

On max-min rodeg index of graphs

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Abstract: Among the defined 148 discrete Adriatic indices, the max-min rodeg index is one. It is a good predictor for the enthalpy of vaporization and standard enthalpy of vaporization for octane isomers, as well as the log water activity coefficient for polychlorobiphenyls. For a graph G , here we concentrate on the max-min rodeg index, defined as

$$Mm_{sde}(G) = \sum_{x \sim y} \sqrt{\frac{\max\{d_x, d_y\}}{\min\{d_x, d_y\}}},$$

where $x \sim y$ and d_x represents the adjacency of two vertices x and y , and the degree of the vertex x , respectively. First, we present some bounds for the max-min rodeg index via standard inequalities. Then we provide upper bounds via some graph parameters for the max-min rodeg index of G . Also, we obtain a relation between the max-min degree index and the energy of G . Finally, we study the extremal value problem over chemical graphs concerning the max-min rodeg index.

Keywords: max-min rodeg index; Diaz-metcalf inequality, clique number, energy, chemical graph.

AMS Subject classification: .

1. Introduction

Let $G = (V(G), E(G))$ be a simple, undirected graph. For an edge $e = xy$ of G , we write e as a (d_x, d_y) -edge. Also, by d_i and $E_{i,j}$, we denote the number of i -degree vertices and (i, j) -edges of G , respectively. By $\omega(G)$, $\nu(G)$, and λ_1 , we denote the clique number, vertex connectivity, and index of a graph G , respectively. A graph

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with *chemical graph* is a graph with vertex degree at most four. By K_n , $K_{i_n, n-1}$ and $\mathcal{G}_{n, m, \delta, \Delta}$, we denote the n -vertex complete graph, the kite graph and the family of n -vertex connected graphs having m edges, maximum degree Δ and minimum degrees δ , respectively.

A topological index is a molecular descriptor of the molecular graph of some molecular structure. Many topological descriptors are special because of their necessity in chemistry, especially in QSPR/QSAR research. In chemical graph theory, one of the most famous and challenging problems is to characterize the extremal graphs concerning different topological indices. We refer to [4, 5, 7–10] for recent advances. There are several vertex degree-based topological indices. Among these indices, some indices such as Randić index, Sombor index, ABC index, AG index, etc, play a prominent role in mathematical chemistry. The Randić index [12] and the reciprocal Randić index of a graph G , denoted by $R(G)$ and $RR(G)$, are defined as

$$R(G) = \sum_{i \sim j} \frac{1}{\sqrt{d_i d_j}} \quad \text{and} \quad RR(G) = \sum_{i \sim j} \sqrt{d_i d_j}.$$

The Sombor index [5] and the arithmetic-geometric index [14] of a graph G , denoted by $SO(G)$ and $AG(G)$, are defined as

$$SO(G) = \sum_{i \sim j} \sqrt{d_i^2 + d_j^2} \quad \text{and} \quad AG(G) = \sum_{i \sim j} \frac{d_i + d_j}{2\sqrt{d_i d_j}}.$$

The atom-bond connectivity index of a graph G is defined as

$$ABC(G) = \sum_{u \sim v} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

The Max-min rodeg index is one of them. For its application, chemical importance, and other related results, we refer to [16–18].

In this paper, in Section 2, we obtain sharp lower bounds on max-min rodeg index via some inequalities and upper bounds via various graph parameters. Also, we provide bounds on the max-min rodeg index of a triangle-free graph. In Section 3, we establish its mathematical relation with other topological indices. Then, in Section 4, we establish a relation between the energy of a graph and the max-min rodeg index of a graph. Finally, in Section 5, we characterize the graph extremal concerning the max-min rodeg index over chemical graphs.

2. Sharp bounds on max-min rodeg index

First, we obtain sharp bounds on max-min rodeg index via the following Diaz-Metcalf inequality [11].

Lemma 1. Let p_t and q_t , $t = 1, \dots, n$, be real numbers such that $Pp_t \leq q_t \leq Qp_t$ for each $t = 1, 2, \dots, n$. Then

$$(P + Q) \sum_{t=1}^n p_t q_t \geq \sum_{t=1}^n q_t^2 + PQ \sum_{t=1}^n p_t^2.$$

Equality occurs if and only if either $q_t = Pp_t$ or $q_t = Qp_t$ for each $t = 1, 2, \dots, n$.

Theorem 1. Let $G \in \mathcal{G}_{n,m,\delta,\Delta}$. Then

$$Mm_{sde}(G) \geq \frac{\delta^2[m + \Delta^2 M_2^*(G)]}{\Delta^2 + \delta^2}. \quad (2.1)$$

Equality occurs if and only if G is regular.

Proof. By the definition of the max-min rodeg index,

$$\begin{aligned} Mm_{sde}(G) &= \sum_{x \sim y} \sqrt{\frac{d_x}{d_y}}, \text{ where } d_x \geq d_y \\ &= \sum_{x \sim y} \sqrt{\frac{d_x^2}{d_x d_y}}. \end{aligned}$$

If $e = xy$ is an edge of G , then $\frac{\delta^4}{d_x d_y} \leq d_x^2 \leq \frac{\Delta^4}{d_x d_y}$ results

$$\frac{\delta^2}{\sqrt{d_x d_y}} \leq \sqrt{d_x^2} \leq \frac{\Delta^2}{\sqrt{d_x d_y}}. \quad (2.2)$$

Equality occurs on the left of Equation 2.2 if and only if $d_x = d_y = \delta$, and in the right if and only if $d_x = d_y = \Delta$ for any edge $xy \in E(G)$.

Assuming $P = \delta^2$ and $Q = \Delta^2$ in Lemma 1, we have

$$\begin{aligned} Mm_{sde}(G) &= \sum_{x \sim y} \sqrt{\frac{d_x^2}{d_x d_y}} = \sum_{x \sim y} \frac{d_x}{\sqrt{d_x d_y}} \\ &= \frac{1}{\delta^2 + \Delta^2} (\delta^2 + \Delta^2) \times \sum_{x \sim y} \frac{d_x}{\sqrt{d_x d_y}} \\ &\geq \frac{1}{\delta^2 + \Delta^2} \left[\sum_{x \sim y} d_x^2 + \Delta^2 \delta^2 \sum_{x \sim y} \frac{1}{d_x d_y} \right] \\ &\geq \frac{1}{\delta^2 + \Delta^2} [\delta^2 m + \Delta^2 \delta^2 M_2^*(G)] \\ &= \frac{\delta^2 [m + \Delta^2 M_2^*(G)]}{\Delta^2 + \delta^2}. \end{aligned} \quad (2.3)$$

If equality occurs in Equation 2.1, then all inequalities in Equation 2.3 become equal. From the equality condition of 2.2 and Lemma 1, we have $d_x = \frac{\delta^2}{\sqrt{d_x d_y}}$ or $d_x = \frac{\Delta^2}{\sqrt{d_x d_y}}$ for any edge $xy \in E(G)$. From the equality conditions in Lemma 1 and Equation 2.2, it is clear that G is regular. \square

Recently, Ali et al. [1] obtained a sharp lower bound on $M_2^*(G)$ stated in the next result.

Corollary 1. *Let $G \in \mathcal{G}_{n,m,\delta,\Delta}$. Then*

$$M_2^*(G) \geq \frac{n(\delta + \Delta) - 2m}{\Delta^2 + \delta^2}.$$

Equality occurs if and only if G is a regular or semiregular bipartite graph.

From Theorem 1 and Corollary 1, the following result is immediate.

Corollary 2. *Let $G \in \mathcal{G}_{n,m,\Delta,\delta}$. Then*

$$Mm_{sde}(G) \geq \frac{\delta^2(\delta^2 m + \Delta^3 n + \delta \Delta^2 n - m \Delta^2)}{(\Delta^2 + \delta^2)^2},$$

with equality if and only if G is regular.

Proposition 1. *Let $G \in \mathcal{G}_{n,m,\delta,\Delta}$. Then*

$$m\sqrt{\frac{\delta}{\Delta}} \leq Mm_{sde}(G) \leq m\sqrt{\frac{\Delta}{\delta}}.$$

Equality occurs in the left case if and only if G is regular, and in the right if and only if G is regular or semiregular bipartite graph.

Proof. We have $\sqrt{\delta} \leq \sqrt{d_x} \leq \sqrt{\Delta}$ and $\frac{1}{\sqrt{\Delta}} \leq \frac{1}{\sqrt{d_y}} \leq \frac{1}{\sqrt{\delta}}$, which implies $\sqrt{\frac{\delta}{\Delta}} \leq \sqrt{\frac{d_x}{d_y}} \leq \sqrt{\frac{\Delta}{\delta}}$. Consequently, we have $m\sqrt{\frac{\delta}{\Delta}} \leq Mm_{sde}(G) \leq m\sqrt{\frac{\Delta}{\delta}}$. Clearly, equality in the left case occurs if and only if $\Delta = \delta$, i.e., G is regular. Equality in the right case occurs if and only if $d_x = \Delta$ and $d_y = \delta$ or $d_x = d_y = \Delta = \delta$, i.e., G is a regular or semiregular bipartite graph. \square

Lemma 2. [15] *Let $G \in \mathcal{G}_{n,m}$ such that G is K_{t+1} free. Then $m \leq \frac{(t-1)n^2}{2t}$, with equality if and only if G is a balanced complete t -partite graph.*

Corollary 3. *Let $G \in \mathcal{G}_{n,m,\delta,\Delta}$ be with the clique number ω . Then*

$$Mm_{sde}(G) \leq \frac{n^2(\omega - 1)}{2\omega} \sqrt{\frac{\Delta}{\delta}}.$$

The equality occurs if and only if G is a complete ω -partite graph in which all classes have equal cardinality.

Proof. Clearly, G is a $K_{\omega+1}$ free graph. Therefore, by Proposition 1 and Lemma 2, we have

$$Mm_{sde}(G) \leq m \sqrt{\frac{\Delta}{\delta}} \leq \frac{n^2(\omega - 1)}{2\omega} \sqrt{\frac{\Delta}{\delta}}.$$

It is easy to observe from Proposition 1 and Lemma 2 that the equality occurs if and only if G is a complete ω -partite graph in which all classes have equal cardinality. \square

Lemma 3. [13] *Let G be a connected graph on $n \geq 3$ vertices, $G \not\cong K_3$, with clique number ω and algebraic connectivity a . Then $\frac{\omega}{a} \leq n - 1$, with equality if and only if G is a short kite.*

Applying Corollary 3 and Lemma 3, we have the following immediate result.

Corollary 4. *Let $G \in \mathcal{G}_{n,m,\delta,\Delta}$ with $n \geq 4$, and algebraic connectivity a . Then*

$$Mm_{sde}(G) < \left(1 - \frac{1}{a(n-1)}\right) \frac{n^2}{2} \sqrt{\frac{\Delta}{\delta}}.$$

Lemma 4. [13] *Let G be a connected graph on $n \geq 3$ vertices, with clique number ω , vertex connectivity v , and index λ_1 . Then $\omega \leq v + n - 2$ with equality if and only if $G \cong K_{i,n-i}$ or $G \cong K_3$, and $\omega \leq 1 + \lambda_1$ with equality if and only if $G \cong K_n$.*

By Corollary 3 and Lemma 4, we have the following result.

Corollary 5. *Let $G \in \mathcal{G}_{n,m,\delta,\Delta}$ with $n \geq 3$, vertex connectivity v and index λ_1 . Then*

$$(a) \ Mm_{sde}(G) \leq \left(1 - \frac{1}{v+n-2}\right) \frac{n^2}{2} \sqrt{\frac{\Delta}{\delta}} \text{ with equality if and only if } G \cong K_3.$$

$$(b) \ Mm_{sde}(G) \leq \left(1 - \frac{1}{1+\lambda_1}\right) \frac{n^2}{2} \sqrt{\frac{\Delta}{\delta}} \text{ with equality if and only if } G \cong K_n.$$

Theorem 2. *Let $G \in \mathcal{G}_{n,m,\delta,\Delta}$ be such that it is a triangle-free graph. Then*

$$\sqrt{\frac{\delta}{n-\delta}}(n-1) \leq Mm_{sde}(G) \leq \frac{n^2}{4} \sqrt{\frac{n-\delta}{\delta}}. \quad (2.4)$$

Equality on the left of equation 2.4 occurs if and only if $G \cong K_2$, and on the right if and only if G is a balanced complete bipartite graph.

Proof. Let G be a triangle-free graph. If $e = xy$ is an edge of G , then $N(x) \cap N(y) = \emptyset$ and hence $\Delta \leq n - \delta$. Then

$$\begin{aligned} Mm_{sde}(G) &= \sum_{\delta \leq d_y \leq d_x \leq \Delta} \sqrt{\frac{d_x}{d_y}} E_{d_x, d_y} \\ &\geq \sqrt{\frac{\delta}{n - \delta}} \sum_{\delta \leq d_y \leq d_x \leq n - \delta} E_{d_x, d_y} \\ &\geq \sqrt{\frac{\delta}{n - \delta}} (n - 1). \end{aligned} \tag{2.5}$$

In the first inequality in equation 2.5, the equality holds if and only if $d_x + d_y = n$ for every edge xy of G . Thus, if $d_x = p$ for an edge uv , then each of the p neighbors, including v , of u should have degree $n - p$. Similarly, each of $n - p$ neighbors of v has degree p . Therefore, $m = p(n - p)$ $G \cong K_{p, n-p}$ for some natural number p . Also, we know in a connected graph G , $m \geq n - 1$, with equality if and only if G is a tree. Hence the equality occurs on the left of equation 2.4 if all the above inequalities must be equalities, which is only possible if and only if $G \cong K_2$.

Since G is triangle-free, from Proposition 1, Lemma 2 and the fact that $\Delta \leq n - \delta$, we have

$$\begin{aligned} Mm_{sde}(G) &\leq \frac{n^2(\omega - 1)}{2\omega} \sqrt{\frac{\Delta}{\delta}} \\ &\leq \frac{n^2(2 - 1)}{4} \sqrt{\frac{n - \delta}{\delta}} \\ &= \frac{n^2}{4} \sqrt{\frac{n - \delta}{\delta}}. \end{aligned}$$

Equality on the right of equation 2.4 holds if and only if G is a balanced complete bipartite graph. \square

Corollary 6. *Let G be a tree of order n . Then*

$$\sqrt{n - 1} \leq Mm_{sde}(G) \leq \frac{n^2}{4} \sqrt{n - 1}.$$

Equality holds if and only if $G \cong K_2$.

3. Relation with other topological indices

The max-min degree index of a graph G is defined as

$$Mm_{deg}(G) = \sum_{x \sim y} \frac{\max\{d_x, d_y\}}{\min\{d_x, d_y\}} = \sum_{x \sim y} \frac{d_x}{d_y} \quad \text{where } d_x \geq d_y.$$

For other related works on max-min degree index, we refer to [4, 8, 16, 17].

Theorem 3. *Let $G \in \mathcal{G}_{n,m,\Delta,\delta}$. Then*

$$\sqrt{\frac{\delta}{\Delta}} Mm_{deg}(G) \leq Mm_{sde}(G) \leq \sqrt{\frac{\Delta}{\delta}} Mm_{deg}(G).$$

In the left case, equality occurs if and only if G is regular or semiregular bipartite graph, and in the right case if and only if G is regular. Also, we have $Mm_{sde}(G) \leq \sqrt{mMm_{sde}(G)}$ with equality if and only if $\frac{d_x}{d_y}$ is a constant for each edge $xy \in G$ with $d_x \geq d_y$.

Proof. From the definition of max-min rodeg index, we have

$$Mm_{sde}(G) = \sum_{x \sim y} \sqrt{\frac{d_x}{d_y}} = \sum_{x \sim y} \frac{d_x}{d_y} \sqrt{\frac{d_y}{d_x}} \geq \sqrt{\frac{\delta}{\Delta}} Mm_{deg}(G). \quad (3.1)$$

Equality occurs in equation 3.1 if and only if G is regular or semiregular.

Similarly, we can prove that $Mm_{sde}(G) \leq \sqrt{\frac{\Delta}{\delta}} Mm_{deg}(G)$ with equality if and only if G is regular.

Also, by the Cauchy-Schwarz inequality, we have

$$Mm_{sde}(G) = \sum_{x \sim y} \sqrt{\frac{d_x}{d_y}} \leq \sqrt{\sum_{x \sim y} (1) \sum_{x \sim y} \frac{d_x}{d_y}} = \sqrt{mMm_{deg}(G)}.$$

The equality occurs in the above if and only if $\frac{d_x}{d_y}$ is a constant for each edge $xy \in G$ with $d_x \geq d_y$. \square

Theorem 4. *Let $G \in \mathcal{G}_{n,m,\Delta,\delta}$. Then*

$$\delta R(G) \leq Mm_{sde}(G) \leq \Delta R(G).$$

The equality on the left occurs if and only if G is regular and on the right if and only if every edge in G contains a vertex of maximum degree. Also,

$$\frac{1}{\Delta} RR(G) \leq Mm_{sde}(G) \leq \frac{1}{\delta} RR(G).$$

The equality occurs on the left if and only if G is regular, and on the right if and only if each edge in G contains a vertex of minimum degree.

Proof. From the definition of max-min rodeg index, we have

$$Mm_{sde}(G) = \sum_{x \sim y} \sqrt{\frac{d_x}{d_y}} = \sum_{x \sim y} \frac{d_x}{\sqrt{d_x d_y}} \leq \Delta R(G).$$

Equality occurs if and only if each edge in G contains a vertex of maximum degree. Similarly, $Mm_{sde} \geq \delta R(G)$ with equality if and only if G is regular. Again,

$$Mm_{sde}(G) = \sum_{x \sim y} \sqrt{\frac{d_x}{d_y}} = \sum_{x \sim y} \frac{\sqrt{d_x d_y}}{d_y} \leq \frac{1}{\delta} RR(G).$$

Equality occurs if and only if each edge in G contains a vertex of minimum degree. Similarly, $Mm_{sde}(G) \geq \frac{1}{\Delta} RR(G)$ such that equality occurs if and only if G is regular. \square

Theorem 5. *Let $G \in \mathcal{G}_{n,m,\delta,\Delta}$. Then*

$$\frac{SO(G)}{\sqrt{2}\Delta} \leq Mm_{sde}(G) \leq \frac{SO(G)}{\sqrt{2}\delta}.$$

Equality on each side occurs if and only if G is regular.

Proof. If $\delta \leq q \leq p \leq \Delta$, consider the function

$$f(p, q) = \frac{\sqrt{\frac{p}{q}}}{\sqrt{p^2 + q^2}} = \sqrt{\frac{p}{p^2 q + q^3}}.$$

We have

$$\frac{\partial f}{\partial q} = \frac{1}{2} \sqrt{\frac{p^2 q + q^3}{p}} \cdot \frac{(0 - p^3 - 3pq^2)}{(p^2 q + q^3)^2} < 0.$$

and

$$\frac{\partial f}{\partial p} = \frac{1}{2} \sqrt{\frac{p^2 q + q^3}{p}} \cdot \frac{q(q^2 - p^2)}{(p^2 q + q^3)^2} \leq 0, \quad \text{since } p \geq q.$$

Thus f is decreasing in each variable and hence

$$\begin{aligned} \frac{\sqrt{\frac{p}{q}}}{\sqrt{p^2 + q^2}} &\leq \sqrt{\frac{\delta}{\delta^3 + \delta^3}} = \frac{1}{\sqrt{2}\delta}, \\ \frac{\sqrt{\frac{p}{q}}}{\sqrt{p^2 + q^2}} &\geq \frac{1}{\sqrt{2}\Delta}, \\ \frac{\sqrt{d_x^2 + d_y^2}}{\sqrt{2}\Delta} &\leq \sqrt{\frac{d_x}{d_y}} \leq \frac{\sqrt{d_x^2 + d_y^2}}{\sqrt{2}\delta}, \end{aligned}$$

for each edge $xy \in E(G)$. Hence,

$$\frac{SO(G)}{\sqrt{2}\Delta} \leq Mm_{sde}(G) \leq \frac{SO(G)}{\sqrt{2}\delta},$$

and the equality on the left (resp. right) occurs if and only if G is regular. \square

Theorem 6. *Let $G \in \mathcal{G}_{n,m,\delta,\Delta}$. Then*

$$2AG(G) - \sqrt{\frac{\Delta}{\delta}}m \leq Mm_{sde}(G) \leq 2AG(G) - \sqrt{\frac{\delta}{\Delta}}m,$$

and the equality in the left occurs if and only if G is regular, and in the right if and only if G is regular or semiregular bipartite graph.

Proof. We have

$$\begin{aligned} Mm_{sde}(G) &= \sum_{x \sim y} \sqrt{\frac{d_x}{d_y}} \\ &= \sum_{x \sim y} \frac{d_x + d_y - d_y}{\sqrt{d_x d_y}} \\ &= \sum_{x \sim y} \left\{ \frac{2(d_x + d_y)}{2\sqrt{d_x d_y}} - \sqrt{\frac{d_y}{d_x}} \right\} \\ &\geq 2AG(G) - \sqrt{\frac{\Delta}{\delta}}m. \end{aligned}$$

Equality occurs if and only if G is regular.

Similarly, $Mm_{sde}(G) \leq 2AG(G) - \sqrt{\frac{\delta}{\Delta}}m$ so that equality occurs if and only if G is regular or semiregular bipartite graph. \square

Lemma 5. *Let p and q be real numbers such that $p \geq q \geq 0$. Then*

(a) $\sqrt{p-q} \geq \sqrt{p} - \sqrt{q}$ with equality if and only if $p = q$ or $q = 0$.

(b) $\sqrt{p+q} \geq \frac{1}{\sqrt{2}}(\sqrt{p} + \sqrt{q})$ with equality if and only if $p = q$.

Proof. we know

$$\sqrt{p} - \sqrt{q} - \sqrt{p-q} = \frac{p-p+q}{\sqrt{p} + \sqrt{p-q}} - \sqrt{q} = \frac{q}{\sqrt{p} + \sqrt{p-q}} - \sqrt{q}.$$

Since $p \geq q$, we have $\sqrt{p} - \sqrt{q} - \sqrt{p-q} \leq \frac{q}{\sqrt{q}} - \sqrt{q} = 0$. Consequently, $\sqrt{p} - \sqrt{q} \leq \sqrt{p-q}$ with equality if and only if $p = q$ or $q = 0$.

Again, we have $(\sqrt{p} - \sqrt{q})^2 \geq 0$ which implies $2(p+q) \geq p + 2\sqrt{pq} + q$. i.e.,

$$p + q \geq \frac{1}{2}(\sqrt{p} + \sqrt{q})^2$$

resulting in,

$$\sqrt{p+q} \geq \frac{1}{\sqrt{2}}(\sqrt{p} + \sqrt{q}).$$

The equality occurs if and only if $p = q$. □

Theorem 7. *Let G be a graph of size m with maximum and minimum degrees Δ and δ , respectively. Then*

$$Mm_{sde}(G) \geq \sqrt{\frac{\delta}{2}}ABC(G) + \frac{m}{\sqrt{\Delta}} - m, \quad (3.2)$$

with equality if and only if $G \cong nK_1$.

Proof. We have

$$\begin{aligned} Mm_{sde}(G) &= \sum_{x \sim y} \sqrt{\frac{d_x}{d_y}} \\ &= \sum_{x \sim y} \sqrt{\frac{d_x + d_y}{d_y} - 1} \\ &\geq \sum_{x \sim y} \sqrt{\frac{d_x + d_y - 2 + 2}{d_y}} - m \quad \text{by Lemma 5} \\ &\geq \sum_{x \sim y} \sqrt{\frac{d_x + d_y - 2}{2d_y}} + \sum_{x \sim y} \sqrt{\frac{2}{2d_y}} - m \quad \text{by Lemma 5} \\ &= \sum_{x \sim y} \sqrt{\frac{d_x}{2}} \cdot \sqrt{\frac{d_x + d_y - 2}{d_x d_y}} + \sum_{x \sim y} \frac{1}{\sqrt{d_y}} - m \\ &\geq \sqrt{\frac{\delta}{2}}ABC(G) + \frac{m}{\sqrt{\Delta}} - m. \end{aligned}$$

The equality occurs in equation 3.2 if the inequalities above become equalities. Applying Lemma 5 for equalities in the above inequalities, we must have $G \cong nK_1$. Conversely, if $G = nK_1$, then $Mm_{sde}(G) = 0 = \sqrt{\frac{1}{2}}.0 + m - m$. Hence, the result follows. □

Corollary 7. *Let G be a nontrivial connected graph of size m with maximum and minimum degrees Δ and δ , respectively. Then*

$$Mm_{sde}(G) > \sqrt{\frac{\delta}{2}} ABC(G) + \frac{m}{\sqrt{\Delta}} - m.$$

4. Graph energy and max-min rodeg index

In [3], Arizmendi et al. showed that the energy of a graph G can be expressed as $\epsilon(G) = \sum_{i=1}^n \epsilon_{v_i}$, where ϵ_{v_i} is the energy of a vertex v_i . Also, they proved that if $e = xy$ is an edge of G , then

$$\epsilon(e) = \frac{\epsilon_x}{d_x} + \frac{\epsilon_y}{d_y}.$$

Theorem 8. ([2], Theorem 3) *If $e = xy$ is an edge of a simple (undirected) graph. Then $\epsilon_x \epsilon_y \geq 1$.*

Theorem 9. *For a graph G with maximum degree Δ and minimum degree δ , we have*

$$\frac{\delta \epsilon(G)}{2\sqrt{\Delta}} \leq Mm_{sde}(G) \leq \frac{\epsilon(G)\Delta}{2}.$$

Equality holds on left if and only if G is union of K_2 , and on right if and only if G is a disjoint union of complete bipartite graphs.

Proof. For an edge $e = xy$ of G , we have

$$\epsilon(G) = \sum_{x \sim y} \left(\frac{\epsilon_x}{d_x} + \frac{\epsilon_y}{d_y} \right). \quad (4.1)$$

If $e = xy$, then by applying the AM-GM inequality and the condition $\epsilon_x \epsilon_y \geq 1$ (see Theorem 8), we have

$$\epsilon(e) = \frac{\epsilon_x}{d_x} + \frac{\epsilon_y}{d_y} \geq 2\sqrt{\frac{\epsilon_x \epsilon_y}{d_x d_y}} \geq \frac{2}{d_x} \sqrt{\frac{d_x}{d_y}}.$$

Consequently, we have $\epsilon(G) = \sum_{x \sim y} \left(\frac{\epsilon_x}{d_x} + \frac{\epsilon_y}{d_y} \right) \geq \sum_{x \sim y} \frac{2}{d_x} \sqrt{\frac{d_x}{d_y}} \geq \frac{2Mm_{sde}(G)}{\Delta}$. If $Mm_{sde}(G) = \frac{\epsilon(G)\Delta}{2}$, then all the above inequalities become equality. Then we must have $\frac{\epsilon_x}{d_x} + \frac{\epsilon_y}{d_y} = 2\sqrt{\frac{\epsilon_x \epsilon_y}{d_x d_y}}$, which is the only possible if $\frac{\epsilon_x}{d_x} = \frac{\epsilon_y}{d_y}$. Also, from $\epsilon_x \epsilon_y = 1$, we have

$$\epsilon_x = \sqrt{\frac{d_x}{d_y}}.$$

As the left-hand side is independent of y , $d_{n_x} = d_y$, where n_x is a neighbor of x . Similarly, $d_{n_y} = d_x$, where n_y is a neighbor of y . So, two cases arise:

- (a) If $d_x = d_y = d$, then G is d -regular and hence $Mm_{sde}(G) = \frac{dn}{2}$. For $\epsilon(G) = \frac{2Mm_{sde}(G)}{\Delta} = \frac{2}{d} \cdot \frac{dn}{2} = n$, G must be $K_{d,d}$ for some positive integers d ([6], Theorem 3).
- (b) If $d_x \neq d_y$, we can write $V(G) = V_1 \cup V_2$, where any vertex in V_i is of degree d_{v_i} for $i \in \{1, 2\}$ and end vertices of any edge belongs to both V_1 and V_2 . Hence G is a bipartite semiregular graph. If $|V_1| = n_1$, $|V_2| = n_2$, and $d_{v_1} \geq d_{v_2}$ then

$$Mm_{sde}(G) = n_1 d_{v_1} \sqrt{\frac{d_{v_1}}{d_{v_2}}} = n_2 d_{v_2} \sqrt{\frac{d_{v_1}}{d_{v_2}}}.$$

Now, for $Mm_{sde}(G) = \frac{\epsilon(G)\Delta}{2}$, we must have $\epsilon(G) = n_1 \sqrt{\frac{d_{v_1}}{d_{v_2}}} + n_2 \sqrt{\frac{d_{v_2}}{d_{v_1}}}$, because then

$$\begin{aligned} \epsilon(G) &= n_1 \sqrt{\frac{d_{v_1}}{d_{v_2}}} + n_2 \sqrt{\frac{d_{v_2}}{d_{v_1}}} \\ &= \frac{1}{\Delta} [n_1 \Delta \sqrt{\frac{d_{v_1}}{d_{v_2}}} + n_2 \Delta \sqrt{\frac{d_{v_2}}{d_{v_1}}}] \\ &= \frac{1}{\Delta} [n_1 d_{v_1} \sqrt{\frac{d_{v_1}}{d_{v_2}}} + n_2 d_{v_2} \sqrt{\frac{d_{v_1}}{d_{v_2}}}] \\ &= \frac{2Mm_{sde}(G)}{\Delta}. \end{aligned}$$

This occurs only if $G \cong K_{d_{v_1}, d_{v_2}}$ ([6], Theorem 5).

Again, by the definition of the energy of a graph and the fact that $\epsilon_{x_i} \leq \sqrt{d_{x_i}}$ for any vertex $x_i \in V(G)$ ([3], Proposition 3.2), we have

$$\begin{aligned} \epsilon(G) &= \sum_{e \in E(G)} \epsilon(e) = \sum_{x \sim y} \left(\frac{\epsilon_x}{d_x} + \frac{\epsilon_y}{d_y} \right) \\ &\leq \sum_{x \sim y} \left(\frac{\sqrt{d_x}}{d_x} + \frac{\sqrt{d_y}}{d_y} \right) \\ &= \sum_{x \sim y} \frac{\sqrt{d_x} + \sqrt{d_y}}{\sqrt{d_x d_y}} \\ &= \sum_{x \sim y} \frac{\sqrt{d_x} + \sqrt{d_y}}{d_x} \cdot \sqrt{\frac{d_x}{d_y}} \\ &\leq \frac{2\sqrt{\Delta} Mm_{sde}(G)}{\delta}. \end{aligned}$$

Consequently, $Mm_{sde}(G) \geq \frac{\delta \epsilon(G)}{2\sqrt{\Delta}}$. Equality will exist if and only if G is union of K_2 ([3], Proposition 3.2). \square

5. Max-min rodeg index of chemical graphs

For a chemical graph G with $\delta(G) \geq 1$, one can easily observe that

$$d_1 + d_2 + d_3 + d_4 = n \quad (5.1)$$

and

$$\begin{aligned} 2E_{1,1} + E_{1,2} + E_{1,3} + E_{1,4} &= d_1 \\ E_{1,2} + 2E_{2,2} + E_{2,3} + E_{2,4} &= 2d_2 \\ E_{1,3} + E_{2,3} + 2E_{3,3} + E_{3,4} &= 3d_3 \\ E_{1,4} + E_{2,4} + E_{3,4} + 2E_{4,4} &= 4d_4. \end{aligned} \quad (5.2)$$

Let $\mathbb{A} = \{(s, t) \in \mathbb{N} \times \mathbb{N} : 1 \leq s \leq t \leq 4\}$. Then from Equation 5.1 and 5.2, we have

$$n = \sum_{(x,y) \in \mathbb{A}} \frac{x+y}{xy} E_{x,y}. \quad (5.3)$$

Also we have

$$Mm_{sde}(G) = \sum_{(x,y) \in \mathbb{A}} \sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} E_{x,y}. \quad (5.4)$$

Theorem 10. *For a n -vertex chemical graph G , we have*

$$Mm_{sde}(G) \leq 2n,$$

with equality if and only if G is a 4-regular graph.

Proof. Applying Equation 5.4, we have

$$\begin{aligned} Mm_{sde}(G) &= \sum_{(x,y) \in \mathbb{A}} \sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} E_{x,y} \\ &= E_{4,4} + \sum_{(x,y) \in \mathbb{A} - \{(4,4)\}} \sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} E_{x,y} \\ &= 2n - \sum_{(x,y) \in \mathbb{A} - \{(4,4)\}} \frac{2x+2y}{xy} E_{x,y} + \sum_{(x,y) \in \mathbb{A} - \{(4,4)\}} \sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} E_{x,y} \\ &= 2n + \sum_{(x,y) \in \mathbb{A} - \{(4,4)\}} \left(\sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} - \frac{2x+2y}{xy} \right) E_{x,y}. \end{aligned}$$

One can easily check that $\sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} - \frac{2x+2y}{xy} < 0$ for all $(x,y) \in \mathbb{A} - \{(4,4)\}$. Therefore,

$$Mm_{sde}(G) \leq 2n. \quad (5.5)$$

If $Mm_{sde}(G) = 2n$, then we have $2n = 2n + \sum_{(x,y) \in \mathbb{A} - \{(4,4)\}} (\sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} - \frac{2x+2y}{xy}) E_{x,y}$. Since $\sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} - \frac{2x+2y}{xy} < 0$ for all $(x,y) \in \mathbb{A} - \{(4,4)\}$, we have $E_{x,y} = 0$ for all $(x,y) \in \mathbb{A} - \{(4,4)\}$. Hence, G is a 4-regular graph.

Conversely, if G is a 4 regular graph, then $Mm_{sde} = E_{4,4} = m = \frac{4n}{2} = 2n$. \square

Theorem 11. For a n -vertex chemical graph G , we have

$$Mm_{sde}(G) \geq \begin{cases} \frac{n}{2} & \text{if } n \text{ is even} \\ \frac{n-3}{2} + 2\sqrt{2} & \text{if } n \text{ is odd.} \end{cases}$$

Equality occurs if and only if $G \cong \frac{n}{2}P_2$ (when n is even) or $G \cong \frac{n-3}{2}P_2 \oplus P_3$ (when n is odd).

Proof. From Equation 5.4, we have

$$\begin{aligned} Mm_{sde}(G) &= E_{1,1} + \sum_{(x,y) \in \mathbb{A} - \{(1,1)\}} \sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} \\ &= \frac{1}{2}(n - \sum_{(x,y) \in \mathbb{A} - \{(1,1)\}} \frac{x+y}{xy} E_{x,y}) + \sum_{(x,y) \in \mathbb{A} - \{(1,1)\}} \sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} \\ &= \frac{n}{2} + \sum_{(x,y) \in \mathbb{A} - \{(1,1)\}} (\sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} - \frac{x+y}{2xy}) E_{x,y}. \end{aligned}$$

One can easily check that

$$\sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} - \frac{x+y}{2xy} > 0 \quad (5.6)$$

for all $(x,y) \in \mathbb{A} - \{(1,1)\}$. Therefore

$$Mm_{sde} \geq \frac{n}{2}. \quad (5.7)$$

If $Mm_{sde} = \frac{n}{2}$, then

$\frac{n}{2} = \frac{n}{2} + \sum_{(x,y) \in \mathbb{A} - \{(1,1)\}} (\sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} - \frac{x+y}{2xy}) E_{x,y}$. Applying relation 5.6, we have $E_{x,y} = 0$ for all $(x,y) \in \mathbb{A} - \{(1,1)\}$. Since n is even clearly $G \cong \frac{n}{2}P_2$. Conversely, if $G \cong \frac{n}{2}P_2$ then $Mm_{sde}(G) = \frac{n}{2}$.

Let $\mathbb{T} = \mathbb{A} - \{(1, 1), (1, 2)\}$. Therefore

$$\begin{aligned} Mm_{sde}(G) &= E_{1,1} + \sqrt{2}E_{1,2} + \sum_{(x,y) \in \mathbb{T}} \sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} E_{x,y} \\ &= E_{1,1} + \frac{2\sqrt{2}}{3} \left(n - 2E_{1,1} - \sum_{(x,y) \in \mathbb{T}} \frac{x+y}{xy} E_{x,y} \right) + \sum_{(x,y) \in \mathbb{T}} \sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} \\ &= \frac{2\sqrt{2}n}{3} + \left(1 - \frac{4\sqrt{2}}{3}\right) E_{1,1} + \sum_{(x,y) \in \mathbb{T}} \left(\sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} - \frac{2\sqrt{2}(x+y)}{3xy} \right) E_{x,y}. \end{aligned}$$

Since $\delta(G) \geq 1$, we have $E_{1,1} \leq \frac{n-3}{2}$. Also, one can easily check that

$$\sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}} - \frac{2\sqrt{2}(x+y)}{3xy} > 0 \quad (5.8)$$

for all $(x, y) \in \mathbb{T}$. Hence, applying all these conditions, we have

$$Mm_{sde}(G) \geq \frac{2\sqrt{2}n}{3} + \left(1 - \frac{4\sqrt{2}}{3}\right) \frac{n-3}{2} = \frac{n-3}{2} + 2\sqrt{2}.$$

If $Mm_{sde}(G) = \frac{n-3}{2} + 2\sqrt{2}$, we have $E_{1,1} = \frac{n-3}{2}$ and $E_{x,y} = 0$ for all $(x, y) \in \mathbb{T}$. This implies $G \cong \frac{n-3}{2} P_2 \oplus P_3$.

Conversely, if $G \cong \frac{n-3}{2} P_2 \oplus P_3$, then $Mm_{sde}(G) = \frac{n-3}{2} + 2\sqrt{2}$. \square

By applying Theorem 10 and Theorem 2 of [16], the following result is immediate.

Theorem 12. *Let G be a connected chemical graph. Then*

$$2\sqrt{2} + n - 3 \leq Mm_{sde}(G) \leq 2n.$$

Equality occurs on the left if and only if $G \cong P_n$, and on the right if and only if G is a connected 4-regular graph.

Conclusion

In this paper, we have analyzed the max-min rodeg index of a graph. Here, we present some lower bounds for max-min rodeg index using some established inequalities and upper bounds in terms of some graph parameters such as clique number, algebraic connectivity, vertex connectivity, and spectral radius. We provide sharp bounds for the max-min rodeg index of a triangle-free graph. Also, we establish a mathematical relation between the max-min rodeg index and other topological indices. Then, we obtain a relation between the energy of a graph and the max-min rodeg index of a

graph, and also characterize the corresponding extremal graphs. Finally, we characterize the graph extremal with respect to the max-min rodeg index over chemical graphs.

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