or the Schultz index found a modest use in the structure-property-activity modeling [e.g., 11].

In the present article, we investigate the properties of reciprocal molecular topological index RMTI, in particular, its relationship with the first Zagreb index M_1, derive upper bounds for RMTI in terms of the number of vertices and the number of edges for various classes of graphs. We also considered a Nordhaus-Gaddum-type result [12] for RMTI.

2 Preliminaries

Let G be a simple connected graph with vertex set $V(G) = \{v_1, v_2 \ldots, v_n\}$. For $u \in V(G)$, $\Gamma(u)$ denotes the set of its (first) neighbors in G and the degree of u is $d_u = |\Gamma(u)|$. The adjacency matrix $\mathbf{A}$ of G is an $n \times n$ matrix $(\mathbf{A}_{ij})$ such that $\mathbf{A}_{ij} = 1$ if the vertices v_i and v_j are adjacent and 0 otherwise [13].

Let G be a connected graph with n vertices. The distance matrix $\mathbf{D}$ of G is an $n \times n$ matrix $(\mathbf{D}_{ij})$ such that $\mathbf{D}_{ij}$ is just the distance between the vertices v_i and v_j in G [14]. The molecular topological index of the graph G is defined as

$$\mathrm{MTI} = \mathrm{MTI}(G) = \underline{d}(\mathbf{A} + \mathbf{D})\underline{1}$$

where $\underline{d} = (d_1, d_2, \ldots, d_n)$ with $d_i = d_{v_i}$ for $i = 1, 2, \ldots, n$, and $\underline{1}$ is the all 1's $n \times 1$vector. Setting $D_i = \sum_{j=1}^{n} \mathbf{D}_{ij}$, we have

$$\mathrm{MTI}(G) = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i D_i. \tag{1}$$

Recall the Hosoya definition of the Wiener index [15]

$$\mathrm{W}(G) = \sum_{i<j} \mathbf{D}_{ij}.$$

For a connected graph G with n vertices, the reciprocal distance matrix, also called the Harary matrix $\mathbf{R}$ [13,16,17], is defined as an $n \times n$ matrix $(\mathbf{R}_{ij})$ such that $\mathbf{R}_{ij} = 1/\mathbf{D}_{ij}$ if $i \neq j$ and 0 otherwise. The reciprocal molecular topological index RMTI [6] of G is defined as

$$\mathrm{RMTI} = \mathrm{RMTI}(G) = \underline{d}(\mathbf{A} + \mathbf{R})\underline{1}$$

Setting $R_i = \sum_{j=1}^{n} \mathbf{R}_{ij}$, we have

$$R\,\mathrm{MTI}(G) = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i R_i. \tag{2}$$

In [6], RMTI and other formulations of reciprocal and constant-interval reciprocal Schultz-type topological indices have been discussed and their use illustrated by the QSPR studies on physical constants of alkanes and cycloalkanes.

The Harary index H of a graph G has been defined similarly as the Wiener index [16–19]

$$\mathrm{H}(G) = \sum_{i<j} \mathbf{R}_{ij}.$$

The term $\sum_{i=1}^{n} d_i^2 = \sum_{u \in V(G)} d_u^2$ in (1) and (2) is known as the first Zagreb index of G, denoted by $\mathrm{M}_1(G)$ [20,21]. See [22,23] for its main properties and [24–28] for recent results.

3 Properties of RMTI

Let S_n and K_n be respectively the star and the complete graph with n vertices. We first give a relation between RMTI and the Harary index.

Theorem 1 *Let G be a connected graph with n vertices, m edges, minimum vertex degree δ and maximum vertex degree Δ. Then*

$$2\delta\,(m + \mathrm{H}(G)) \le \mathrm{RMTI}(G) \le 2\Delta\,(m + \mathrm{H}(G)) \tag{3}$$

with either equality if and only if G is a regular graph.

Proof From (2), we have

$$\delta \left(\sum_{i=1}^{n} d_i + \sum_{i=1}^{n} R_i \right) \le \mathrm{RMTI}(G) \le \Delta \left(\sum_{i=1}^{n} d_i + \sum_{i=1}^{n} R_i \right)$$

with either equality if and only if G is regular. Note that $\sum_{i=1}^{n} d_i + \sum_{i=1}^{n} R_i = 2m + 2\mathrm{H}(G)$. Thus, the above result follows. □

Let G be a connected graph with n vertices, minimum vertex degree δ and maximum vertex degree Δ. Note that $m \le \mathrm{H}(G)$ with equality if and only if $G = K_n$, where m is the number of edges of G. By Theorem 1, we have

$$2\delta\mathrm{H}(G) < \mathrm{RMTI}(G) \le 4\Delta\mathrm{H}(G)$$

with the right equality if and only if $G = K_n$.

Now we present a relation between RMTI and the first Zagreb index M_1.

Theorem 2 *Let Gbe a connected simple graph with n vertices and $m$edges. Then*

$$\mathrm{RMTI}(G) \leq \frac{3}{2}\mathrm{M}_1(G) + (n-1)m \tag{4}$$

with equality if and only if the diameter of $G$is at most two.

Proof Since $R_i \leq d_i + \frac{1}{2}(n - d_i - 1) = \frac{1}{2}(n + d_i - 1)$ for any $v_i \in V(G)$, we have

$$\sum_{i=1}^{n} d_i R_i \leq \sum_{i=1}^{n} \frac{1}{2} d_i (n + d_i - 1) = \frac{1}{2}\sum_{i=1}^{n} d_i^2 + \frac{1}{2}(n-1)\sum_{i=1}^{n} d_i$$
$$= \frac{1}{2}\mathrm{M}_1(G) + (n-1)m.$$

This, together with Eq. (2), implies (4).

From the arguments above, equality holds in (4) if and only if $R_i = d_i + \frac{1}{2}(n - d_i - 1)$ for every vertex v_i, i.e., the diameter of $G$is at most two. □

For any class of graphs $\mathbb{G}$, if $\mathrm{M}_1(G)$ is maximum in $\mathbb{G}$ and the diameter of G is at most two, then by Theorem 2, RMTI(G) is also maximum in $\mathbb{G}$. Therefore, we can find upper bounds for RMTI of various classes of graphs.

A universal vertex is a vertex adjacent to every other vertex. Let U_n with $n \geq 3$ be the graph obtained by adding a universal vertex to a graph consisting of a path of length 1 and $n - 3$ isolated vertices, and let B_n with $n \geq 4$ be the graph obtained by adding a universal vertex to a graph consisting of a path of length 2 and $n - 4$ isolated vertices. From [14], among all connected graphs with n vertices and m edges, the ones for which the first Zagreb index is maximum are obtained by adding a universal vertex to the graphs with n vertices and $m - n + 1$ edges for which the first Zagreb index is maximum. Note that $\mathrm{M}_1(S_n) = n(n-1)$, $\mathrm{M}_1(U_n) = n^2 - n + 6$, and $\mathrm{M}_1(B_n) = n^2 - n + 14$.

Let G be a graph on $n \geq 4$ vertices. If G is a tree, then $\mathrm{RMTI}(G) \leq \frac{1}{2}(n-1)(5n-2)$ with equality if and only if $G = S_n$. If G is unicyclic, then $\mathrm{RMTI}(G) \leq \frac{1}{2}(5n^2 - 5n + 18)$ with equality if and only if $G = U_n$. If G is bicyclic, then $\mathrm{RMTI}(G) \leq \frac{1}{2}(5n^2 - 3n + 40)$ with equality if and only $G = B_n$.

Let G be a graph with n vertices and $m$edges. Then [25]

$$\mathrm{M}_1(G) \leq m\left(\frac{2m}{n-1} + n - 2\right)$$

with equality if and only if G is S_n or K_n.

Corollary 3 *Let G be a connected graph with n vertices and $m$edges. Then*

$$\mathrm{RMTI}(G) \leq m\left(\frac{3m}{n-1} + \frac{5n-8}{2}\right)$$

with equality if and only if G is S_n or K_n.

Let W_n be the graph obtained from the star S_n by adding $\lfloor (n-1)/2 \rfloor$ independent edges. Let $even(n) = 1$ if n is even, and 0 otherwise.

Let G be a connected graph with $n \geq 2$ vertices and m edges. If G be a K_{r+1}-free graph, where $2 \leq r \leq n-1$, then [26]

$$\mathrm{M}_1(G) \leq \frac{2r-2}{r} nm$$

with equality if and only if G is a complete bipartite graph for $r = 2$ and the regular complete r-partite graph for $r \geq 3$. If G is a quadrangle-free graph, then [27]

$$\mathrm{M}_1(G) \leq n(n-1) + 2m - 2\mathrm{even}(n)$$

with equality if and only if G is W_n. If G is a triangle- and a quadrangle-free graph, then [27]

$$\mathrm{M}_1(G) \leq n(n-1)$$

with equality if and only if G is S_n or a Moore graph of diameter 2.

Corollary 4 *Let G be a connected graph with $n \geq 2$ vertices and m edges.*

(i) If G is K_{r+1}-free graph, where $2 \leq r \leq n-1$, then

$$\mathrm{RMTI}(G) \leq \frac{3r-3}{r} nm + (n-1)m$$

with equality if and only if G is a complete bipartite graph for $r = 2$ and the regular complete r-partite graph for $r \geq 3$.

(ii) If G is quadrangle-free graph, then

$$\mathrm{RMTI}(G) \leq \frac{3}{2}\left[n(n-1) - 2even(n)\right] + (n+2)m$$

with equality if and only if G is W_n.

(iii) If G is a triangle- and a quadrangle-free graph, then

$$\mathrm{RMTI}(G) \leq (n-1)\left(\frac{3}{2}n + m\right)$$

with equality if and only if G is S_n or a Moore graph of diameter 2.

A graph is called a cactus if any two of its cycles have at most one common vertex. Note that trees and unicyclic graphs are special cacti. For $0 \leq k \leq \lfloor (n-1)/2 \rfloor$, let $W_{n,k}$ be the graph obtained by adding k independent edges to the star graph S_n. In particular $W_{n,\lfloor (n-1)/2 \rfloor} = W_n$.

Lemma 5 *Let G be a connected cactus with n vertices and k cycles, where* $0 \le k \le \lfloor (n-1)/2 \rfloor$. *Then*

$$\mathrm{M}_1(G) \le n(n-1) + 6k$$

with equality if and only if G is $W_{n,k}$.

Proof If $k = 0$, then it is easy to see that the result holds. Suppose that $k \ge 1$. Assume that G is a connected cactus with n vertices and k cycles such that $\mathrm{M}_1(G)$ is as large as possible.

Suppose that there is a vertex u outside all cycles such that except one neighbor v of u with $d_v \ge 2$, all other neighbors, $u_1, u_2, \ldots, u_s$, of u are pendant vertices, where $d_u = s + 1 \ge 2$. Then for $\mathrm{H} = G - \{uu_1, \ldots, uu_s\} + \{vu_1, \ldots, vu_s\}$, we have

$$\mathrm{M}_1(H) - \mathrm{M}_1(G) = (d_v + s)^2 + 1 - d_v^2 - (s+1)^2 = 2(s-1)d_v + 1 > 0,$$

a contradiction. So each vertex outside all cycles is a pendant vertex adjacent to some vertex of a cycle.

Suppose that there are two vertex-disjoint cycles C_p and C_q in G. Then, there is a path, say $v_1 v_2 \ldots v_l$, joining C_p and C_q, where v_1 belongs to C_p, v_l belongs to C_q, and $l - 1 \ge 1$. Suppose that $d_{v_1} \ge d_{v_l}$. Denote by v_{l+1} and v_{l+2} neighbors of v_l in C_q. For $G' = G - \{v_l v_{l+1}, v_l v_{l+2}\} + \{v_1 v_{l+1}, v_1 v_{l+2}\}$, we have

$$\mathrm{M}_1(G') - \mathrm{M}_1(G) = (d_{v_1} + 2)^2 + (d_{v_l} - 2)^2 - d_{v_1}^2 - d_{v_l}^2 = 2(d_{v_1} + 4 - d_{v_l}) > 0,$$

a contradiction. So any two cycles of G have exactly one common vertex, and then all cycles of G have exactly one common vertex, denoted by v_1. If G contains exactly one cycle, choose v_1 to be any vertex with maximum degree.

If $y_1, y_2, \ldots, y_t$ are pendant vertices adjacent to v_i with $v_i \ne v_1$ then for $G'' = G - \{v_i y_1, \ldots, v_i y_t\} + \{v_1 y_1, \ldots, v_1 y_t\}$, we have

$$\mathrm{M}_1(G'') - \mathrm{M}_1(G) = (d_{v_1} + t)^2 + (d_{v_i} - t)^2 - d_{v_1}^2 - d_{v_i}^2 = 2t(d_{v_1} + t - d_{v_i}) > 0,$$

a contradiction. Hence G is a graph in which all cycles have exactly one common vertex v_1 and all other vertices outside cycles are pendent vertices adjacent to v_1.

If there is a cycle $C_p = v_1 v_2 \ldots v_p v_1$ of length $p \ge 4$, then for $G^* = G - \{v_2 v_3\} + \{v_1 v_3\}$, we have

$$\mathrm{M}_1(G^*) - \mathrm{M}_1(G) = (d_{v_1} + 1)^2 + 1 - d_{v_1}^2 - 4 = 2(d_{v_1} - 1) > 0,$$

a contradiction. Thus all cycles of G have length 3. This proves the lemma. □

By Theorem 2 and Lemma 5, we have

Corollary 6 *Let G be a connected cactus with* $n \ge 2$ *vertices and k cycles, where* $0 \le k \le \lfloor (n-1)/2 \rfloor$. *Then*

$$\mathrm{RMTI}(G) \le \frac{(n-1)(5n-2)}{2} + (n+8)k$$

with equality ifand only if G is $W_{n,k}$.

In the following we give a result on RMTI of the Nordhaus–Gaddum type [12]. For a graph G, $\overline{G}$ denotes its complement. We need a following lemma.

Lemma 7 *Let G be a connected graph on $n \geq 4$ vertices with a connected $\overline{G}$. Then*

$$\mathrm{M}_1(G) + \mathrm{M}_1(\overline{G}) \leq n^3 - 4n^2 + 3n + 8$$

with equality if and only if G or $\overline{G}$ is the graph S'_n, which is obtained by attaching a pendant vertex to a pendant vertex of the star S_{n-1}.

Proof It is obvious for $n = 4$. Suppose that $n \geq 5$. First note that

$$\begin{aligned}\mathrm{M}_1(G) + \mathrm{M}_1(\overline{G}) &= \sum_{u \in V(G)} \left[d_u^2 + (n-1-d_u)^2 \right] \\ &= n(n-1)^2 - 2 \sum_{u \in V(G)} d_u(n-1-d_u).\end{aligned}$$

Since both G and $\overline{G}$ are connected, we have $d_u(n-1-d_u) \geq n-2$ with equality if and only if $d_u = 1$ or $d_u = n-2$. Suppose that $d_u = 1$ and $d_v = n-2$ in G. Assume that uv is an edge in G. Let $N = \Gamma(v) \backslash \{u\}$. Then for the unique vertex w in $V(G) \backslash (\Gamma(v) \cup \backslash \{v\})$, $1 \leq d_w \leq n-3$. If $d_w = 1$ and $G[N]$ (the subgraph of G induced by N) is empty, then $G = S'_n$. If $d_w = n-3$ and $G[N]$ is complete, then $G = \overline{S'_n}$. Otherwise, there are at least two vertices whose degrees are at least 2 and at most $n-3$. Thus $\sum_{u \in V(G)} d_u(n-1-d_u)$ achieves its minimum value $(n-1)(n-2) + 2(n-3) = n^2 - n - 4$ if and only if G is S'_n or $\overline{S'_n}$. Now the desired result follows easily. □

Theorem 8 *Let G be a connected graph on $n \geq 4$ vertices with a connected $\overline{G}$. Then*

$$\mathrm{RMTI}(G) + \mathrm{RMTI}(\overline{G}) < 2n^3 - 7n^2 + 5n + 12.$$

Proof By Theorem 2 and Lemma 7,

$$\begin{aligned}\mathrm{RMTI}(G) + \mathrm{RMTI}(G) &\leq \frac{3}{2}\left[\mathrm{M}_1(G) + \mathrm{M}_1(\overline{G})\right] + \frac{1}{2}n(n-1)^2 \\ &\leq \frac{3}{2}\left(n^3 - 4n^2 + 3n + 8\right) + \frac{1}{2}n(n-1)^2 \\ &= 2n^3 - 7n^2 + 5n + 12.\end{aligned}$$

Note that if the upper bound in Lemma 7 is attained, then the diameter of G is 3. Hence the upper bound in Theorem 2 and in Lemma 7 cannot be achieved at the same time. The theorem is thus proved. □

Similarly to Theorem 2, we give a lower bound for RMTI.

Theorem 9 *Let G be a connected graph with $n \geq 2$ vertices, m edges and diameter D. Then*

$$\mathrm{RMTI}(G) \geq \left(2 - \frac{1}{D}\right) \mathrm{M}_1(G) + \frac{2}{D}(n-1)m$$

with equality if and only if the diameter of Gs at most two.

Proof Since $R_i \geq d_i + \frac{1}{D}(n - d_i - 1) = \frac{1}{D}(n-1) + \left(1 - \frac{1}{D}\right) d_i$ for any vertex v_i, it follows that

$$\begin{aligned} \mathrm{RMTI}(G) &\geq \mathrm{M}_1(G) + \sum_{i=1}^{n} d_i \left[\frac{1}{D}(n-1) + \left(1 - \frac{1}{D}\right) d_i\right] \\ &= \left(2 - \frac{1}{D}\right) \mathrm{M}_1(G) + \frac{2}{D}(n-1)m. \end{aligned}$$

From the arguments above, the lower bound is attained if and only if $R_i = d_i + \frac{1}{D}(n - d_i - 1)$ for every vertex v_i, i.e., the diameter of G is at most two. □

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