Research Article

On the Randić Index of Corona Product Graphs

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Let G be a graph with vertex set $V = (v_1, v_2, \dots, v_n)$. Let $\delta(v_i)$ be the degree of the vertex $v_i \in V$. If the vertices $v_{i_1}, v_{i_2}, \dots, v_{i_{h+1}}$ form a path of length $h \geq 1$ in the graph G , then the h th order Randić index R_h of G is defined as the sum of the terms $1/\sqrt{\delta(v_{i_1})\delta(v_{i_2})\cdots\delta(v_{i_{h+1}})}$ over all paths of length h contained (as subgraphs) in G . Lower and upper bounds for R_h , in terms of the vertex degree sequence of its factors, are obtained for corona product graphs. Moreover, closed formulas are obtained when the factors are regular graphs.

1. Introduction

In this work we consider simple graphs $G = (V, E)$ with n vertices and m edges. Let $V = (v_1, v_2, \dots, v_n)$ be the vertex set of G . For every vertex $v_i \in V$, $\delta(v_i)$ represents the degree of the vertex v_i in G . The maximum and minimum degree of the vertices of G will be denoted by Δ and δ , respectively.

The Randić index $R_1(G)$ of a graph G was introduced in 1975 [1] and defined as

$$R_1(G) = \sum_{v_i v_j \in E} \frac{1}{\sqrt{\delta(v_i)\delta(v_j)}}. \quad (1.1)$$

This graph invariant, sometimes referred to as connectivity index, has been successfully related to a variety of physical, chemical, and pharmacological properties of organic molecules, and it has become into one of the most popular molecular-structure descriptors. After the publication of the first paper [1], mathematical properties of R_1 were extensively studied, see [2–6] and the references cited therein.

The higher-order Randić indices are also of interest in chemical graph theory. For $h \geq 1$, the h th order Randić index $R_h(G)$ of a graph G is defined as

$$R_h(G) = \sum_{v_{i_1} v_{i_2} \dots v_{i_{h+1}} \in \mathcal{P}_h(G)} \frac{1}{\sqrt{\delta(v_{i_1}) \delta(v_{i_2}) \dots \delta(v_{i_{h+1}})}}, \quad (1.2)$$

where $\mathcal{P}_h(G)$ denotes the set of paths of length h contained (as subgraphs) in G . Of the higher-order Randić indices the most frequently applied is R_2 [7–10]. Estimations of the higher-order Randić index of regular graphs and semiregular bipartite graphs are given in [10]. In this paper we are interested in studying the higher-order Randić index, R_h , for corona product graphs. Roughly speaking, we study the cases $h = 1$, $h = 2$ for arbitrary graphs and the case $h \geq 3$ when the second factor of the corona product is an empty graph. As an example of a chemical compound whose graph is obtained as a corona product graph we consider the Cycloalkanes with a single ring, whose chemical formula is $C_k H_{2k}$, and whose molecular graph can be expressed as $C_k \odot N_2$, where C_k is the cycle graph of order k and N_2 is the empty graph of order two. We recall that, given two graphs G and H of order n_1 and n_2 , respectively, the corona product $G \odot H$ is defined as the graph obtained from G and H by taking one copy of G and n_1 copies of H and then joining by an edge each vertex of the i th copy of H with the i th vertex of G .

2. Estimating R_h for Corona Graphs

Theorem 2.1. For $i \in \{1, 2\}$, let G_i be a graph of minimum degree δ_i , maximum degree Δ_i , order n_i and size m_i . Then,

$$\begin{aligned} R_1(G_1 \odot G_2) &\leq \frac{m_1}{\delta_1 + n_2} + \frac{n_1 m_2}{\delta_2 + 1} + \frac{n_1 n_2}{\sqrt{(\delta_1 + n_2)(\delta_2 + 1)}}, \\ R_1(G_1 \odot G_2) &\geq \frac{m_1}{\Delta_1 + n_2} + \frac{n_1 m_2}{\Delta_2 + 1} + \frac{n_1 n_2}{\sqrt{(\Delta_1 + n_2)(\Delta_2 + 1)}}. \end{aligned} \quad (2.1)$$

Proof. Let $G_i = (V_i, E_i)$, $i \in \{1, 2\}$, and let $G_1 \odot G_2 = (V, E)$. We have

$$R_1(G_1 \odot G_2) = \sum_{xy \in E} \frac{1}{\sqrt{\delta(x) \delta(y)}} = Q_1 + Q_2 + Q_3, \quad (2.2)$$

where

$$\begin{aligned} Q_1 &= \sum_{ab \in E_1} \frac{1}{\sqrt{(\delta(a) + n_2)(\delta(b) + n_2)}} \geq \frac{m_1}{\Delta_1 + n_2}, \\ Q_2 &= \sum_{uv \in E_2} \frac{1}{\sqrt{(\delta(u) + 1)(\delta(v) + 1)}} \geq \frac{n_1 m_2}{\Delta_2 + 1}, \\ Q_3 &= \sum_{a \in V_1, u \in V_2} \frac{1}{\sqrt{(\delta(a) + n_2)(\delta(u) + 1)}} \geq \frac{n_1 n_2}{\sqrt{(\Delta_1 + n_2)(\Delta_2 + 1)}}. \end{aligned} \quad (2.3)$$

Thus, the lower bound follows. Analogously we deduce the upper bound. $\square$

Corollary 2.2. For $i \in \{1, 2\}$, let G_i be a δ_i -regular graph of order n_i . Then,

$$R_1(G_1 \odot G_2) = \frac{n_1 \delta_1}{2(\delta_1 + n_2)} + \frac{n_1 n_2 \delta_2}{2(\delta_2 + 1)} + \frac{n_1 n_2}{\sqrt{(\delta_1 + n_2)(\delta_2 + 1)}}. \quad (2.4)$$

Theorem 2.3. For $i \in \{1, 2\}$, let G_i be a graph of minimum degree δ_i , maximum degree Δ_i , order n_i , and size m_i . Then,

$$\begin{aligned} R_2(G_1 \odot G_2) &\leq \frac{n_1}{(\delta_2 + 1)\sqrt{\delta_1 + n_2}} \left(\frac{n_2(n_2 - 1)}{2} + 2m_2 \right) \\ &\quad + \frac{1}{\delta_1 + n_2} \left(\frac{2n_2 m_1}{\sqrt{\delta_2 + 1}} + \sum_{\delta(v_i) \geq 2} \frac{\delta(v_i)(\delta(v_i) - 1)}{2\sqrt{\delta(v_i) + n_2}} \right) \\ &\quad + \frac{1}{2(\delta_2 + 1)} \sum_{\delta(u_i) \geq 2} \frac{\delta(u_i)(\delta(u_i) - 1)}{\sqrt{\delta(u_i) + 1}}, \\ R_2(G_1 \odot G_2) &\geq \frac{n_1}{(\Delta_2 + 1)\sqrt{\Delta_1 + n_2}} \left(\frac{n_2(n_2 - 1)}{2} + 2m_2 \right) \\ &\quad + \frac{1}{\Delta_1 + n_2} \left(\frac{2n_2 m_1}{\sqrt{\Delta_2 + 1}} + \sum_{\delta(v_i) \geq 2} \frac{\delta(v_i)(\delta(v_i) - 1)}{2\sqrt{\delta(v_i) + n_2}} \right) \\ &\quad + \frac{1}{2(\Delta_2 + 1)} \sum_{\delta(u_i) \geq 2} \frac{\delta(u_i)(\delta(u_i) - 1)}{\sqrt{\delta(u_i) + 1}}. \end{aligned} \quad (2.5)$$

Proof. Let $V_1 = \{v_1, v_2, \dots, v_{n_1}\}$ and $V_2 = \{u_1, u_2, \dots, u_{n_2}\}$ be the set of vertices of G_1 and G_2 , respectively. Given a vertex $v \in V_i$, we denote by $N_{G_i}(v)$ the set of neighbors that v has in G_i . The paths of length two in $G_1 \odot G_2$ are obtained as follows:

- (i) paths $u_i v_j u_k$, $i \neq k$, where $u_i, u_k \in V_2$ and $v_j \in V_1$,
- (ii) paths $u_i v_j v_k$, $j \neq k$, where $u_i \in V_2$ and $v_j, v_k \in V_1$,
- (iii) paths $v_i u_j u_k$, $j \neq k$, where $v_i \in V_1$ and $u_j, u_k \in V_2$,
- (iv) paths of length two belonging to G_1 ,
- (v) paths of length two belonging to the n_1 copies of G_2 .

So, we have $R_2(G_1 \odot G_2) = \sum_{i=1}^5 Q_i$, where

$$\begin{aligned} Q_1 &= \sum_{v_j \in V_1; u_i, u_k \in V_2} \frac{1}{\sqrt{(\delta(u_i) + 1)(\delta(v_j) + n_2)(\delta(u_k) + 1)}} \\ &= \sum_{j=1}^{n_1} \frac{1}{\sqrt{\delta(v_j) + n_2}} \cdot \sum_{i=1}^{n_2-1} \sum_{l=i+1}^{n_2} \frac{1}{\sqrt{(\delta(u_i) + 1)(\delta(u_l) + 1)}} \\ &\geq \frac{n_1 n_2 (n_2 - 1)}{2(\Delta_2 + 1)\sqrt{\Delta_1 + n_2}} \end{aligned} \quad (2.6)$$

corresponds to the paths type (i),

$$\begin{aligned}
 Q_2 &= \sum_{u_i \in V_2; v_j, v_k \in V_1} \frac{1}{\sqrt{(\delta(u_i) + 1)(\delta(v_j) + n_2)(\delta(v_k) + n_2)}} \\
 &= \sum_{i=1}^{n_2} \frac{1}{\sqrt{\delta(u_i) + 1}} \cdot \sum_{j=1}^{n_1} \sum_{v_l \in N_{G_1}(v_j)} \frac{1}{\sqrt{(\delta(v_j) + n_2)(\delta(v_l) + n_2)}} \\
 &\geq \frac{2m_1 n_2}{(\Delta_1 + n_2)\sqrt{\Delta_2 + 1}}
 \end{aligned} \tag{2.7}$$

corresponds to the paths type (ii),

$$\begin{aligned}
 Q_3 &= \sum_{v_i \in V_1; u_j, u_k \in V_2} \frac{1}{\sqrt{(\delta(v_i) + n_2)(\delta(u_j) + 1)(\delta(u_k) + 1)}} \\
 &= \sum_{i=1}^{n_1} \frac{1}{\sqrt{\delta(v_i) + n_2}} \cdot \sum_{j=1}^{n_2} \sum_{u_l \in N_{G_2}(u_j)} \frac{1}{\sqrt{(\delta(u_j) + 1)(\delta(u_l) + 1)}} \\
 &\geq \frac{2n_1 m_2}{(\Delta_2 + 1)\sqrt{\Delta_1 + n_2}}
 \end{aligned} \tag{2.8}$$

corresponds to the paths type (iii),

$$\begin{aligned}
 Q_4 &= \sum_{v_i, v_j, v_k \in \mathcal{P}(G_1)} \frac{1}{\sqrt{(\delta(v_i) + n_2)(\delta(v_j) + n_2)(\delta(v_k) + n_2)}} \\
 &\geq \frac{1}{2(\Delta_1 + n_2)} \sum_{\delta(v_i) \geq 2} \frac{\delta(v_i)(\delta(v_i) - 1)}{\sqrt{\delta(v_i) + n_2}}
 \end{aligned} \tag{2.9}$$

corresponds to the paths type (iv), and

$$\begin{aligned}
 Q_5 &= \sum_{u_i, u_j, u_k \in \mathcal{P}(G_2)} \frac{1}{\sqrt{(\delta(u_i) + 1)(\delta(u_j) + 1)(\delta(u_k) + 1)}} \\
 &\geq \frac{1}{2(\Delta_2 + 1)} \sum_{\delta(u_i) \geq 2} \frac{\delta(u_i)(\delta(u_i) - 1)}{\sqrt{\delta(u_i) + 1}}
 \end{aligned} \tag{2.10}$$

corresponds to the paths type (v). Thus, the lower bound follows. The upper bound is obtained by analogy. $\square$

Corollary 2.4. For $i \in \{1, 2\}$, let G_i be a δ_i -regular graph of order n_i . Then,

$$\begin{aligned} R_2(G_1 \odot G_2) &= \frac{n_1 n_2}{(\delta_2 + 1)\sqrt{\delta_1 + n_2}} \left(\frac{n_2 - 1}{2} + \delta_2 \right) \\ &\quad + \frac{n_1 \delta_1}{2(\delta_1 + n_2)} \left(\frac{2n_2}{\sqrt{\delta_2 + 1}} + \frac{\delta_1 - 1}{\sqrt{\delta_1 + n_2}} \right) + \frac{n_2 \delta_2 (\delta_2 - 1)}{2(\delta_2 + 1)\sqrt{\delta_2 + 1}}. \end{aligned} \quad (2.11)$$

The girth of a graph is the size of its smallest cycle. For instance, the molecular graphs of benzenoid hydrocarbons have girth 6. The molecular graphs of biphenylene and azulene have girth 4 and 5, respectively [11].

The following result, and its proof, was implicitly obtained in the proof of Theorem 1 of [10]. By completeness, here we present it as a separate result.

Lemma 2.5. Let $G = (V, E)$ be a graph with girth $g(G)$. If $\delta \geq 2$ and $g(G) > h$, then the number of paths of length h in G is bounded by

$$\frac{(\delta - 1)^{h-2}}{2} \sum_{u \in V} \delta(u)(\delta(u) - 1) \leq |\mathcal{P}_h(G)| \leq \frac{(\Delta - 1)^{h-2}}{2} \sum_{u \in V} \delta(u)(\delta(u) - 1). \quad (2.12)$$

Proof. Since $\delta \geq 2$, for every $v \in V$, the number of paths of length 2 in G of the form $v_i v v_j$ is $\delta(v)(\delta(v) - 1)/2$. Therefore, the result follows for $h = 2$.

Suppose now that $h \geq 3$. Given a vertex $u \in V$, let $\mathcal{P}_h(u)$ be the set of paths of length h whose second vertex is u , that is, paths of the form $u_1 u u_2 \cdots u_h$. We denote by $N(v)$ the set of neighbors of an arbitrary vertex $v \in V$. Note that the degree of v is $\delta(v) = |N(v)|$. If $\delta \geq 2$, then for every $v \in V$ and $w \in N(v)$ we have $N(w) \setminus \{v\} \neq \emptyset$. So, for every $u \in V$, there exists a vertex sequence $u_1 u u_2 \cdots u_h$ such that $u_1, u_2 \in N(u)$, $u_3 \in N(u_2) \setminus \{u\}$, $u_4 \in N(u_3) \setminus \{u_2\}, \dots$, and $u_h \in N(u_{h-1}) \setminus \{u_{h-2}\}$. If $g(G) > h$, then the sequence $u_1 u u_2 \cdots u_h$ is a path. Conversely, every path of length h whose second vertex is u can be constructed as above. Hence, the number of paths of length h whose second vertex is u is bounded by

$$\begin{aligned} |\mathcal{P}_h(u)| &\geq \min_{u_1 u u_2 \cdots u_h \in \mathcal{P}_h(u)} \left\{ \delta(u)(\delta(u) - 1) \prod_{j=2}^{h-1} (\delta(u_j) - 1) \right\} \\ &\geq \delta(u)(\delta(u) - 1)(\delta - 1)^{h-2}, \\ |\mathcal{P}_h(u)| &\leq \max_{u_1 u u_2 \cdots u_h \in \mathcal{P}_h(u)} \left\{ \delta(u)(\delta(u) - 1) \prod_{j=2}^{h-1} (\delta(u_j) - 1) \right\} \\ &\leq \delta(u)(\delta(u) - 1)(\Delta - 1)^{h-2}. \end{aligned} \quad (2.13)$$

Thus, the result follows. □

Now N_k denotes the empty graph of order k .

Theorem 2.6. Let $G = (V, E)$ be a graph with girth $g(G)$, minimum degree δ , and maximum degree Δ . If $\delta \geq 2$ and $g(G) > h \geq 3$, then

$$\begin{aligned} R_h(G \odot N_k) &\leq \left(\frac{\Delta - 1}{2\sqrt{\delta + k}} + k \right) \frac{(\Delta - 1)^{h-3}}{(\delta + k)^{h/2}} \sum_{u \in V} \delta(u)(\delta(u) - 1), \\ R_h(G \odot N_k) &\geq \left(\frac{\delta - 1}{2\sqrt{\Delta + k}} + k \right) \frac{(\delta - 1)^{h-3}}{(\Delta + k)^{h/2}} \sum_{u \in V} \delta(u)(\delta(u) - 1). \end{aligned} \quad (2.14)$$

Proof. The paths of length h in G contribute to $R_h(G \odot N_k)$ in

$$\sum_{v_{i_1} v_{i_2} \dots v_{i_{h+1}} \in \mathcal{P}_h(G)} \frac{1}{\sqrt{\prod_{l=1}^{h+1} (\delta(v_{i_l}) + k)}}. \quad (2.15)$$

Moreover, each path of length $h - 1$ in G leads to $2k$ paths of length h in $G \odot N_k$; thus, the paths of length $h - 1$ in G contribute to $R_h(G \odot N_k)$ in

$$\sum_{v_{i_1} v_{i_2} \dots v_{i_h} \in \mathcal{P}_{h-1}(G)} \frac{2k}{\sqrt{\prod_{l=1}^h (\delta(v_{i_l}) + k)}}. \quad (2.16)$$

Hence,

$$\begin{aligned} R_h(G \odot N_k) &= \sum_{v_{i_1} v_{i_2} \dots v_{i_{h+1}} \in \mathcal{P}_h(G)} \frac{1}{\sqrt{\prod_{l=1}^{h+1} (\delta(v_{i_l}) + k)}} + \sum_{v_{i_1} v_{i_2} \dots v_{i_h} \in \mathcal{P}_{h-1}(G)} \frac{2k}{\sqrt{\prod_{l=1}^h (\delta(v_{i_l}) + k)}} \\ &\leq \frac{|\mathcal{P}_h(G)|}{\sqrt{(\delta + k)^{h+1}}} + 2k \frac{|\mathcal{P}_{h-1}(G)|}{\sqrt{(\delta + k)^h}}. \end{aligned} \quad (2.17)$$

By Lemma 2.5 we obtain the upper bound and the lower bound is obtained by analogy. $\square$

Corollary 2.7. Let $G = (V, E)$ be a δ -regular graph of order n and girth $g(G)$. If $\delta \geq 2$ and $g(G) > h \geq 3$, then

$$R_h(G \odot N_k) = \left(\frac{\delta - 1}{2\sqrt{\delta + k}} + k \right) \frac{n\delta(\delta - 1)^{h-2}}{(\delta + k)^{h/2}}. \quad (2.18)$$

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