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ON ZEROTH-ORDER GENERAL RANDIĆ INDICES OF TREES AND UNICYCLIC GRAPHS

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Abstract

Let G be a graph with vertex set $V(G)$. The zeroth-order general Randić index of G is defined as

$$\chi_\alpha(G) = \sum_{v \in V(G)} (d_v)^\alpha$$

where d_v is the degree of the vertex v in G and α is a real number. For $\alpha > 1$ or $\alpha < 0$, we characterize respectively the n-vertex trees and the n-vertex unicyclic graphs of fixed number of pendent vertices with the first three largest zeroth-order general Randić indices, and we also characterize respectively the n-vertex trees and the n-vertex unicyclic graphs of fixed maximum degree with the first two largest zeroth-order general Randić indices.

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INTRODUCTION

A topological index is a numeric quantity from the structural graph of a molecule. It is a structural invariant, i.e., it does not depend on the labelling or the pictorial representation of a graph.

Let G denote a graph with vertex set $V(G)$ and edge set $E(G)$. Let d_v denote the degree of the vertex v in G. Recently, Li and Zheng [1] introduced a kind of topological index — the zeroth-order general Randić index of a graph G as

$$\chi_\alpha(G) = \sum_{v \in V(G)} (d_v)^\alpha$$

where α is a real number. The cases $\alpha = 0, 1$ are trivial. For $\alpha = 2, -1/2$, the zeroth-order general Randić index χ_α reduces to the the first Zagreb index M_1 [2, 3] and the zeroth-order Randić index χ^0 [4, 5], respectively.

In [6] all trees with the first three largest and smallest zeroth-order general Randić indices were determined when $\alpha \in \{k, -k, -1/k\}$, and in [7] all unicyclic graphs with the largest zeroth-order general Randić index when $\alpha \in \{k, -k, -1/k\}$ were determined, where $k \geq 2$ is an integer. In [8] zeroth-order general Randić index of unicyclic graphs was investigated in more detail when the length of the unique cycle is fixed. In [9] the molecular (n, m)-graphs with the largest and smallest zeroth-order general Randić indices were characterized.

For $\alpha > 1$ or $\alpha < 0$ (resp. $0 < \alpha < 1$), we characterize respectively the n-vertex trees and the n-vertex unicyclic graphs of fixed number of pendent vertices with the first three largest (resp. smallest) zeroth-order general Randić indices, and we also characterize respectively the n-vertex trees and the n-vertex unicyclic graphs of fixed maximum degree with the first two largest (resp. smallest) zeroth-order general Randić indices.

RESULTS

For a graph G, $N(v)$ denotes the set of the (first) neighbors of $v \in V(G)$.

If the degree sequence of a graph G is $\delta_1, \delta_2, \ldots, \delta_n$, we write $D(G) = [\delta_1, \delta_2, \ldots, \delta_n]$. Furthermore $D(G) = [x_1^{a_1}, x_2^{a_2}, \ldots, x_t^{a_t}]$ means that the degree sequence of G consists of x_i (a_i times), where $i = 1, 2, \ldots, t$, and we drop the superscript 1 of x_i if $a_i = 1$.

Let G be a graph with $D(G) = [\delta_1, \delta_2, \ldots, \delta_n]$ such that $\delta_i \geq \delta_j \geq 2$ for some pair of distinct i, j. Then for vertices u and v such that $d_u = \delta_i$, $d_v = \delta_j$ and $N(v) \setminus (N(u) \cup \{u\}) \neq \emptyset$, let G' be the graph obtained from G by increasing the degree of vertex u by 1 and reducing the degree of vertex v by 1. So $D(G') = [\delta_1, \delta_2, \ldots, \delta_{i-1}, \delta_i + 1, \delta_{i+1}, \ldots, \delta_{j-1}, \delta_j - 1, \delta_{j+1}, \ldots, \delta_n]$. We will say G' is obtained from G by replacing the pair (δ_i, δ_j) by $(\delta_i + 1, \delta_j - 1)$. For $\alpha \neq 0, 1$, by Lagrange's mean-value theorem and noting that $\alpha x^{\alpha-1}$ is increasing for $x > 0$ if and only if $\alpha > 1$ or $\alpha < 0$, we have

Lemma 1. [9] *For the graphs G and G', $\chi_\alpha(G) < \chi_\alpha(G')$ if $\alpha > 1$ or $\alpha < 0$, and $\chi_\alpha(G) > \chi_\alpha(G')$ if $0 < \alpha < 1$.*

In view of Lemma 1, we consider any topological index $f(G)$ such that $f(G) < f(G')$ (resp. $f(G) > f(G')$) instead of χ_α for $\alpha > 1$ or $\alpha < 0$ (resp. $0 < \alpha < 1$).

We first consider trees with fixed number of pendent vertices.

Theorem 2. *Let $f(G)$ be a topological index such that $f(G) < f(G')$ (resp. $f(G) > f(G')$). Let T be a tree with n vertices, p of which are pendent vertices, $3 \leq p \leq n-2$.*

(i) *$f(T)$ attains the largest (resp. smallest) value if and only if $D(T) = [p, 2^{n-p-1}, 1^p]$.*

(ii) *For $p \geq 4$, $f(T)$ attains the second largest (resp. smallest) value if and only if $D(T) = [p-1, 3, 2^{n-p-2}, 1^p]$.*

(iii) *For $p = 5$, $f(T)$ attains the third largest (resp. smallest) value if and only if $D(T) = [3^3, 2^{n-8}, 1^5]$, and for $p \geq 6$, $f(T)$ attains the third largest (resp. smallest) value if and only if $D(T) = [p-2, 4, 2^{n-p-2}, 1^p]$.*

Proof. Suppose that $D(T) \neq [p, 2^{n-p-1}, 1^p]$ and v is a vertex with maximum degree. Then there must be a vertex $w \neq v$ such that $d_w \geq 3$. Let $N(w) = \{w_1, \ldots, w_l\}$, where w_1 lies on the path from v to w and $l = d_w$. Let $T_i = T - ww_3 - \cdots - ww_{i+2} + vw_3 + \cdots + vw_{i+2}$ for $i = 1, 2, \ldots, l-2$. By the condition of the theorem, $f(T) < f(T_1) < \cdots < f(T_{l-2})$. Repeating the operations above, we obtain a tree sequence $T, T_1, \ldots, T_s$ with n vertices, p of which are pendent vertices, such that $f(T) < f(T_1) < \cdots < f(T_s)$, and there is no pair of distinct vertices in T_s with degree greater than or equal to 3. Obviously, $D(T_s) = [p, 2^{n-p-1}, 1^p]$. This proves (i).

Suppose that $p \geq 4$. Since T_s is obtained from T_{s-1} by replacing some pair (δ_i, δ_j) by the pair $(\delta_i + 1, \delta_j - 1)$ and $D(T_s) = [p, 2^{n-p-1}, 1^p]$, where $D(T_{s-1}) = [\delta_1, \delta_2, \ldots, \delta_n]$ and $\delta_i \geq \delta_j \geq 3$, one can see that $D(T_{s-1}) = [p-1, 3, 2^{n-p-2}, 1^p]$. This proves (ii).

Similarly, $T_{s-2} = T^1_{s-2}$ for $p \geq 6$ or T^2_{s-2} for $p \geq 5$, where $D(T^1_{s-2}) = [p-2, 4, 2^{n-p-1}, 1^p]$ and $D(T^2_{s-2}) = [p-2, 3^2, 2^{n-p-2}, 1^p]$. Since T^1_{s-2} can be obtained from T^2_{s-2} by replacing the pair $(3,3)$ by $(4,2)$, we have $f(T^2_{s-2}) < f(T^1_{s-2})$. It follows that

$D(T_{s-2}) = [p-2, 3^2, 2^{n-p-2}, 1^p]$ for $p = 5$ and $D(T_{s-2}) = [p-2, 4, 2^{n-p-1}, 1^p]$ for $p \geq 6$. This proves (iii). $\square$

Now we consider trees with fixed maximum degree. Motivated by [6, Theorem 3], we prove the following.

Theorem 3. *Let $f(G)$ be a topological index such that $f(G) < f(G')$ (resp. $f(G) > f(G')$). Let T be a tree with n vertices and maximum degree Δ, where $n - 2 = a(\Delta - 1) + k - 1$, a is an integer, $k = 1, 2, 3, \ldots, \Delta - 1$, and $3 \leq \Delta \leq n - 2$.*

(i) *$f(T)$ attains the largest (resp. smallest) value if and only if $D(T) = [\Delta^a, 1^{n-a}]$ if $k = 1$ and $D(T) = [\Delta^a, k, 1^{n-a-1}]$ if $k > 1$.*

(ii) *For $a = 1$ (and then $k \geq 3$), $f(T)$ attains the second largest (resp. smallest) value if and only if $D(T) = [\Delta, k - 1, 2, 1^{n-3}]$, and for $a \geq 2$, $f(T)$ attains the second largest (resp. smallest) value if and only if*

(a) *$D(T) = [\Delta^{a-1}, \Delta - 1, 2, 1^{n-a-1}]$ if $k = 1$,*

(b) *$D(T) = [\Delta^{a-1}, \Delta - 1, 2^2, 1^{n-a-2}]$ for $\Delta = 3$ and $D(T) = [\Delta^{a-1}, \Delta - 1, 3, 1^{n-a-1}]$ for $\Delta \geq 4$ if $k = 2$,*

(c) *$D(T) = [\Delta^{a-1}, (\Delta - 1)^2, 2, 1^{n-a-2}]$ for $\Delta = 3$ and $D(T) = [\Delta^a, \Delta - 2, 2, 1^{n-a-2}]$ for $\Delta \geq 4$ if $k = \Delta - 1$,*

(d) *$D(T) = D(T^i)$ where $i = 1, 2$, $f(T^i) = \max\{f(T^1), f(T^2)\}$ with $D(T^1) = [\Delta^{a-1}, \Delta - 1, k + 1, 1^{n-1-a}]$ and $D(T^2) = [\Delta^a, k - 1, 2, 1^{n-a-2}]$ if $3 \leq k \leq \Delta - 2$.*

Proof. Suppose that $f(G) < f(G')$. The proof for the case $f(G) > f(G')$ is similar.

Let T be a tree with n vertices and maximum degree Δ. Let $D(T) = [x_1, x_2, \ldots, x_n]$. If $\Delta > x_i \geq x_j \geq 2$, $i \neq j$, then construct a tree T_1 by increasing x_i by 1 and reducing x_j by 1. By the condition of the theorem, $f(T) < f(T_1)$. Repeating the operation above, we obtain a tree sequence $T, T_1, T_2, \ldots, T_s$ with n vertices and maximum degree Δ, such that $f(T) < f(T_1) < f(T_2) < \cdots < f(T_s)$, and there is no pair y_i, y_j such that $\Delta > y_i \geq y_j \geq 2$, $i \neq j$, where $D(T_s) = [y_1, y_2, \ldots, y_n]$. Thus except at most one vertex of degree k for some $k = 2, 3, \ldots, \Delta - 1$, all vertices of T_s have degree $\Delta, 1$. Denote by a, b and c the number of vertices of degree Δ, k and 1, respectively. Then $a\Delta + bk + c = 2n - 2$, $a + b + c = n$ and $b \leq 1$.

If $n - 2 \equiv 0 \pmod{(\Delta - 1)}$, then $a = \frac{n-2}{\Delta-1}$, $b = 0$, $c = n - a$ and so $D(T_s) = [\Delta^a, 1^{n-a}]$. If $n - 1 - k \equiv 0 \pmod{(\Delta - 1)}$, then $a = \frac{n-1-k}{\Delta-1}$, $b = 1$, $c = n - 1 - a$ and so $D(T_s) = [\Delta^a, k, 1^{n-1-a}]$. Hence (i) follows.

If $a = 1$, then $k \geq 3$ and so $D(T_{s-1}) = [\Delta, k-1, 2, 1^{n-3}]$.

Suppose in the following that $a \geq 2$.

If $k = 1$, since $D(T_s) = [\Delta^{a-1}, 1^{n-a}]$, we have $D(T_{s-1}) = [\Delta^{a-1}, \Delta - 1, 2, 1^{n-1-a}]$.

If $k = 2$, since $D(T_s) = [\Delta^a, 2, 1^{n-a-1}]$, we have $T_{s-1} = T^1_{s-1}$ for $\Delta \geq 4$ or T^2_{s-1} for $\Delta \geq 3$, where $D(T^1_{s-1}) = [\Delta^{a-1}, \Delta - 1, 3, 1^{n-a-1}]$ and $D(T^2_{s-1}) = [\Delta^{a-1}, \Delta - 1, 2^2, 1^{n-a-2}]$. Note that $f(T^2_{s-1}) < f(T^1_{s-1})$ for $\Delta \geq 4$. It follows that $D(T_{s-1}) = [\Delta^{a-1}, \Delta - 1, 2^2, 1^{n-a-2}]$ for $\Delta = 3$ and $D(T_{s-1}) = [\Delta^{a-1}, \Delta - 1, 3, 1^{n-a-1}]$ for $\Delta \geq 4$.

If $k = \Delta - 1$, then $T_{s-1} = T^1_{s-1}$ for $\Delta \geq 4$ or T^2_{s-1} for $\Delta \geq 3$, where $D(T^1_{s-1}) = [\Delta^a, \Delta - 2, 2, 1^{n-a-2}]$ and $D(T^2_{s-1}) = [\Delta^{a-1}, (\Delta - 1)^2, 2, 1^{n-a-2}]$. Note that $f(T^2_{s-1}) < f(T^1_{s-1})$. It follows that $D(T_{s-1}) = [\Delta^{a-1}, (\Delta - 1)^2, 2,\ 1^{n-a-2}]$ for $\Delta = 3$, $D(T_{s-1}) = [\Delta^a, \Delta - 2, 2, 1^{n-a-2}]$ for $\Delta \geq 4$.

If $3 \leq k \leq \Delta - 2$, then $T_{s-1} = T^i_{s-1}$ for $i = 1, 2, 3$, where $D(T^1_{s-1}) = [\Delta^{a-1}, \Delta - 1, k + 1, 1^{n-a-1}]$, $D(T^2_{s-1}) = [\Delta^a, k-1, 2, 1^{n-a-2}]$ and $D(T^3_{s-1}) = [\Delta^{a-1}, \Delta - 1, k, 2, 1^{n-a-2}]$. Note that $f(T^1_{s-1}), f(T^2_{s-1}) > f(T^3_{s-1})$. It follows that $D(T) = D(T^i)$ where $i = 1, 2$, $f(T^i) = \max\{f(T^1), f(T^2)\}$ with $D(T^1) = [\Delta^{a-1}, \Delta - 1, k + 1,\ 1^{n-1-a}]$ and $D(T^2) = [\Delta^a, k - 1, 2, 1^{n-a-2}]$ if $3 \leq k \leq \Delta - 2$.

Hence (ii) holds. $\square$

Now we turn to unicyclic graphs.

Theorem 4. *Let $f(G)$ be a topological index such that $f(G) < f(G')$ (resp. $f(G) > f(G')$). Let U be a unicyclic graph with n vertices, p of which are pendent vertices, $2 \leq p \leq n - 3$.*

(i) *$f(U)$ attains the largest (resp. smallest) value if and only if $D(U) = [p + 2, 2^{n-p-1}, 1^p]$.*

(ii) *$f(U)$ attains the second largest (resp. smallest) value if and only if $D(U) = [p + 1, 3, 2^{n-p-2}, 1^p]$.*

(iii) *$f(U)$ attains the third largest (resp. smallest) value if and only if $D(U) = [3^3, 2^{n-6}, 1^3]$ for $p = 3$ and $D(U) = [p, 4, 2^{n-p-2}, 1^p]$ for $p \geq 4$.*

Proof. Suppose that $f(G) < f(G')$. The proof for the case $f(G) > f(G')$ is similar.

Suppose that $D(U) \neq [p + 2, 2^{n-p-1}, 1^p]$. There are two vertices v, w such that $d_v \geq d_w \geq 3$. Let the neighbors of w be $w_1, w_2, \ldots, w_l$ with $l = d_w$. If both v and w lie on the unique cycle, let w_1, w_2 be the two neighbors of w on the cycle. If v lies on the cycle but w does not, let w_1 be the neighbor of w on the path from v to w. If w lies on the cycle but v does not, let w_1 be the neighbor of w on the path from v to w and w_2 be one of the two neighbors of w on the cycle. Let $U_i = U - ww_3 - \cdots - ww_{i+2} + vw_3 + \cdots + vw_{i+2}$ for $i = 1, \ldots, l-2$. By the condition of the theorem $f(U) < f(U_1) < \cdots < f(U_{l-2})$. Repeating the operations above, we obtain a unicyclic graph sequence $U, U_1, U_2, \ldots, U_s$ with n vertices, p of which are pendent vertices, such that $f(U) < f(U_1) < f(U_2) < \cdots < f(U_s)$, and there is no pair of distinct vertices in U_s with degree greater than or equal to 3. Obviously $D(U_s) = [p+2, 1^p, 2^{n-p-1}]$. This proves (i).

Since U_s is obtained from U_{s-1} by replacing some pair (δ_i, δ_j) by the pair $(\delta_i - 1, \delta_j + 1)$ and $D(U_s) = [p+2, 1^p, 2^{n-p-1}]$, where $D(U_{s-1}) = [\delta_1, \delta_2, \ldots, \delta_n]$ and $\delta_i \geq \delta_j \geq 3$, one can see that $D(U_{s-1}) = [p+1, 3, 2^{n-p-2}, 1^p]$. This proves (ii).

Suppose that $p \geq 3$. Then $U_{s-2} = U^1_{s-2}$ for $p \geq 4$ or U^2_{s-2} for $p \geq 3$, where $D(U^1_{s-2}) = [p, 4, 2^{n-p-2}, 1^p]$ and $D(U^2_{s-2}) = [p, 3^2, 2^{n-p-3}, 1^p]$. Note that U^1_{s-2} can be obtained from U^2_{s-2} by replacing the pair $(3,3)$ by $(4,2)$. So $f(U^2_{s-2}) < f(U^1_{s-2})$ for $p \geq 4$. It follows that $D(U_{s-2}) = [p, 3^2, 2^{n-p-3}, 1^p]$ for $p = 3$ and $[p, 4, 2^{n-p-2}, 1^p]$ for $p \geq 4$. This proves (iii). $\square$

Theorem 5. *Let $f(G)$ be a topological index such that $f(G) < f(G')$ (resp. $f(G) > f(G')$). Let U be a unicyclic graph with n vertices and maximum degree Δ, where $n = a(\Delta - 1) + k - 1$, a is an integer, $k = 1, 2, 3, \ldots, \Delta - 1$, and $3 \leq \Delta \leq n - 2$.*

(i) *For $a = 1$ (and then $k \geq 3$), $f(U)$ attains the largest (resp. smallest) value if and only if $D(U) = [\Delta, k-1, 2, 1^{n-3}]$, and for $k \geq 4$, $f(U)$ attains the second largest (resp. smallest) value if and only if $D(U) = [\Delta, k-2, 3, 1^{n-3}]$ if $k \geq 5$ and $D(U) = [\Delta, 2^3, 1^{n-4}]$ if $k = 4$.*

(ii) *For $a = 2$ and $k = 1$, $f(U)$ attains the largest (resp. smallest) value if and only if $D(U) = [\Delta, \Delta - 1, 2, 1^{n-3}]$, and $f(U)$ attains the second largest (resp. smallest) value if and only if $D(U) = [4, 2^3, 1^2]$ for $\Delta = 4$ and $D(U) = [\Delta, \Delta - 2, 3, 1^{n-3}]$ for $\Delta \geq 5$.*

(iii) *For $a \geq 3$ and $k = 1$, $f(U)$ attains the largest (resp. smallest) value if and only if $D(U) = [\Delta^a, 1^{n-a}]$, and $f(U)$ attains the second largest (resp. smallest) value if and only if $D(U) = [\Delta^{a-1}, \Delta - 1, 2, 1^{n-a-1}]$.*

(iv) *For $a \geq 2$ and $k \geq 2$, $f(U)$ attains the largest (resp. smallest) value if and only if $D(U) = [\Delta^a, k, 1^{n-a-1}]$, and $f(U)$ attains the second largest (resp. smallest) value if and only if*

(a) *$D(U) = [\Delta^{a-1}, \Delta - 1, 2^2, 1^{n-a-2}]$ for $\Delta = 3$ and $D(T) = [\Delta^{a-1}, \Delta - 1, 3, 1^{n-a-1}]$ for $\Delta \geq 4$ if $k = 2$,*

(b) $D(U) = [\Delta^{a-1}, (\Delta-1)^2, 2, 1^{n-a-2}]$ *for* $\Delta = 3$ *and* $D(U) = [\Delta^a, \Delta - 2, 2, 1^{n-a-2}]$ *for* $\Delta \geq 4$ *if* $k = \Delta - 1$,

(c) $D(U) = D(U^i)$ *where* $i = 1, 2$, $f(U^i) = \max\{f(U^1), f(U^2)\}$ *with* $D(U^1) = [\Delta^{a-1}, \Delta - 1, k+1, 1^{n-1-a}]$ *and* $D(U^2) = [\Delta^a, k-1, 2, 1^{n-a-2}]$ *if* $3 \leq k \leq \Delta - 2$.

Proof. If $a \geq 3$ or if $a = 2$ and $k \geq 2$, then by similar arguments as in the proof of Theorem 3, (iii) and (iv) follow.

Suppose that $a = 1$. Then $n = \Delta + k - 2$ with $k \geq 3$. Let $D(U) = [x_1, x_2, \ldots, x_n]$. We claim that $D(U) \neq [\Delta^r, 1^r]$ for any integer r with $1 \leq r \leq n-1$. Otherwise $r\Delta + (n-r) = 2n$, which is obviously impossible for $r = 1$. Suppose that $r \geq 2$. Then $r\Delta - r = \Delta + k - 2 \leq 2\Delta - 3$ from which we have $(r-2)\Delta \leq r - 3$, also a contradiction. Similarly, we have $D(U) \neq [\Delta^r, l, 1^{n-r-1}]$ for any integer r and l with $1 \leq r \leq n-2$ and $2 \leq l \leq \Delta - 1$. If $D(U) \neq [\Delta, k-1, 2, 1^{n-3}]$, then by repeating the operation to replace some pair (x_i, x_j) by the pair $(x_i + 1, x_j - 1)$ for $\Delta > x_i \geq x_j \geq 2$, we obtain a unicyclic graph sequence $U, U_1, \ldots, U_s$ with n vertices and maximum degree Δ, such that $f(U) < f(U_1) < \cdots < f(U_s)$, and except two vertices of degree l and 2 respectively, all vertices of U_s have degree Δ, 1, where l is an integer with $2 \leq l < \Delta$. Let r be the number of vertices of degree Δ in U_s. Then $r\Delta + l + 2 + (n-r-2) = 2n$, i.e., $(r-1)(\Delta-1) = k - l - 1$, from which we have $r = 1$ and $l = k-1$. So $D(U_s) = [\Delta, k-1, 2, 1^{n-3}]$. Furthermore $U_{s-1} = U^1_{s-1}$ for $k \geq 5$ or U^2_{s-1} for $k \geq 4$, where $D(U^1_{s-1}) = [\Delta, k-2, 3, 1^{n-3}]$ and $D(U^2_{s-1}) = [\Delta, k-2, 2^2, 1^{n-4}]$. Since $f(U^1_{s-1}) > f(U^2_{s-1})$ for $k \geq 5$, (i) follows.

Finally, suppose that $a = 2$ and $k = 1$. Then $n = 2(\Delta - 1)$ with $\Delta \geq 4$. By similar argument as above, $f(U)$ attains the largest value if and only if except two vertices of degree l and 2 respectively, all vertices of U have degree Δ, 1, where l is an integer with $2 \leq l < \Delta$. It is easy to see that the number of vertices of degree Δ is one and $l = \Delta - 1$. Now (ii) follows easily. $\square$

If we replace the part "Let $f(G)$ be a topological index such that $f(G) < f(G')$ (resp. $f(G) > f(G')$)" in Theorems 2–5 by "Let α satisfy $\alpha > 1$ or $\alpha < 0$ (resp. $0 < \alpha < 1$)" and replace the topological index f of other places in Theorems 2–5 by χ_α, then by Lemma 1, the corresponding results follow. Thus for $\alpha > 1$ or $\alpha < 0$ (resp. $0 < \alpha < 1$), we have determined the n-vertex trees and the n-vertex unicyclic graphs of fixed number of pendent vertices with the first three largest (resp. smallest) zeroth-order general Randić indices, and the n-vertex trees and the n-vertex unicyclic graphs of fixed maximum degree with the first two largest (resp. smallest) zeroth-order general Randić indices.

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References

[1] X. Li, J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 195–208.

[2] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.

[3] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

[4] L. B. Kier, L. H. Hall, *Molecular connectivity in structure-activity analysis*, Research Studies Press, Chichester, 1986.

[5] L. Pavlović, Maximal value of the zeroth-order Randić index, *Discr. Appl. Math.* **127** (2003) 615–626.

[6] X. Li, H. Zhao, Trees with first three smallest and largest generalized topological indices, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 57–62.

[7] H. Wang, H. Deng, Unicycle graphs with maximum generalized topological indices, *J. Math. Chem.*, in press.

[8] H. Hua, H. Deng, On unicycle graphs with maximum and minmum zeroth-order general Randić index, *J. Math. Chem.*, in press.

[9] Y. Hu, X. Li, Y. Shi, T. Xu, I. Gutman, On molecular graphs with smallest and greatest zeroth-order general Randić index, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 425–434.