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Extremal Chemical (n, m, k)-Graphs with Maximum Randić Index

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Abstract

The Randić index of an organic molecule whose molecular graph is G is the sum of the weights $(d(u)d(v))^{-\frac{1}{2}}$ of all edges uv of G, where $d(u)$ and $d(v)$ are the degrees of the vertices u and v in G. In this paper, we present a upper bound on the Randić index for all chemical graphs with n vertices, $m \geq n$ edges and $k > 0$ pendant vertices, and determine corresponding extremal graphs.

1. Introduction and Notations

In studying branching properties of alkanes, several numbering schemes for the edges of the associated hydrogen-suppressed graph were proposed based on the degrees of the end-vertices of an edge. To preserve rankings of certain molecules, some inequalities involving the weights of edges needed to be satisfied. The Randić index

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of an organic molecule whose molecular graph is G is defined (see [25]) as

$$R(G) = \sum_{uv} (d(u)d(v))^{-\frac{1}{2}}$$

where $d(u)$ denotes the degree of the vertex u of the molecular graph G, the summation goes over all pairs of adjacent vertices of G. The research background of Randić index together with its generalization appears in chemistry or mathematical chemistry and can be found in the literature (see [8, 9, 26]). An important direction is to find bounds for the Randić index or the general Randić index of graphs and determine the graphs with maximal or minimal (general) Randić index in a given class of graphs. Up to now, many results are given (see [1], [3]-[6], [11]-[24], [27]-[30]), but most of them are lower bounds. In this paper, we present a upper bound on the Randić index for all chemical graphs with n vertices, $m \geq n$ edges and $k > 0$ pendant vertices, and determine corresponding extremal graphs.

In order to discuss our results, we first introduce some terminologies and notations of graphs. For other undefined notations, the reader is referred to [2]. We only consider finite, undirected and simple graphs. For a vertex x of a graph G, we denote the neighborhood and the degree of x by $N_G(x)$ and $d_G(x)$, respectively. A *pendant vertex* is a vertex of degree 1. The maximum degree of G is denoted by $\Delta(G)$. An edge is *symmetric* if it connects two vertices of equal degree; otherwise it is said to be *asymmetric*. We use $G - xy$ to denote the graph that arises from G by deleting the edge $xy \in E(G)$. Similarly, $G + xy$ is a graph that arises from G by adding an edge $xy \notin E(G)$, where $x,\ y \in V(G)$. Let $P_s = v_0 v_1 \cdots v_s$ be a path of G with $d(v_1) = \cdots = d(v_{s-1}) = 2$ (unless $s = 1$). If $d(v_0) = 1$ and $d(v_s) \geq 3$, then we call P_s a *pendant chain* of G.

A (n, m, k)-graph is a connected graph that has n vertices, m edges and k pendant vertices. Clearly, a $(n, n-1, k)$-graph is a tree, a (n, n, k)-graph is a unicyclic graph, a $(n, n+1, k)$-graph is a bicyclic graph and a $(n, n+2, k)$-graph is a tricyclic graph. A connected graph is called *chemical* if its maximum degree is at most 4.

Let $G = (V, E)$ be a graph. Denote

$$V_i(G) = \{v : v \in V(G), d_G(v) = i\},\ n_i(G) = |V_i(G)|,$$

$E_1 = \{uv \in E(G) : d_G(u) = 1,\ d_G(v) = 2\}$, $E_2 = \{uv \in E(G) : d_G(u) = d_G(v) = 2\}$, $E_3 = \{uv \in E(G) : d_G(u) = 2,\ d_G(v) \geq 3\}$, $E_4 = \{uv \in E(G) : d_G(u), d_G(v) \geq 3\}$ and $E_5 = \{uv \in E(G) : d_G(u) = 1,\ d_G(v) \geq 3\}$. Note that any edge in $E_1 \cup E_3 \cup E_5$ is an asymmetric edge.

2. Preliminaries

The proof of our results are carried out mainly by the following lemma.

Lemma 2.1 (see [3]). *Let G be a connected graph with n vertices. Then*

$$R(G) = \frac{n}{2} - \sum_{e \in E(G)} w^*(e), \qquad (*)$$

where $w^*(e) = \frac{1}{2}\left(\frac{1}{\sqrt{d_G(u)}} - \frac{1}{\sqrt{d_G(v)}}\right)^2$ *for* $e = uv$. ■

The above result can be for formulated also as follows: The Randić index of a connected graph is maximum if and only if G does not possess edges connecting vertices of different degrees (see [13]). This method has been successfully applied in the study of the extremal values of Randić index in some classes of graphs. Moreover, it can simplify the proof of some known results (see [3, 13]).

Note that an asymmetry edge has a positive-valued weight w^*, whereas the weight w^* of any symmetry edge is zero. Therefore, symmetry edges do not contribute to the right-hand side summations in $(*)$. With regard to this, the most obvious consequence of $(*)$ is the known results (see [3]).

Let G be a (n, m, k)-graph, then $m \geq n - 1$ and $k \geq 0$. If $k = 0$, then the chemical $(n, m, 0)$-graphs with extremal Randić index are determined by Gutman et al (see [7]). Also, the chemical $(n, n-1, k)$-graphs with extremal Randić index are determined by Hansen and Mélot (see [10]). So in the following, we assume that $k > 0$ and $m \geq n$. Note that if $k > 0$, then $E_1 \cup E_5 \neq \emptyset$ and any (n, m, k)-graph necessarily possess asymmetry edges.

Denoted by $\mathscr{G}_{n,m,k}$ the set of all (n, m, k)-graphs with $k > 0$ and $m \geq n$.

Next we will give another lemma which will be used in the proofs of our results.

Lemma 2.2. *Suppose $G \in \mathscr{G}_{n,m,k}$, $v \in V(G)$ vertex of degree 2 not contained in any pendant chain and not contained in any cycle of length 3. Let degrees of adjacent vertices of v be at least 2. Then, there is a graph $G' \in \mathscr{G}_{n,m,k}$ such that one of the following holds:*

(i) $R(G) < R(G')$;

(ii) $R(G) = R(G')$ *and G' has more vertices in pendant chains then G.*

Proof. Denote $N_G(v) = \{u, w\}$ with $d_G(v) = 2$ and $d_G(u) = s \geq 2$, $d_G(w) = t \geq 2$. Let x be a pendant vertex of G and y its neighbor. Then $d_G(y) = l \geq 2$. Let

$G' = G - uv - vw - xy + uw + xv + yv$. Then $G' \in \mathscr{G}_{n,m,k}$. Note that

$$\begin{aligned} R(G) - R(G') &= \frac{1}{\sqrt{2s}} + \frac{1}{\sqrt{2t}} + \frac{1}{\sqrt{l}} - \frac{1}{\sqrt{st}} - \frac{1}{\sqrt{2l}} - \frac{1}{\sqrt{2}} \\ &= \left(\frac{1}{\sqrt{s}} - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{t}}\right) + \left(\frac{1}{\sqrt{2}} - 1\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{l}}\right). \end{aligned}$$

If $l > 2$ or $s, t > 2$, then $R(G) < R(G')$. Otherwise, if $l = 2$, then only one pendant chain is altered (one that corresponds to pendant vertex x and in that chain v is included). Hence $R(G) = R(G')$ and G' has more vertices in pendant chains. ■

From Lemma 2.2, we may assume that all vertices of degree 2 (except for some vertices on the 3-cycles) in a (n, m, k)-graph G with maximum Randić index lie on the pendant chains of G.

Let s, t, k be three positive integers with $s \geq 6$ and $t = \frac{3s-2k}{2} \geq s$. We call G *a* $(s, t, k, 3)$*-semi-regular graph* if G is a (s, t, k)-graph with $|V_1(G)| = k$ and $d_G(v) = 3$ for any vertex $v \in V(G) \backslash V_1(G)$. Note that for a $(s, t, k, 3)$-semi-regular graph, we have $k \geq 3$ if $t = s$, $k \geq 2$ if $t = s + 1$ and $k \geq 1$ if $t \geq s + 2$. In Fig. 1, we have drawn four $(10, 10, 5, 3)$-semi-regular graphs.

Let n, m, k be three positive integers with $m \geq n$ and $3n \geq 2m + 3k$. Let $\mathscr{G}^*_{n,m,k} = \{G : G$ is a (n, m, k)-graph obtained from a $(s, t, k, 3)$-semi-regular graph by adding at least one new vertex on each pendant edge, and total number of new vertices is $3n - 2m - 2k\}$. Then $\mathscr{G}^*_{n,m,k} \subseteq \mathscr{G}_{n,m,k}$. In Fig. 2, we have drawn four (15,15,5)-graphs in $\mathscr{G}^*_{15,15,5}$.

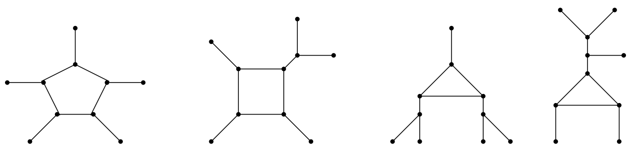


Fig. 1 $(10, 10, 5, 3)$-semi-regular graphs

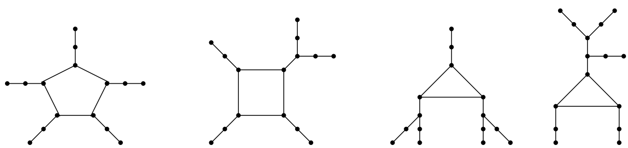


Fig. 2 Four graphs in $\mathscr{G}^*_{15,15,5}$

3. Chemical (n, m, k)-Graphs with Maximum Randić Index

In this section, we first consider (n, m, k)-graphs and determine the extremal (n, m, k)-graphs with maximum Randić index.

Theorem 3.1. *Suppose $G \in \mathscr{G}_{n,m,k}$ with $R(G)$ being as large as possible, where $n = m$ and $k \geq 3$, or $n = m + 1$ and $k \geq 2$, or $n \geq m + 2$. If no vertex of degree 2 is on the cycle of length 3 of G, then*

$$R(G) \leq \frac{n}{2} - \frac{(7 - 3\sqrt{2} - \sqrt{6})k}{6}. \tag{1}$$

Moreover, the equality in (1) holds if and only if $3n \geq 3k + 2m$ and $G \in \mathscr{G}^*_{n,m,k}$.

Proof. First we note that if $G \in \mathscr{G}^*_{n,m,k}$ and $3n \geq 3k + 2m$, then the equality in (1) holds.

Now, we prove that if $G \in \mathscr{G}_{n,m,k}$ with $R(G)$ is as large as possible, where $n = m$ and $k \geq 3$, or $n = m + 1$ and $k \geq 2$, or $n \geq m + 2$, then (1) holds and equality in (1) holds only if $3n \geq 3k + 2m$ and $G \in \mathscr{G}^*_{n,m,k}$. By assumption and the proof of Lemma 2.2, we can assume, without loss of generality, that all vertices of G with degree 2 are on the pendant chains of G. Thus $E(G) = E_1 \cup E_2 \cup E_3 \cup E_4 \cup E_5$ and $|E_3| = |E_1|$. Note that $|E_1| + |E_5| = k$, and hence by Lemma 2.1,

$$\begin{aligned}
R(G) &= \frac{n}{2} - \sum_{e \in E(G)} w^*(e) \\
&= \frac{n}{2} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)^2 |E_1| - \sum_{uv \in E_3} \frac{1}{2}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d(v)}}\right)^2 \\
&\quad - \sum_{uv \in E_4} \frac{1}{2}\left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}}\right)^2 - \sum_{uv \in E_5} \frac{1}{2}\left(1 - \frac{1}{\sqrt{d(v)}}\right)^2 \\
&\leq \frac{n}{2} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)^2 |E_1| - \sum_{uv \in E_3} \frac{1}{2}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d(v)}}\right)^2 - \sum_{uv \in E_5} \frac{1}{2}\left(1 - \frac{1}{\sqrt{d(v)}}\right)^2 \\
&\leq \frac{n}{2} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)^2 |E_1| - \frac{1}{2}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 |E_3| - \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right)^2 |E_5| \\
&= \frac{n}{2} + \frac{(3\sqrt{2} + \sqrt{6} - 7)k}{6} - \left(1 - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)|E_5| \\
&\leq \frac{n}{2} + \frac{(3\sqrt{2} + \sqrt{6} - 7)k}{6}.
\end{aligned}$$

In order for equality to hold, all inequalities in the above argument should be equalities. Thus we have (i) $|E_5| = 0$; (ii) for any $uv \in E_3$, $d_G(u) = 2$, $d_G(v) = 3$; (iii) for any $uv \in E_4$, $d_G(u) = d_G(v)$. Since each edge of E_3 are incident to an edge of E_4 and a vertex of degree 2, respectively, we have $d_G(u) = d_G(v) = 3$ for any $uv \in E_4$ and $n_2 \geq k$. Thus the maximum degree of G is 3. Since G is an (n, m, k)-graph, we have $n_1 + 2n_2 + 3n_3 = 2m$ and $n_1 + n_2 + n_3 = n$. Hence $3n \geq 3k + 2m$ and $G \in \mathscr{G}^*_{n,m,k}$. ■

Let n_2^* be the number of the cycles C of length 3 in G with $V_2 \cap V(C) \neq \emptyset$.

Theorem 3.2. *Suppose $G \in \mathscr{G}_{n,m,k}$ with $R(G)$ being as large as possible and $n_2^* > 0$. Then*

$$R(G) \leq \frac{n}{2} - \frac{(7 - 3\sqrt{2} - \sqrt{6})k}{6} - \frac{5 - 2\sqrt{6}}{6} n_2^*.$$

Proof. Let $G \in \mathscr{G}_{n,m,k}$ with $R(G)$ being as large as possible. By the proof of Lemma 2.2, we can assume, without loss of generality, that all vertices of G with degree 2 are on the pendant chains of G or on the cycles of length 3 of G. Thus $E(G) = E_1 \cup E_2 \cup E_3 \cup E_4 \cup E_5$ and $|E_3| = |E_1| + 2n_2^*$. Note that $|E_1| + |E_5| = k$, and hence by Lemma 2.1,

$$\begin{aligned}
& R(G) \\
= \; & \frac{n}{2} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)^2 |E_1| - \sum_{uv \in E_3} \frac{1}{2}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d(v)}}\right)^2 \\
& - \sum_{uv \in E_4} \frac{1}{2}\left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}}\right)^2 - \sum_{uv \in E_5} \frac{1}{2}\left(1 - \frac{1}{\sqrt{d(v)}}\right)^2 \\
\leq \; & \frac{n}{2} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)^2 |E_1| - \sum_{uv \in E_3} \frac{1}{2}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{d(v)}}\right)^2 - \sum_{uv \in E_5} \frac{1}{2}\left(1 - \frac{1}{\sqrt{d(v)}}\right)^2 \\
\leq \; & \frac{n}{2} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)^2 |E_1| - \frac{1}{2}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 |E_3| - \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right)^2 |E_5| \\
= \; & \frac{n}{2} + \frac{(3\sqrt{2} + \sqrt{6} - 7)k}{6} - \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 n_2^* \\
& + \frac{|E_5|}{2}\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 - \left(1 - \frac{1}{\sqrt{3}}\right)^2\right] \\
\leq \; & \frac{n}{2} + \frac{(3\sqrt{2} + \sqrt{6} - 7)k}{6} - \frac{5 - 2\sqrt{6}}{6} n_2^*.
\end{aligned}$$

■

Note that if $G \in \mathscr{G}_{n,n,1} \cup \mathscr{G}_{n,n,2} \cup \mathscr{G}_{n,n+1,1}$, then there is at least a cycle containing a vertex of degree 2 in G. Thus, by an argument similar to the proof of Theorem 3.2, we have

Theorem 3.3 *(i) For $G \in \mathscr{G}_{n,m,1}$ with $n = m$ or $m = n+1$, we have*

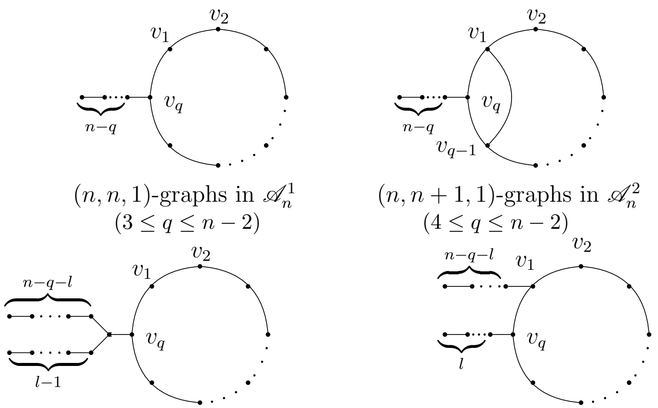
$$R(G) \le \frac{n}{2} - \frac{4-\sqrt{2}-\sqrt{6}}{2}$$

and equality holds if and only if $G \in \mathscr{A}_n^1$, $n \ge 5$ or $G \in \mathscr{A}_n^2$, $n \ge 6$ (see Fig. 3);

(ii) For $G \in \mathscr{G}_{n,n,2}$, we have

$$R(G) \le \frac{n}{2} - \frac{19-6\sqrt{2}-4\sqrt{6}}{6}$$

and equality holds if and only if $G \in \mathscr{B}_n^1$, $n \ge 8$ or $G \in \mathscr{C}_n^1$, $n \ge 7$ (see Fig. 3).



$(n,n,1)$-graphs in $\mathscr{A}_n^1$ $(3 \le q \le n-2)$

$(n,n+1,1)$-graphs in $\mathscr{A}_n^2$ $(4 \le q \le n-2)$

$(n,n,2)$-graphs in $\mathscr{B}_n^1$ $(l \ge 3,\ 3 \le q \le n-5)$

$(n,n,2)$-graphs in $\mathscr{C}_n^1$ $(l \ge 2,\ 3 \le q \le n-4)$

Fig. 3

For any graph $G \in \mathscr{G}_{n,n,1} \cup \mathscr{G}_{n,n,2} \cup \mathscr{G}_{n,n+1,1}$ or $G \in \mathscr{G}^*_{n,m,k}$, the maximum degree of G is 4, thus Theorems 3.1, 3.2 and 3.3 hold for chemical graphs. Thus we have

Corollary 3.4. *For any chemical graph $G \in \mathscr{G}_{n,m,k}$, $m \ge n+2$,*

$$R(G) \le \frac{n}{2} - \frac{(7-3\sqrt{2}-\sqrt{6})k}{6}. \tag{2}$$

Moreover the equality in (2) holds if and only if $G \in \mathscr{G}^*_{n,m,k}$ and $3n \ge 2m+3k$.

Corollary 3.5. *Let chemical graph* $G \in \mathscr{G}_{n,n,k}$. *Then, for* $k = 1$,

$$R(G) \leq \frac{n}{2} - \frac{4-\sqrt{2}-\sqrt{6}}{2}$$

and equality holds if and only if $G \in \mathscr{A}_n^1$ *and* $n \geq 5$*; and for* $k = 2$,

$$R(G) \leq \frac{n}{2} - \frac{19-6\sqrt{2}-4\sqrt{6}}{6}$$

and equality holds if and only if $G \in \mathscr{B}_n^1$ $(n \geq 8)$ *or* $G \in \mathscr{C}_n^1$ $(n \geq 7)$*; and for* $k \geq 3$,

$$R(G) \leq \frac{n}{2} - \frac{(7-3\sqrt{2}-\sqrt{6})k}{6}$$

and equality holds if and only if $n \geq 3k$ *and* $G \in \mathscr{G}^*_{n,n,k}$.

Corollary 3.6. *Let chemical graph* $G \in \mathscr{G}_{n,n+1,k}$. *Then, for* $k = 1$,

$$R(G) \leq \frac{n}{2} - \frac{4-\sqrt{2}-\sqrt{6}}{2}$$

and equality holds if and only if $G \in \mathscr{A}_n^2$ *and* $n \geq 6$*; and for* $k \geq 2$,

$$R(G) \leq \frac{n}{2} - \frac{(7-3\sqrt{2}-\sqrt{6})k}{6}$$

and equality holds if and only if $n \geq 3k+2$ *and* $G \in \mathscr{G}^*_{n,n+1,k}$.

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