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On the Higher Randić Index

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ABSTRACT

Let G be a simple graph with vertex set $V(G)=\{v_1,v_2,...v_n\}$. For every vertex v_i, $\delta(v_i)$ represents the degree of vertex v_i. The h-th order of Randić index, R_h is defined as the sum of terms $\frac{1}{\sqrt{\delta(v_{i_1}),\delta(v_{i_2})...\delta(v_{i_{h+1}})}}$ over all paths of length h contained (as sub graphs) in G. In this paper, some bounds for higher Randić index and a method for computing the higher Randic index of a simple graph is presented. Also, the higher Randić index of coronene/circumcoronene is computed.

Keywords: Randić index, higher Randić index, coronene/circumcoronene.

1. INTRODUCTION

In this paper, we consider simple graph G with vertex set $V(G)=\{v_1,v_2,...v_n\}$. Degree of vertex v is denoted by $\delta(v)$. We denote the minimum and maximum degree of vertices by δ and Δ respectively. A topological index is a real number derived from the structure of a graph in a way that is invariant under graph isomorphism. Most of the more useful invariants belong to one of two broad classes: they are either distance based, or bond-additive. The first class contains the indices that are defined in terms of distances between pairs of vertices; the second class contains the indices defined as the sum of contributions over all edges. Wiener index and Randic index are two graph invariants of these two classes.

In 1975, Milan Randić [1] proposed a topological index under the name branching index, suitable for measuring the extent of branching of the carbon-atom skeleton of

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saturated hydrocarbons. Randic noticed that there is a good correlation between the Randić index and several physico–chemical properties of alkanes: boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapor pressure, surface areas.The Randić index of graph G is defined as:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\delta(u)\delta(v)}}$$

Mathematical properties of the Randić index were extensively studied, see [2–6]. The Randić index of graph *G*, *R(G)* on *n* vertices has the following bounds [7],

$$\sqrt{n-1} \le R(G) \le \frac{n}{2}.$$

Equality on the right-hand side holds if and only if *G* is a graph whose all components are regular of (not necessarily equal) degrees greater than zero. Equality on the left-hand side holds if and only if *G* is a star [7]. The h–th order of Randić index of graph *G*, denoted by $R_h(G)$ [8] is defined as:

$$R_h(G) = \sum_{v_{i_1} v_{i_2} \dots v_{i_{h+1}}} \frac{1}{\sqrt{\delta(v_{i_1}), \delta(v_{i_2}) \dots \delta(v_{i_{h+1}})}}$$

where summation is over all paths of length of *h* contained in *G*. Some results about the higher Randić index have been obtained in [5, 9, 10, 11, 12, 13].

2. MAIN RESULTS

For vertex $v \in V(G)$, let $P_t : v_0 v_1 v_2 \dots v_t$ be a path of length *t* (not longest path) contained in *G* with an end vertex *v*. We consider the weight of P_t as $w(P_t) = \frac{1}{\sqrt{\delta(v)\delta(v_1)\dots\delta(v_t)}}$. For path P_t, there are $\delta(v_t) - 1$ paths of length $t+1$ that start from vertex *v* and contain P_t.

Theorem 1. Let *G* be a connected graph and *d* be the length of longest path contained in *G*. Then for every *t*, $1 \le t \le d-1$

$$\frac{\delta - 1}{\sqrt{\Delta}} R_t(G) \le R_{t+1}(G) \le \frac{\Delta - 1}{\sqrt{\delta}} R_t(G)$$

Proof. For every vertex $v \in V(G)$ and path $P_t : v_0 v_1 v_2 \dots v_t$ start from *v*, there are $\delta(v_t) - 1$ paths of length $t+1$ that maximum and minimum of their weights are $\frac{1}{\sqrt{\delta}} w(P_t)$ and

$\frac{1}{\sqrt{\Delta}}w(P_t)$ respectively. Hence for every path of length of t, there are at least $\delta - 1$ paths of length of *t+1* with minimum weight $\frac{1}{\sqrt{\delta}}$ and also there are at most $\Delta - 1$ paths of length of *t+1* with maximum weight $\frac{1}{\sqrt{\Delta}}$. Therefore,

$$R_{t+1}(G) = \sum_{P_{t+1}\subseteq G} w(P_{t+1}) \le \sum_{P_t \subseteq G} \frac{\Delta - 1}{\sqrt{\delta}} w(P_t) = \frac{\Delta - 1}{\sqrt{\delta}} \sum_{P_t \subseteq G} P_t = \frac{\Delta - 1}{\sqrt{\delta}} R_t(G).$$

Analogously $R_{t+1}(G) \ge \frac{\delta - 1}{\sqrt{\Delta}} R_t(G)$ and the proof is completed.

Corollary 1. Let G be a connected k-regular graph and d be the length of longest path contained in G. Then for every t, $1 \le t \le d-1$, $R_{t+1} = \frac{k-1}{\sqrt{k}} R_t(G)$.

Corollary 2. For a graph with above conditions,

$$R_{t+1}(G) = \left(\frac{k-1}{\sqrt{k}}\right)^t \frac{n}{2}$$

where n is the number of vertices G.

Proof. Since G is a k-regular graph, hence $R_1(G) = \frac{n}{2}$. By induction on t in Corollary 2.2, it concludes that $R_{t+1}(G) = \left(\frac{k-1}{\sqrt{k}}\right)^t R_1(G)$.

Example. Let C_n, F_n and K_n be Cycle, fullerene graph and complete graph on n vertices respectively. C_n, F_n and K_n are regular graphs of degrees 2, 3 and $n-1$ respectively. By Corollary 2, we have:

$$R_t(C_n) = n\left(\frac{1}{\sqrt{2}}\right)^{t+1}, \quad 1 \le t \le n-1,$$

$$R_t(F_n) = \left(\frac{2}{\sqrt{3}}\right)^{t-1} \frac{n}{2}, \quad 1 \le t \le d$$

where d is the length of longest path contained in F_n.

$$R_t(K_n) = \frac{n}{2}\left(\frac{n-2}{\sqrt{n-1}}\right)^{t-1}, \ 1 \le t \le n-1.$$

3. COMPUTING THE HIGHER RANDIĆ INDEX

Many methods and algorithms for computing topological indices were proposed, see [14–18]. In this section, a GAP program is given to compute h–order of Randić index of any simple graph when $1 \le h \le 7$. Also, by using this program, the higher Randić index for coronene/circumcoronene graph is computed. The coronene/circumcoronene is denoted by H_n and its structure is illustrated in Figure 1.

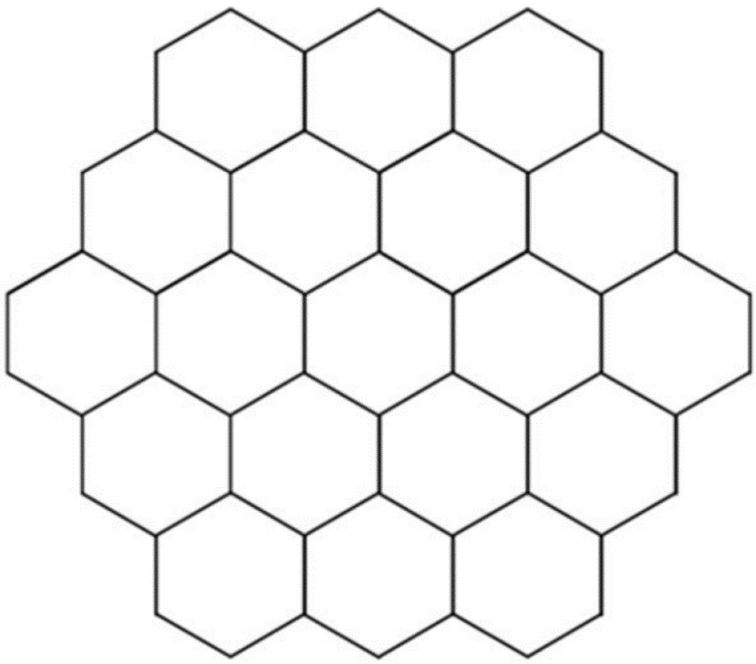

Figure 1. Coronene/Circumcoronene H_3.

Input of the program is the adjacent vertices set of any vertex. $N(i)$ denotes the adjacent vertices set of vertex *i*. The paths of length 1 are edges of graph. Let $P_t : v_0 v_1 ... v_t$ be a path of length *t* contained in *G*. By adding any vertex in the adjacent vertices set of v_t to P_t except vertices of P_t a path of length $t+1$ is obtained. Therefore by induction, all paths of length t, $(1 \le t)$ can be determined and the higher Randić index is computed by summing the weights of such paths. In the following, a GAP program is presented for computing the R_7 of a simple graph:

```
Input N (the adjacent vertices set of each vertex)
for i in [1..n] do
    deg[i]:=Size(N[i]);
od;
R7:=0;
for i in [1..n] do
    for j in N[i] do
        for x in Difference(N[j],[i]) do
            for y in Difference(N[x],[i,j]) do
                for s in Difference(N[y],[i,j,x]) do
                    for t in Difference(N[s],[i,j,x,y]) do
                        for w in Difference(N[t],[i,j,x,y,s]) do
                            for m in Difference(N[w],[i,j,x,y,s,t]) do
                             R7:=R7+1;
                            od;
                        od;
                    od;
                od;
            od;
        od;
    od;
od;
R7:=R7/2;
```

Using the above program, the values $R_h(H_3),\ 1 \le h \le 7$ are computed and the results are shown in the Table1.

h	$R_h(H_3)$
1	$17+4\sqrt{6}$
2	$12\sqrt{3}+5\sqrt{2}$
3	$\frac{55}{3}+\frac{35}{6}\sqrt{6}$
4	$8+\frac{64}{9}\sqrt{3}+\frac{19}{2}\sqrt{2}$
5	$\frac{361}{18}+5\sqrt{6}$
6	$\frac{739}{12}\sqrt{2}+\frac{277}{2}\sqrt{3}$
7	$\frac{965}{54}+\frac{229}{54}\sqrt{6}$

Table 1. The Higher Randić Index of H_3.

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