ON N-VERTEX CHEMICAL GRAPHS WITH A FIXED CYCLOMATIC NUMBER AND MINIMUM GENERAL RANDIĆ INDEX

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The general Randić index of a graph G is defined as $R_\alpha(G) = \sum_{uv\in E(G)}(d_u d_v)^\alpha$, where d_u and d_v denote the degrees of the vertices u and v, respectively, α is a real number, and $E(G)$ is the edge set of G. The minimum number of edges of a graph G whose removal makes G as acyclic is known as the cyclomatic number and it is usually denoted by ν. A graph with the maximum degree at most 4 is known as a chemical graph. For $\nu = 0, 1, 2$ and $\alpha > 1$, the problem of finding graph(s) with the minimum general Randić index R_α among all n-vertex chemical graphs with the cyclomatic number ν has already been solved. In this paper, this problem is solved for the case when $\nu \geq 3$, $n \geq 5(\nu - 1)$, and $1 < \alpha < \alpha_0$, where $\alpha_0 \approx 11.4496$ is the unique positive root of the equation $4(8^\alpha - 6^\alpha) + 4^\alpha - 9^\alpha = 0$.

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1. INTRODUCTION AND STATEMENT OF THE MAIN RESULT

Every graph discussed in this paper is finite, simple, and connected. For a graph G, its vertex set and edge set are denoted by $V(G)$ and $E(G)$, respectively. The edge connecting the vertices $u, v \in V(G)$ and the degree of a vertex u are denoted by uv and d_u, respectively. By an n-vertex graph, we mean a graph of order n. The minimum and maximum vertex degrees of a graph are denoted by δ and Δ, respectively. The notation and terminology from (chemical) graph theory used in this paper, but not defined here, can be found in some standard books.

Chemical structures can be represented by graphs, in which vertices correspond to atoms and edges represent the covalent bond between atoms. Since an atom cannot be attached with more than four covalent bonds in a chemical compound, every graph of maximum degree at most 4 is called a chemical

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graph. Usually, only hydrogen-depleted chemical graphs are considered in literature, and we do the same here in this paper.

The graph invariants which have some chemical applicability are usually known as the topological indices in chemical graph theory [8]. One of the most studied and applied topological indices is the branching index (nowadays, also known as the connectivity index as well as the Randić index), which was proposed by Randić [29] within the study of molecular branching. For a graph G, this index is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} .$$

Detail about the chemical applicability of the Randić index can be found in the books [32, 16], surveys [30, 31] and related references cited therein. For the mathematical properties of this topological index, we refer the readers to the survey papers [27, 20], books [12, 18] and the related references cited therein.

Bollobás and Erdős [2] generalized the Randić index by replacing "$-\frac{1}{2}$" with an arbitrary real number α:

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha .$$

Nowadays, this topological index is known as the general Randić index. Here, we note that $R_1(G)$ is the well-known second Zagreb index [3, 11, 13].

Finding mathematical properties of the general Randić index is a topic of many publications. Li and Yang [23] addressed the problem of finding minimum and maximum general Randić indices of general graphs for any α. (An unsolved case was recently solved by Rada and Cruz [28].) Cavers *et al.* [5] derived an upper bound of R_{-1} for connected graphs and established a relation between $R_{-1}(G)$ and the normalized Laplacian eigenvalues of a graph G. Hu *et al.* [14, 15] found the minimum general Randić index of trees for any α and the maximum general Randić index of trees for $\alpha \leq -2$ and $\alpha \geq -\frac{1}{2}$. Li *et al.* [22] gave the minimum general Randić index of chemical trees with given number of pendent vertices for arbitrary α and characterized the corresponding extremal graphs. Guji and Vumar [10] attacked the problem of finding the maximum general Randić index of bicyclic graphs for $\alpha \geq 1$.

In [25], Liu *et al.* obtained a sharp lower bound and an upper bound of the general Randić index of trees with n vertices and k pendent vertices for $3 \leq k \leq n-2$ and $-1 \leq \alpha < 0$. Cui and Zhong [7] determined the maximum general Randić indices of trees and chemical trees with n vertices and k pendent vertices for $4 \leq k \leq \left\lfloor \frac{n+2}{3} \right\rfloor$ and $\alpha_0 \leq \alpha < 0$, where $\alpha_0 \approx -0.5122$. Further properties of the general Randicć index can be found in the papers [6, 9, 17, 19, 21, 24, 33].

The degree set of a graph is the set of all vertex degrees of the graph. A graph whose degree set consists of only two elements is called bidegreed graph. The minimum number of edges of a graph G whose removal makes G acyclic is known as the cyclomatic number and, usually, it is denoted by ν. Let $\mathcal{CG}_{n,\nu}$ be the class of all n-vertex chemical graphs with cyclomatic number ν. When $\alpha > 1$, the problem of finding graph(s) with minimum general Randić index R_α in the class $\mathcal{CG}_{n,\nu}$ was solved in: [14] for $\nu = 0$, [34] for $\nu = 1$, [26] for $\nu = 2$ (the references [14], [34] and [26] are actually concerned with the tree, unicyclic and bicyclic graphs, respectively. But the extremal graphs, determined there, are the chemical graphs and hence these graphs are also extremal in the corresponding classes of chemical graphs). In this paper, we attack this problem for $\nu \geq 3$ and prove the following theorem.

THEOREM 1. *If $\nu \geq 3$, $n \geq 5(\nu - 1)$ and $1 < \alpha < \alpha_0$, then only those bidegreed graphs with the degree set $\{2, 3\}$ whose no two vertices of degree 3 are adjacent, have the minimum R_α value (which is equal to $[n - 5(\nu - 1)]4^\alpha + 6(\nu - 1)6^\alpha$) in $\mathcal{CG}_{n,\nu}$, where $\alpha_0 \approx 11.4496$ is the unique positive root of the equation $4(8^\alpha - 6^\alpha) + 4^\alpha - 9^\alpha = 0$.*

2. PROOF OF THEOREM 1

In order to prove Theorem 1, we establish some preliminary lemmas. For this, we need to define some terminology and notation first. A vertex $v \in V(G)$ of degree 1 is called pendant vertex and a vertex with degree greater than 2 is known as the branching vertex. Let P: $v_1 v_2 \cdots v_r$ be a path in a graph G. If $r \geq 3$ then the vertices of P other than v_1, v_r are called internal vertices. A pendant path in a graph G is a path of length at least 1 in which every internal vertex (if it exists) has degree 2 in G and one of its remaining (non-internal) vertices is pendant and the other is branching. Let $A \subseteq E(G)$ and $B \subseteq E(\overline{G})$, where $\overline{G}$ is the complement of the graph G. Denote by $G - A + B$ the graph obtained from G by removing the edges of A and adding the edges of B. In what follows, whenever the graphs G and $G - A + B$ are under consideration, by writing d_u we mean the degree of the vertex u in G.

LEMMA 1. *For $\alpha > 1$ and $\nu \geq 1$, if H is a graph with minimum R_α value in $\mathcal{CG}_{n,\nu}$, then minimum degree of H is at least 2.*

Proof. Contrarily, we assume that the graph G contradicts the lemma for some n, ν and α (where $\alpha > 1$ and $\nu \geq 1$). Let $v v_1 v_2 \cdots v_r$ be a pendant path of length $r \geq 1$ in G, where v_r is a pendant vertex and v is a branching vertex. Suppose that u is a neighbor of v different from v_1 and let $G^{(1)} \cong$

$G - \{uv\} + \{uv_r\}$. It is evident that both graphs G and $G^{(1)}$ have the same cyclomatic number.

Case 1. $r = 1$.

We note that

$$\begin{aligned} R_\alpha(G) - R_\alpha(G^{(1)}) = &\sum_{x \in N_G(v)\setminus\{v_1,u\}} [(d_x d_v)^\alpha - (d_x(d_v-1))^\alpha] \\ &+ (d_u d_v)^\alpha - (2d_u)^\alpha + d_v^\alpha - (2(d_v-1))^\alpha \\ \geq &[(d_v)^\alpha - (d_v-1)^\alpha]\left((d_u)^\alpha + \sum_{x \in N_G(v)\setminus\{v_1,u\}} (d_x)^\alpha\right) \\ &- ((2(d_v-1))^\alpha - (d_v)^\alpha) \end{aligned} \tag{1}$$

Because of Lagrange's mean value theorem, there exist real numbers Θ_1, Θ_2 such that $d_v - 1 < \Theta_1 < d_v < \Theta_2 < 2(d_v - 1)$ and

$$\begin{aligned} &[(d_v)^\alpha - (d_v-1)^\alpha]\left((d_u)^\alpha + \sum_{x \in N_G(v)\setminus\{v_1,u\}} (d_x)^\alpha\right) \\ &\quad - ((2(d_v-1))^\alpha - (d_v)^\alpha) \\ &= \alpha\Theta_1^{\alpha-1}\left((d_u)^\alpha + \sum_{x \in N_G(v)\setminus\{v_1,u\}} (d_x)^\alpha\right) - \alpha(d_v-2)\Theta_2^{\alpha-1} \end{aligned} \tag{2}$$

Since G is not a star graph, the vertex v has at least one non-pendant neighbor and hence

$$\begin{aligned} &\alpha\Theta_1^{\alpha-1}\left((d_u)^\alpha + \sum_{x \in N_G(v)\setminus\{v_1,u\}} (d_x)^\alpha\right) - \alpha(d_v-2)\Theta_2^{\alpha-1} \\ &\quad > \alpha(2^\alpha\Theta_1^{\alpha-1} - (d_v-2)\Theta_2^{\alpha-1}) \end{aligned} \tag{3}$$

If $d_v = 3$ then $\Theta_2^{\alpha-1} < 2^{2\alpha-2} < 2^{2\alpha-1} < 2^\alpha\Theta_1^{\alpha-1}$ and hence from (1), (2) and (3), it follows that $R_\alpha(G) - R_\alpha(G^{(1)}) > 0$, which is a contradiction to the minimality of $R_\alpha(G)$.

If $d_v = 4$ then $2\Theta_2^{\alpha-1} < 2 \cdot 6^{\alpha-1} < 2^\alpha\Theta_1^{\alpha-1}$ and hence by using (1), (2) and (3), we have $R_\alpha(G) - R_\alpha(G^{(1)}) > 0$, which is again a contradiction.

Case 2. $r \geq 2$. In this case, we have

$$\begin{aligned} R_\alpha(G) - R_\alpha(G^{(1)}) = &\sum_{x \in N_G(v)\setminus\{v_1,u\}} [(d_x d_v)^\alpha - (d_x(d_v-1))^\alpha] \\ &+ (d_u d_v)^\alpha - (2d_u)^\alpha + (2d_v)^\alpha - (2(d_v-1))^\alpha - (4^\alpha - 2^\alpha) \end{aligned} \tag{4}$$

Bearing in mind the fact $d_v \geq 3$, we note that there exist real numbers θ_1, θ_2 such that $2 < \theta_2 < 4 \leq 2(d_v - 1) < \theta_1 < 2d_v$ and

$$(2d_v)^\alpha - (2(d_v-1))^\alpha - (4^\alpha - 2^\alpha) = 2\alpha\left(\theta_1^{\alpha-1} - \theta_2^{\alpha-1}\right),$$

which is positive for every $\alpha > 1$; this fact, together with, Equation (4) yield again a contradiction. □

LEMMA 2 ([1]). *For $n \geq 5(\nu-1)$, if $H \in \mathcal{CG}_{n,\nu}$ such that $\delta \geq 2$ and $\Delta \geq 4$, then H contains at least four vertices of degree 2.*

LEMMA 3 ([4]). *For $n \geq 5(\nu-1)$, if $H \in \mathcal{CG}_{n,\nu}$ such that $\delta \geq 2$ and $\Delta \geq 4$, then H contains at least one pair of adjacent vertices both of degree 2.*

LEMMA 4. *For $\nu \geq 3$, $1 < \alpha < \alpha_0$ and $n \geq 5(\nu-1)$, if H is a graph with the minimum R_α value in $\mathcal{CG}_{n,\nu}$, then maximum degree of H is 3, where $\alpha_0 \approx 11.4496$ is the unique positive root of the equation $4\cdot 8^\alpha + 4^\alpha - 3\cdot 6^\alpha - 9^\alpha = 0$.*

Proof. Suppose to the contrary that the graph G is a counter-example to the lemma for some n, ν and α. From Lemma 1, it follows that minimum degree of G is at least 2. Also, the assumption $\nu \geq 3$ implies that the maximum degree of G must be 4 because G is a counter-example to the lemma. From Lemma 3, it follows that G has at least one pair of adjacent vertices both of degree 2.

Case 1. G contains a pair of adjacent vertices both of degree 2 such that at least one of them is adjacent to a vertex having maximum degree.

Assume that $t_0, w_0 \in V(G)$ is a pair of adjacent vertices (both) of degree 2 such that $N_G(w_0) = \{u_0, t_0\}$ where u_0 is a vertex with maximum degree. Evidently, the vertex w_0 is not adjacent to at least two neighbors of u_0 (because $d_{u_0} = 4$ and $d_{w_0} = 2$). Let v_0 be one of such neighbors of u_0. If $G^{(1)} \cong G - \{u_0v_0\} + \{v_0w_0\}$ then

$$\begin{aligned} R_\alpha(G) - R_\alpha(G^{(1)}) &= \sum_{x \in N_G(u_0)\setminus\{v_0,w_0\}} [(4d_x)^\alpha - (3d_x)^\alpha] + (4d_{v_0})^\alpha - (3d_{v_0})^\alpha \\ &\quad + 8^\alpha - 9^\alpha + 4^\alpha - 6^\alpha \\ &\geq 2\left[8^\alpha - 6^\alpha\right] + 8^\alpha - 6^\alpha + 8^\alpha - 9^\alpha + 4^\alpha - 6^\alpha \\ &= 4(8^\alpha - 6^\alpha) + 4^\alpha - 9^\alpha \end{aligned}$$

which is positive for all values of α in the interval $(1, \alpha_0)$. Thus, $R_\alpha(G) - R_\alpha(G^{(1)}) > 0$, which is a contradiction to the minimality of $R_\alpha(G)$.

Case 2. For every pair of adjacent vertices $a, b \in V(G)$ of degree 2, neither of a, b is adjacent to a vertex having maximum degree.

Let $w_1, w_2, w_3 \in V(G)$ such that $d_{w_1} = d_{w_2} = 2$ and $w_1w_2, w_2w_3 \in E(G)$. Lemma 2 forces that G contains at least four vertices of degree 2.

Subcase 2.1. G contains a vertex of degree 2 adjacent to a vertex having maximum degree.

Let u be a vertex having maximum degree such that u is adjacent to a vertex w of degree 2 (note that $w \neq w_1, w_2$, otherwise it would come down to Case 1). Let $N_G(w) = \{u, t\}$, where the vertex t may be coincident with the vertex w_3.

Subcase 2.1.1. The vertices w_1 and w_3 are non-adjacent.

Whether the vertex w_3 coincides with the vertex t or not, in either case, we let $G^{(2)} \cong G - \{tw, w_1w_2, w_2w_3\} + \{w_2w, w_2t, w_1w_3\}$. Elementary calculations show that both the graphs G and $G^{(2)}$ have the same R_α value. We note that now the vertex w is adjacent to a vertex, namely w_2, having degree 2 in $G^{(2)}$. Hence, by Case 1, we can construct a graph $G^{(3)}$ from $G^{(2)}$ such that $R_\alpha(G^{(2)}) - R_\alpha(G^{(3)}) > 0$, which is a contradiction.

Subcase 2.1.2. The vertices w_1 and w_3 are adjacent.

If $t \neq w_3$, then the graphs $G^{(4)} \cong G - \{tw, w_1w_2\} + \{w_2w, w_1t\}$ and G have the same R_α value. Thereby, again by Case 1, we can construct graph $G^{(5)}$ from $G^{(4)}$ such that $R_\alpha(G^{(4)}) - R_\alpha(G^{(5)}) > 0$, which is again a contradiction.

Suppose in the following that $t = w_3$. Let $v \in N_G(u) \setminus \{t, w\}$, and we may choose v such that it is not adjacent to t.

If $d_v \geq 3$, then for the graph $G^{(6)} \cong G - \{uv, w_1w_2\} + \{w_1v, w_2u\}$, we have

$$R_\alpha(G) - R_\alpha(G^{(6)}) = (d_ud_v)^\alpha - (2d_u)^\alpha - (2d_v)^\alpha + 4^\alpha = (d_u^\alpha - 2^\alpha)(d_v^\alpha - 2^\alpha) > 0,$$

which contradicts the minimality of $R_\alpha(G)$.

Suppose that $d_v = 2$. Denote by v' the unique neighbor of v in G different from u. Clearly, v' is different from the vertices w, t, w_1, w_2. Let $G^{(7)} \cong G - \{v'v, w_1w_2\} + \{vw_1, v'w_2\}$. Elementary calculations show that both the graphs G and $G^{(7)}$ have the same R_α value. We note that now the vertex v is adjacent to a vertex, namely w_1, having degree 2 in $G^{(7)}$. Hence, by Case 1, we can construct a new graph $G^{(8)}$ having smaller R_α value than that of $G^{(7)}$, which gives again a contradiction.

Subcase 2.2. G does not contain any vertex of degree 2 adjacent to a vertex having maximum degree.

Let $u \in V(G)$ be a vertex with maximum degree. Clearly, there exists a vertex $t' \in V(G) \setminus N_G(u)$ of degree 2 which is not adjacent to at least one neighbor, say z of u, because $d_u = 4$. If $G^{(9)} \cong G - \{uz\} + \{t'z\}$ then

$$\begin{aligned} R_\alpha(G) - R_\alpha(G^{(9)}) = & \sum_{x \in N_G(u) \setminus \{z\}} [(4d_x)^\alpha - (3d_x)^\alpha] + \sum_{y \in N_G(t')} [(2d_y)^\alpha - (3d_y)^\alpha] \\ & + (4d_z)^\alpha - (3d_z)^\alpha. \end{aligned}$$

Since $d_x = 3$ or 4, $d_y = 2$ or 3, and the function $f(x) = (2x)^\alpha - (3x)^\alpha$ is decreasing in x (> 1) for every $\alpha > 1$, we have

$$R_\alpha(G) - R_\alpha(G^{(9)}) > 3\,[12^\alpha - 9^\alpha] + 2\,[6^\alpha - 9^\alpha] = 3\,[12^\alpha - 9^\alpha] - 2\,[9^\alpha - 6^\alpha] > 0$$

for every $\alpha > 1$. But, this is again a contradiction. $\square$

Let $x_{i,j}(G)$ (or simply $x_{i,j}$) be the number of edges in the graph G connecting the vertices of degrees i and j.

Lemma 5 ([1]). *For $\nu \geq 3$, assume that $G \in \mathcal{CG}_{n,\nu}$ has the degree set $\{2, 3\}$.*

(i) *If $n > 5(\nu - 1)$, then $x_{2,2} \geq 1$.*

(ii) *If $n = 5(\nu - 1)$, then $x_{2,2} = x_{3,3}$.*

Lemma 6. *For $\nu \geq 3$, $\alpha > 1$ and $n \geq 5(\nu - 1)$, if H minimizes R_α in $\mathcal{CG}_{n,\nu}$, then $x_{3,3} = 0$.*

Proof. Contrarily, suppose that under the given constrains, the graph G is a counter-example for some n, v and α. Lemmas 1 and 4 guarantee that G has the degree set $\{2, 3\}$. Suppose that $w, t \in V(G)$ are adjacent vertices such that $d_w = d_t = 3$.

If $x_{2,2} = 0$, then Lemma 5(i) implies that $n = 5(v - 1)$, and hence from Lemma 5(ii) it follows that $x_{3,3} = 0$, which is a contradiction.

Assume that $x_{2,2} \geq 1$. Suppose that $u, v \in V(G)$ are adjacent vertices both of degree 2. Let $x \neq u$ be the vertex adjacent to v. The vertex x may be coincident with either of the vertices w and t, and if this is the case, then without loss of generality, we assume that $x = t$.

Case 1. The vertices u and v do not have common neighbor.

If $G^{(1)} \cong G - \{uv, vx, wt\} + \{ux, wv, tv\}$, then $x = t$ or $x \neq t$, in both cases, we have

$$R_\alpha(G) - R_\alpha(G^{(1)}) = 9^\alpha - 2 \cdot 6^\alpha + 4^\alpha > 0, \tag{5}$$

a contradiction to the minimality of $R_\alpha(G)$.

Case 2. The vertices u and v have common neighbor.

It is evident that $d_x = 3$.

If $x \neq t$, then after the same calculations as in (5), we conclude that the graph $G - \{uv, wt\} + \{ut, vw\}$ has a smaller R_α value than that of G, which gives a contradiction.

If $x = t$, then we consider a neighbor $w' \neq t$ of w. Again, after the same calculations as in (5), we conclude that the graph

$$G - \{uv, tw, w'w\} + \{uw, vw, w't\}$$

has a smaller R_α value than that of G, which gives also a contradiction. □

LEMMA 7. [1] *For $\nu \geq 3$ and $n \geq 5(\nu - 1)$, if $H \in \mathcal{CG}_{n,\nu}$ is the graph with the degree set $\{2, 3\}$ such that $x_{3,3} = 0$, then $x_{2,2} = n - 5(\nu - 1)$ and $x_{2,3} = 6(\nu - 1)$.*

From the definition of R_α and Lemma 7, the next lemma follows.

LEMMA 8. *For $\nu \geq 3$ and $n \geq 5(\nu - 1)$, if $H \in \mathcal{CG}_{n,\nu}$ is the graph with the degree set $\{2, 3\}$ such that $x_{3,3} = 0$, then*

$$R_\alpha(H) = [n - 5(\nu - 1)]4^\alpha + 6(\nu - 1)6^\alpha.$$

Now, we are in a position to prove the main result, that is Theorem 1.

Proof of Theorem 1. The theorem follows from Lemmas 1, 4, 6 and 8. □

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