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The Computation of New Versions of Randic Index for $TUC_4C_8(R)$ Nanotubes

[1]A. Mahmiani, [2]O. Khormali and [3]A. Iranmanesh

[1]Department of Mathematics Payame Noor University, 19395-4697 Tehran, Iran
[2]Mathematics and Informatics Research Group, ACECR,
Tarbiat Modares University, P.O. Box: 14115-343, Tehran, Iran
[3]Department of Pure Mathematice, Faculty of Mathematical sciences,
Tarbiat Modares Universiry, P.O. Box: 14115-137, Tehran, Iran

Abstract: Recently, the subdivision Randic index was introduced. In this paper, we present new version of Randic index by using some graph operator and in related to the subdivision Randic index. Next, by using some results about this version, it is computed for $TUC_4C_8(R)$ nanotubes.

Key words: Randic index · Subdivision Randic index · Molecular graph · Nanotubes

INTRODUCTION

In 1975 Randic [1] proposed several numbering schemes for the edges of the associated hydrogen-suppressed graph based on the degrees of the end vertices of an edge in studying the properties of alkane. To preserve rankings of certain molecules, several inequalities involving the weights of edges needed to be satisfied. Randic stated that weighting all edges uv of the associated graph G by $(d(u)d(v))^{-\frac{1}{2}}$ preserved these inequalities, where $d(u)$ denotes the degree of a vertex u in G. The sum of these latter weights over the edges of G is called the Randic index of G, denoted by $R(G)$. Some researchers often call it connectivity index [2]. Randic index is an important molecular descriptor and has been closely correlated with many chemical properties [3]. So, finding the graphs having maximum and minimum Randic indices and related problem of finding lower and upper bounds for the Randic index, attracted recently the attention of many researchers, and many results have been achieved, see [2, 4-7]. Clark and Moon [5] were interested in the former index and they gave a bound for trees. Bollobas and Erdos [4] generalized these indices by replacing $-\frac{1}{2}$ with any real number α, which was called the general Randic index in [5]. Here we denote it by $R_\alpha(G)$. When $\alpha = 1$, it is another important chemical index, called the Zagreb group index M_2, see [8]. In the following, we obtain the lower and upper bounds for the general Randic index among graphs with n vertices, and the corresponding extremal graphs. A clear picture is given depending on the real number α in different intervals.

In the following, the new version of Randic index will be introduced by using subdivision graphs. Next, some bounds and other results are concluded for the new version of Randic index. Finally, it is computed for $TUC_4C_8(R)$ nanotubes.

DISCUSSION AND RESULTS

Firstly, we restate two subdivision graphs which constructed from a graph G.

Suppose $G = (V, E)$ is a connected graph with the vertex set $V(G)$ and the edge set $E(G)$. Give an edge $e = (u, v)$, let $V(e) = \{u, v\}$. The subdivision graph $S(G)$ which is related graphs to graph G have been defined as follows (See [9]):

Subdivision Graph: $S(G)$ is the graph obtained from G by replacing each of its edge by a path of length two, or equivalently, by inserting an additional vertex into each edge of G. See Figure 1(c).

Two extra subdivision operator named $R(G)$ is defined as follows [9]:

$R(G)$ is defined as the graph obtained from G by adding a new vertex corresponding to each edge of G and by joining each new vertex to the end vertices of the edge corresponding to it. See Figure 1(e).

Corresponding Author: O. Khormali, Mathematics and Informatics Research Group, ACECR, Tarbiat Modares University, P.O. Box : 14115-343, Tehran, Iran.

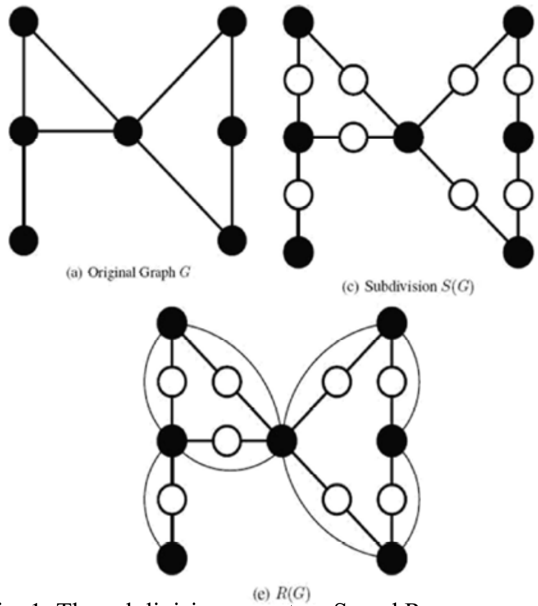

Fig. 1: The subdivision operators S, and R.

Given $G = (V,E)$, where $|E(G)| \subset \binom{V(G)}{2}$, we may define two other sets that we use frequently:

$$EE(G) := \{\{e,e'\} \mid e,e' \in E(G), e \neq e', |V(e) \cap V(e')| = 1\}$$
$$EV(G) := \{\{e,v\} \mid e \in E(G), V(G) \ni v \in V(e)\}$$

We can write the subdivision operators above as follows:

$S(G) := (V(G) \cup E(G), EV(G))$
$R(G) := (V(G) \cup E(G), E(G), \cup EV(G))$

Before stating the new version of Randic index, we state the zeroth-order Randic index and subdivision Randic index.

The zeroth-order Randic index of a graph G, defined by Kier and Hall [10], is

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

Later Li and Zhao in [11] defined the zeroth-order general Randic index $^{0}R_{\alpha}(G)$ of a graph G as

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

for general real number α.

The subdivision Randic index of a graph G, defines by Mahmiani and Khormali [3], is

$$R_S(G) = \sum_{xy=e \in E(S(G))} \frac{1}{\sqrt{d(x)d(y)}}$$

and the general subdivision Randic index of a graph G is

$$(R_s)_{\alpha}(G) = \sum_{xy=e \in E(S(G))} (d(x)d(y))^{\alpha}$$

for general real number α.

Definition 2-1: The R-Randic index of a graph G is

$$R_R(G) = \sum_{xy=e \in E(R(G))} \frac{1}{\sqrt{d(x)d(y)}}$$

and the general R-Randic index of a graph G is

$$(R_R)_{\alpha}(G) = \sum_{xy=e \in E(R(G))} (d(x)d(y))^{\alpha}$$

for general real number α.

Lemma 2-2: [3] Let G be a graph. We have

$$R_S(G) = \frac{1}{\sqrt{2}}\, {}^{0}R(G)$$

Lemma 2-3: [3] Let G be a graph. We have:

$$(R_s)_{\alpha}(G) = 2^{\alpha}\ {}^{0}R_{\alpha+1}(G)$$
$$^{0}R_{\alpha}(G) = 2^{1-\alpha}\ (R_s)_{\alpha-1}(G)$$

Result 2-4: Let G be a graph. We have:

$$R_R(G) = R(G) + R_S(G)$$
$$R_R(G) = R(G) + \frac{\sqrt{2}}{2}\, {}^{0}R(G)$$

Proof: The result can be concluded from the definition of R-Randic index and lemma (2-2). ?

Result 2-5: Let G be a graph. We have:

$$(R_R)_{\alpha}(G) = R_{\alpha}(G) + (R_S)_{\alpha}(G)$$
$$(R_R)_{\alpha}(G) = R_{\alpha}(G) + 2^{\alpha}\ {}^{0}R_{\alpha+1}(G)$$

Proof: The result can be concluded from the definition of R-Randic index and Lemma (2-3). □

In the following, we find the bounds for R-Randic index for trees. At first we restate the definitions of path P_n and star S_n. The path P_n is a tree of order n with exactly two vertices of degree 1. The star of order n, denoted by S_n, is the tree with n- 1 vertices of degree 1

Lemma 2-6: The path P_n which is of order n has the maximum R-Randic index.

Proof: Let the path P_n of order n. In [11], it is proved that the path P_n has the maximum subdivision Randic index. Also, the path P_n has the maximum Randic index. Therefore, due to the Result (2-4), P_n has the maximum R-Randic index. □

Lemma 2-7: The star S_n which is of order n has the minimum R-Randic index.

Proof: Let the star S_n of order n. In [11], it is proved that S_n has the minimum subdivision Randic index. Also, S_n has the minimum Randic index. Therefore, due to the Result (2-4), P_n has the minimum R-Randic index. □

Therorem 2-8: Let T be a tree of order n. The bounds of R-Randic index are

$$\sqrt{n-1}\left(\frac{\sqrt{2}}{2}(\sqrt{n-1}+1)+1\right) \le R_R(G) \le \frac{3n-7+2\sqrt{2}}{2}$$

Proof: Due to the Lemmas (2-6 and 2-7) and the facts that $R(P_n)=\frac{n-3+2\sqrt{2}}{2}, R(S_n)=\sqrt{n-1} R_s(P_n)=n-2+\sqrt{2}$ and $R_s(S_n)=\frac{\sqrt{2}}{2}(n-1+\sqrt{n-1})$, the upper and lower bounds of R-Randic index for trees can be concluded. ?

Now, we compute the R-Randic index for some familiar graphs and next, for TUC_4C_8(R) nanotubes.

Example 2-9: The R-Randic index of the cycle C_n, complete graph K_n and complete bipartite graph $K_{a,b}$ are as follows:

$$R_s(C_n)=\frac{3n}{2},\ R_s(K_n)=\frac{n}{2}(\sqrt{2n-2}+1),$$

$$R_s(K_{a,b})=\sqrt{ab}\left(\frac{\sqrt{2}}{2}\left(\sqrt{b}+\sqrt{a}\right)+1\right)$$

We use the notations q and p for the number of rows of squares and number of squares in a row, respectively in the TUC_4C_8(R) nanotubes which is mentioned in Figure 2 with $q = 4$ and $p = 8$.

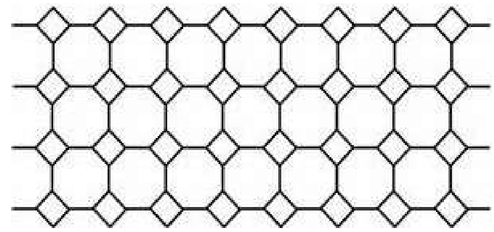

Fig. 2: Two dimensional lattice of $TUC_4C_8(R)$ nanotube, $q = 4, p = 8$

Theorem 2-10: The general subdivision Randic index for TUC_4C_8(R) nanotubes is

$$\left(R_S\right)_\alpha (TUC_4C_8(R)) = 2^{\alpha+1} p(2^{\alpha+1}+(2q-1)3^{\alpha+1})$$

Proof: Due to the Figure 2, number of vertices of TUC_4C_8(R) which is $4pq$ and definition general subdivision Randic index, we can conclude the result easily.□

Result 2-11: The zeroth-order general Randic index for TUC_4C_8(R) nanotubes is

$${}^0R_\alpha(TUC_4C_8(R)) = 2p(2^\alpha+(2q-1)3^\alpha)$$

Proof: Due to Lemma (2-3) and Theorem (2-10), the result can be concluded. □

Result 2-12: The subdivision Randic index and zeroth-order Randic index for TUC_4C_8(R) nanotubes are

$$R_s(TUC_4C_8(R)) = \sqrt{2}p(\sqrt{2}+(4q-1)\sqrt{3})$$

$${}^0R(TUC_4C_8(R)) = p(\sqrt{2}+(4q-2)\frac{\sqrt{3}}{3})$$

Proof: Due to Lemma (2-2) and Theorem (2-10) and Result (2-11), the result can be concluded. □

Theorem 2-13: The general R-Randic index for TUC_4C_8(R) nanotubes is

$$\left(R_R\right)_\alpha (TUC_4C_8(R)) =$$
$$p\left(2^{\alpha+1}(2^{\alpha+1}+(2q-1)3^{\alpha+1})+4(6^\alpha)+(6q-5)9^\alpha\right)$$

Proof: Due to the Result (2-5) and the fact that $R_\alpha(TUC_4C_8(R)) = p\left(4(6^\alpha)+(6q-5)9^\alpha\right)$, we have the desire result.□

Result 2-14: The R-Randic index of TUC_4C_8(R) nanotubes is

$$R_R(TUC_4C_8(R)) = p\left(\frac{6q+1+2\sqrt{6}}{3} + (4q-1)\sqrt{6}\right)$$

Proof: Due to Result (2-4) and Theorem (2-13) and the fact that $R_\alpha(TUC_4C_8(R)) = \frac{p}{3}\left(6q+2\sqrt{6}-5\right)$, the result can be concluded. □

CONCLUSION

The relations between the new version of Randic index which is introduced as R-Randic index and Subdivision Randic index and zeroth-order randic index are found. Also, the relation between general versions of them is found. In addition, the general subdivision Randic index, zeroth-order general Randic index and R-Randic index for TUC_4C_8(R) nanotubes are concluded.

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