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ON MOLECULAR GRAPHS WITH SMALLEST AND GREATEST ZEROTH-ORDER GENERAL RANDIĆ INDEX*

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Abstract

A molecular (n,m)-graph G is a connected simple graph with n vertices, m edges and vertex degrees not exceeding 4. If $d(v)$ denotes the degree of the vertex v, then the zeroth-order general Randić index ${}^0R_\alpha$ of the graph G is defined as $\sum\limits_{v\in V(G)} d(v)^\alpha$, where α is a pertinently chosen real number. We characterize, for any α, the molecular (n,m)-graphs with smallest and greatest ${}^0R_\alpha$.

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1 Introduction

The Randić (or connectivity) index was introduced by Randić in 1975 and is defined as [25]

$$R = R(G) = \sum_{uv \in E(G)} (d(u)\, d(v))^{-1/2}$$

where $d(u)$ denotes the degree of the vertex u of the graph G, and $E(G)$ is the edge set of G. Randić himself demonstrated [25] that this index is well correlated with a variety of physico–chemical properties of various classes of organic compounds. Eventually, this structure–descriptor became one of the most popular topological indices to which two books [15, 17], several reviews [7, 24, 26] and countless research papers are devoted.

Like other successful structure–descriptors, the Randić index received considerable attention also from mathematical chemists and mathematicians. In particular, bounds for R and graphs extremal with regard to R were extensively studied [1, 2, 4, 8, 9, 10, 11, 12].

In 1998 Bollobás and Erdös [3] generalized $R(G)$ by replacing the exponent $-1/2$ by an arbitrary real number α. This graph invariant is called *the general Randić index* and will be denoted by $R_\alpha = R_\alpha(G)$. Li and Yang [20] studied R_α for general n-vertex graphs, obtained lower and upper bounds for it, and characterized the corresponding extremal graphs. Later Hu, Li and Yuan [13, 14] determined the trees extremal with regard to R_α, whereas Li, Wang and Wei [19] gave lower and upper bounds for R_α of molecular (n, m)-graphs. Other mathematical studies of the general Randić index are found in [5, 6].

The zeroth-order Randić index, conceived by Kier and Hall [16], is

$${}^0R = {}^0R(G) = \sum_{v \in V(G)} d(v)^{-1/2}$$

Eventually, Li and Zheng [22] defined the *zeroth-order general Randić index* of a graph G as

$${}^0R_\alpha = {}^0R_\alpha(G) = \sum_{v \in V(G)} d(v)^{\alpha}$$

for any real number α.

Pavlović determined the graphs with maximum ${}^0R$-index [23]. Li et al. [18] investigated the same problem for the topological index $M_1(G)$, one of the Zagreb indices, that is defined as $M_1(G) = \sum_{v \in V(G)} d(v)^2$. (Evidently, $M_1 \equiv {}^0R_\alpha$ for $\alpha = +2$.) They obtained sufficient and necessary conditions under which (n,m)-graphs have minimum M_1, and a necessary condition for an (n,m)-graph having maximum $M_1(G)$. Li and Zhao [21] characterized trees with the first three smallest and largest zeroth-order general Randić index, with the exponent α being equal to k, $-k$, $1/k$, and $-1/k$, where $k \geq 2$ is an integer.

In this paper we investigate the zeroth-order general Randić index of molecular (n,m)-graphs, i. e., connected simple graphs with n vertices, m edges and maximum vertex degree at most 4. We characterize the molecular (n,m)-graphs with extremal (maximum or minimum) zeroth-order general Randić index.

First we need to introduce some notation.

Denote by $D(G) = [d_1, d_2, \cdots, d_n]$ the degree sequence of the graph G, where d_i stands the degree of the i-th vertex of G, and $d_1 \geq d_2 \geq \cdots \geq d_n$.

If there is a graph G, such that $d_i \geq d_j + 2$, let G' be the graph obtained from G by replacing the pair (d_i, d_j) by the pair $(d_i - 1, d_j + 1)$. In other words, if $D(G) = [d_1, d_2, \cdots, d_{i-1}, d_i, d_{i+1}, \cdots, d_{j-1}, d_j, d_{j+1}, \cdots, d_n]$, then $D(G') = [d_1, d_2, \cdots, d_{i-1}, d_i - 1, d_{i+1}, \cdots, d_{j-1}, d_j + 1, d_{j+1}, \cdots, d_n]$.

Note that if $\alpha = 0$ then ${}^0R_\alpha(G) = n$, and if $\alpha = 1$ then ${}^0R_\alpha(G) = 2m$. Therefore, in the following we always assume that $\alpha \neq 0, 1$.

Lemma 1.1 *For the two graphs G and G', specified above, we have*

(i) ${}^0R_\alpha(G) > {}^0R_\alpha(G')$ *for* $\alpha < 0$ *or* $\alpha > 1$

(ii) ${}^0R_\alpha(G) < {}^0R_\alpha(G')$ *for* $0 < \alpha < 1$.

Proof. Since ${}^0R_\alpha(G) = \sum\limits_{v\in V(G)} d(v)^\alpha$, we have

$$\begin{aligned} {}^0R_\alpha(G) - {}^0R_\alpha(G') &= d_i^\alpha + d_j^\alpha - (d_i-1)^\alpha - (d_j+1)^\alpha \\ &= [d_i^\alpha - (d_i-1)^\alpha] - \left[(d_j+1)^\alpha - d_j^\alpha\right] \\ &= \alpha\left(\xi_1^{\alpha-1} - \xi_2^{\alpha-1}\right) \end{aligned}$$

where $\xi_1 \in (d_i-1, d_i)$, and $\xi_2 \in (d_j, d_j+1)$. So, by $d_i \geq d_j + 2$, we have $\xi_1 > \xi_2$. Then ${}^0R_\alpha(G) > {}^0R_\alpha(G')$ for $\alpha < 0$ or $\alpha > 1$, whereas ${}^0R_\alpha(G) < {}^0R_\alpha(G')$ for $0 < \alpha < 1$.

∎

2 Extremal molecular (n, m)-graphs

Denote by n_i the number of vertices of degree i in a molecular (n,m)-graph G . Then we have

$$ {}^0R_\alpha(G) = n_1 + 2^\alpha\, n_2 + 3^\alpha\, n_3 + 4^\alpha\, n_4 \tag{2.1}$$

Theorem 2.1 *Let C^* be a molecular (n,m)-graph with degree sequence $[d_1, d_2, \cdots, d_n]$, such that $|d_i - d_j| \leq 1$ for any $i \neq j$. Then for $\alpha < 0$ or $\alpha > 1$, C^* has the minimum zeroth-order general Randić index among all molecular (n,m)-graphs, whereas for $0 < \alpha < 1$, C^* has the maximum zeroth-order general Randić index among all molecular (n,m)-graphs. Moreover,*

$$ {}^0R_\alpha(C^*) = \begin{cases} 2 + 2^\alpha\,(n-2) & \text{if} \;\; m = n-1 \\ 2^\alpha\,(3n-2m) + 3^\alpha\,(2m-2n) & \text{if} \;\; n \leq m \leq \lfloor 3n/2 \rfloor \\ 3^\alpha\,(4n-2m) + 4^\alpha\,(2m-3n) & \text{if} \;\; \lfloor 3n/2 \rfloor < m \leq 2n \end{cases}$$

Proof. We only consider the case $0 < \alpha < 1$, because the proof for the other case is fully analogous. Let G be a molecular graph and $D(G) = [d_1, d_2, \cdots, d_n]$. If $G \ncong C^*$, then there must exist a pair (d_i, d_j) such that $d_i \geq d_j + 2$. By Lemma 1.1, the graph G' , obtained by replacing the pair (d_i, d_j) by the pair $(d_i - 1, d_j + 1)$, has a greater ${}^0R_\alpha$-value than G . Consequently, G is not a molecular (n,m)-graph with maximum zeroth-order general Randić index.

To show the existence, we construct the extremal (n, m)-graph C^* (with minimum ${}^0R_\alpha$ for $\alpha < 0$ or $\alpha > 1$, and with maximum ${}^0R_\alpha$ for $0 < \alpha < 1$) by adding edges one by one. First, we start from a tree. There must be at least two 1-degree vertices in a tree. By Lemma 1.1, there does not exist any 3-degree vertex, and so the extremal tree must be the path P_n. Next we add an edge joining the two leaves of the path. In this way the degrees of all vertices become equal to two, and then we get a cycle. We continue by adding edges one by one, so as to maximize the number of 3-degree vertices, until either there remain no 2-degree vertices, or remains exactly one. If more edges need to be added, then we first connect the 2-degree vertex (if such does exist) with a non-adjacent 3-degree vertex, and continue by connecting pairs of nonadjacent 3-degree vertices. The construction is shown in Figure 2.1. ∎

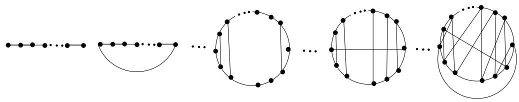

Figure 2.1 Constructing molecular graphs with extremal zeroth-order general Randić index, according to Theorem 2.1.

Theorem 2.2 *Let G^* be a molecular (n, m)-graph with at most one vertex of degree 2 or 3. If one of the following conditions holds:*

(I) $m = n - 1$

(II) $m \geq n \geq 6$, *for* $n = 6$, $m \geq 10$, *and for* $n = 7$, $m \neq 8$

then for $\alpha < 0$ *or* $\alpha > 1$, G^* *has the maximum zeroth-order general Randić index among all molecular* (n, m)*-graphs, whereas for* $0 < \alpha < 1$, *the same graph has the minimum zeroth-order general Randić index among all molecular* (n, m)*-graphs. Moreover,*

$$
{}^0R_\alpha(G^*) = \begin{cases} (4n - 2m)/3 + 4^\alpha\,(2m - n)/3 & \text{if } \; 2m - n \equiv 0 \;(mod\ 3) \\ (4n - 2m - 2)/3 + 2^\alpha + 4^\alpha\,(2m - n - 1)/3 & \text{if } \; 2m - n \equiv 1 \;(mod\ 3) \\ (4n - 2m - 1)/3 + 3^\alpha + 4^\alpha\,(2m - n - 2)/3 & \text{if } \; 2m - n \equiv 2 \;(mod\ 3) \end{cases}
$$

Proof. Again, we only consider the case $0 < \alpha < 1$, because the proof for the other case is similar. Let G' be a molecular (n,m)-graph and $D(G') = [d_1, d_2, \cdots, d_n]$. Let G' possess two vertices of degree 2 or 3, i. e., let there be a pair (d_i, d_j), such that $3 \geq d_i \geq d_j \geq 2$. Then by Lemma 1.1, there is a graph G, obtained by replacing the pair (d_i, d_j) by the pair (d_i+1, d_j-1), that has a smaller ${}^0R_\alpha$-value than G'. Repeating the above operation until there is no pair (d_i, d_j), such that $3 \geq d_i \geq d_j \geq 2$, we arrive at G^* with minimum zeroth-order general Randić index. In view of (2.1), for G^* we have

$$\begin{cases} n_1 + n_2 + n_3 + n_4 & = \; n \\ n_1 + 2\,n_2 + 3\,n_3 + 4\,n_4 & = \; 2m \\ n_2 + n_3 & \leq \; 1 \end{cases}$$

From the above equations, we have one of the following three options:

(1) $n_2 = n_3 = 0$, implying $n_1 = (4n - 2m)/3$, $n_4 = (2m - n)/3$, and $2m - n \equiv 0 \ (mod\ 3)$

(2) $n_2 = 1$, $n_3 = 0$, implying $n_1 = (4n - 2m - 2)/3$, $n_4 = (2m - n - 1)/3$, and $2m - n \equiv 1 \ (mod\ 3)$

(3) $n_2 = 0$, $n_3 = 1$, implying $n_1 = (4n - 2m - 1)/3$, $n_4 = (2m - n - 2)/3$, and $2m - n \equiv 2 \ (mod\ 3)$.

In order to show the existence, we construct G^* by distinguishing the following cases:

(I) $m = n - 1$, i. e., G^* is a tree.

(I.1) If $2m - n \equiv 0 \ (mod\ 3)$, we first construct a path with n_4 vertices, and then add n_1 pendent vertices, taking care that no vertex gets degree greater than 4.

(I.2) If $2m - n \equiv 1 \ (mod\ 3)$, we first construct a path with n_4 vertices, then add n_1 pendent vertices, taking care that no vertex gets degree greater than 4, and finally subdivide an edge by inserting to it a vertex of degree 2.

(I.3) If $2m - n \equiv 2 \ (mod\ 3)$, we first construct a path with $n_4 + 1$ vertices, and then add n_1 pendent vertices, taking care that no vertex gets degree greater than 4.

(II) $m \geq n \geq 6$, for $n = 6$ and $m \geq 10$, or for $n = 7$ and $m \neq 8$.

In Figure 2.2 we show one of the possible graphs G^* for $n_4 \leq 4$, that is for $\lfloor (2m - n)/3 \rfloor \leq 4$. For $n_4 \geq 5$, we construct G^* as follows:

(II.1) If $2m - n \equiv 0 \ (mod\ 3)$, we first construct a 4-regular graph on n_4 vertices, then delete $n_1/2$ edges from it, and then add n_1 pendent vertices, taking care that no vertex gets degree greater than 4.

(II.2) If $2m - n \equiv 1 \ (mod\ 3)$, we first construct a 4-regular graph on n_4 vertices, then delete $n_1/2$ edges from it, then add n_1 pendent vertices, taking care that no vertex gets degree greater than 4, and finally subdivide an edge inserting to it a vertex of degree 2.

(II.3) If $2m - n \equiv 2 \ (mod\ 3)$, we first construct a 4-regular graph on $n_4 + 1$ vertices, then delete $(n_1 + 1)/2$ edges from it, and then add n_1 pendent vertices, taking care that no vertex gets degree greater than 4.

This completes the proof. ∎

Note that Theorem 2.2 holds under the conditions $m = n - 1$, or $n = 6$ and $m \geq 10$, or $n = 7$ and $m \neq 8$, or $m \geq n \geq 8$, since for the other pairs of n and m the extremal degree sequences obtained in Theorem 2.2 are not graphic. It is easy to check that for $n = 1, 2, 3$, and for $n \geq 4$ and $m = \binom{n}{2} - 1$ or $m = \binom{n}{2}$ the (n, m)-graph is unique. For $n = 4$ and $m = 4$, or $n = 5$ and $5 \leq m \leq 8$, or $n = 6$ and $6 \leq m \leq 9$, or $n = 7$ and $m = 8$ we can characterize the extremal graphs by examining all possible degree sequences. These extremal graphs are depicted in Figure 2.3 (minimum ones for $0 < \alpha < 1$, maximum ones for $\alpha < 0$ or $\alpha > 1$, except for $n = 5$ and $m = 7$, in which case (a) is the minimum graph for $0 < \alpha < 1$ and maximum graph for $\alpha < 0$ or $1 < \alpha < 2$, and (b) is the maximum graph for $\alpha \geq 2$).

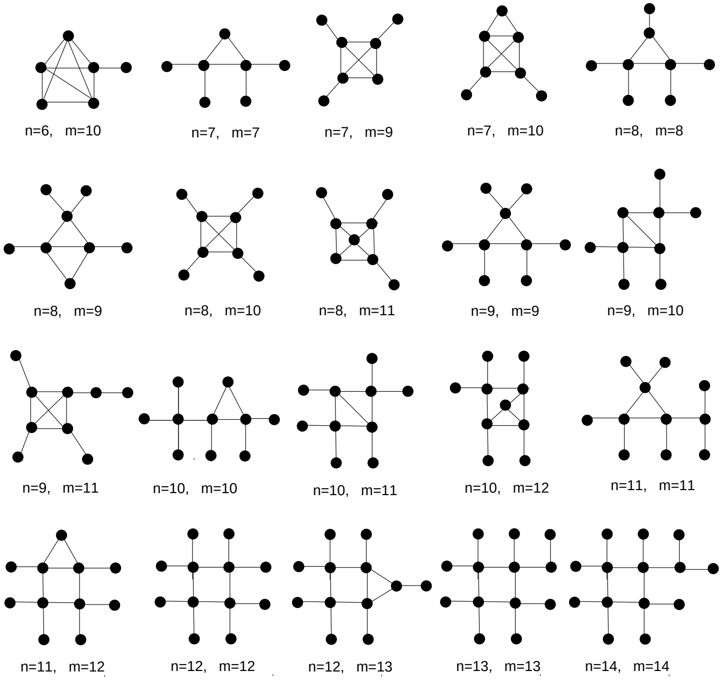

Figure 2.2 Molecular graphs with extremal zeroth-order general Randić index, having four or fewer vertices of degree 4.

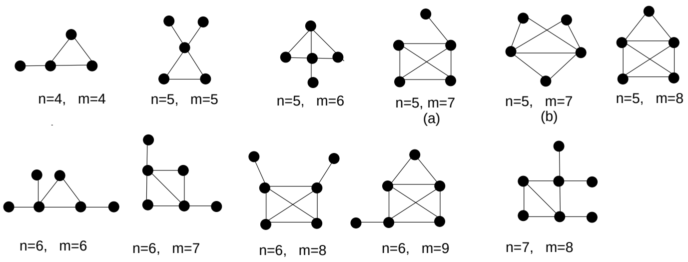

Figure 2.3 Some graphs with extremal zeroth-order general Randić index; for details see text.

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