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SOME BOUNDS ON THE MODIFIED RANDIC INDEX

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ABSTRACT. In this paper, we present some new lower and upper bounds for the modified Randic index in terms of maximum, minimum degree, girth, algebraic connectivity, diameter and average distance. Also we obtained relations between this index with Harmonic and Atom-bond connectivity indices. Finally, as an application we computed this index for some classes of nano-structures and linear chains.

Keywords: Randic index, Girth, Harmonic index, ABC index, Algebraic connectivity, Average distance.

INTRODUCTION

In this paper $G = (V(G), E(G))$ is a simple connected graph, where $V(G)$ is the set vertex of G, and $E(G)$ is the edge set of G. There are many different kinds of chemical indices that some of them are distance based like Wiener index, some of them are based on degree like Randic index. This fact is emphasized in the recent survey [12] which contains uniform approach to the degree- based indices.

The Randic index was proposed by Milan Randic in 1975. This topological index was named Branching index, later called Randic index, which defined as $R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$, where d_u denote the degree of vertex u. This index has been defined to measure the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. Although Milan Randic showed that there is a good correlation between this index and physicochemical properties of alkanes such as boiling points, surface areas and energy levels [1, 3, 27]. There are many applications in organic chemistry, medicinal chemistry and pharmacology that this index became one of the most interesting topic in graph theory which 4 books are devoted [10, 18-19, 23]. In 2011, Z.Dvorak proposed a modified of Randic index, defined as $R'(G) = \sum_{uv\in E(G)} \frac{1}{\max(d_u, d_v)}$, that is more tractable from computational point of view. It is much easier to follow during graph modifications than Randic index see [5] for more details. In [2], the authors showed that for every graph with n vertices, R´(G) is at least 1 no more than $\frac{n}{2}$ and these bounds attained by stars and regular graph. Although they determined graphs with minimal and maximal value of R´(G) among all trees and unicylic graphs, in [4], the authors showed that for all connected graph G the inequality $R'(G) \geq rad\,(G) - \frac{1}{2}$ holds where $rad(G)$ is the minimum eccentricity among all vertices of G, and the eccentricity of the vertex v is the maximum distance from v to any vertex. The maximum and minimim degree of a vertex in G denoted by Δ(G) and δ(G), respectively.

The Laplacian matrix of G is defined as $L_G = D_G - A_G$, where D_G is the diagonal matrix of its vertex degree and A_G is the adjacency matrix. Among all eigenvalues of the Laplacian matrix of G, one of the most popular is the second smallest, which was called the algebraic connectivity of a graph by fiedler [9] in 1973, and denoted by $a(G)$. In [22], the authors get relation between Randic index and algebraic connectivity. The girth of a graph G, denoted by $g(G)$, is the minimum length of its cycles. In [21] the authors computed upper bound of Randic index with girth g. Let $\mu(G)$ be the average distance of G that defined as $\mu(G) = \frac{W(G)}{\binom{n}{2}}$ such that $W(G)$ is the Wiener index defined as the sum of the lengths of the shortest path between all pairs of vertices and diameter of G is the maximum distance over all pairs of vertices u and v of G denoted by $D(G)$. In [30], the authors obtained relation between Randic index and diameter of a graph.

The edge cut of G is a group of edges whose total removal renders the graph disconnected. The edge connectivity $\lambda(G)$ is the size of a smallest edge cut. In this paper, we obtain a new bounds for the modified Randic index in terms of girth, diameter and algebraic connectivity. In continue, we establish some relation between this index and harmonic index and ABC index. The harmonic index of graph G is defined as $H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$. The atom–bond connectivity index of a nontrivial graph G, denoted by $ABC(G)$, is defined as $ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$. For more information about harmonic and ABC index we refer the reader to see [7,11,26,29].

MAIN RESULTS

The aim of this section is to determine some new bounds for R' in terms of girth, diameter and algebraic connectivity minimum and maximum degree.

Theorem 2.1: Let G be a connected triangle-free graph with $n \geq 2$ vertices and m edges. Then we have:

$$R'(G) \geq \frac{m}{n},$$

with equality if and only if G is an (n+1)-vetrex star S_{n+1}.

Proof: Let uv be an edge in G. Since G is triangle-free, we have $d_u \leq n - d_v$. Therefore regarding the definition of $R'(G)$, we have $R'(G) \geq \frac{m}{n}$. Furthermore, If G is the $(n+1)$-vertex star S_{n+1}, then $R'(G) = \frac{n-1}{n} = \frac{m}{n}$.

Conversely, we assume that $R'(G) = \frac{m}{n}$ but G is not isomorphic to S_{n+1}, then there must existan edge uv such that $d_u \leq (n+1) - d_v$, implying that $R'(G) > \frac{m}{n}$, a contradiction. This completes the proof.

Theorem 2.2: Let G be a 2-edge connected graph with n vertices and m edges then
$R'(G) \leq \frac{m}{2}$,
with equality if and only if G is an n-vertex cycle C_n.

Proof: Let uv be an edge in G. Since G is 2-edge connected, we have $d_u \geq 2$ and $d_v \geq 2$. So we have $R'(G) \leq \frac{m}{2}$ with equality if and only if $d_v = 2$ for any vertex v in G, that is $G \cong C_n$.

Note that a 2-connected graph is necessarily a 2-edge connected graph. By above theorem we have:

Corollary 2.3: Let G be a 2-connected graph with n vertices and m edges then we have

$$R'(G) < \frac{m}{2},$$

With equality if and only if G is an n-vertex cycle C_n.

Let S_n^* be a unicyclic graph obtained from star $K_{1,n-1}$ by joining two pendant vertices of $K_{1,n-1}$ by a new edge. (Fig. 1)

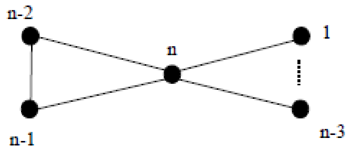

Fig. 1. The graph S_n^*

Theorem 2.4 : Let G be a connected graph on $n \geq 3$ vertices and girth g with $\delta \geq 2$, then the following inequalities hold:

$$R' + g \geq \sqrt{2(n-3)} + \frac{5}{2},\ R'.g \geq 3\sqrt{2(n-3)} - \frac{3}{2}.$$

The equality holds if G$\cong S_5^*$.

Proof: In [5], the authors proved that

$$R'(G) \geq \sqrt{2(n-3)} - \frac{1}{2}. \qquad (1)$$

It is easy to see that G contains at least one cycle since minimum degree δ is at least 2, so the girth of G is at least 3, this implies the inequality. Therefore the equalities hold if G$\cong S_5^*$, so the proof is now completed.

Lemma 2.5: Let G be a graph on n vertices with the algebraic connectivity a, we have:

$$a \geq 2\lambda\left(1 - \cos\frac{\pi}{n}\right),$$

where λ denotes the edge connectivity of G.

Proof: see [9] for more details.

Theorem 2.6: Let G be a graph on n vertices and edge connectivity λ≥ 2 such that $d(G) \geq 3$, we get the following inequality:

$$R'.a \geq 4\sqrt{2(n-3)}\left(1 - \cos\frac{\pi}{n}\right),$$

and if $\lambda = 1$ then we have:

$$R'.a \geq 2\sqrt{2(n-3)}\left(1 - \cos\frac{\pi}{n}\right).$$

Proof: Due to the above Lemma, if the edge connectivity $\lambda \geq 2$, we have $a \geq 4(1 - cos\frac{\pi}{n})$ and by using inequality (1) we can obtain:

$$R'.a \geq 4\sqrt{2(n-3)}\left(1 - cos\frac{\pi}{n}\right).$$

To prove the second part, it is enough to apply lemma 2.5.

Theorem 2.7: Fix a positive integer n. Among all trees on n vertices and maximum degree Δ, the maximum value of algebraic connectivity equals to $\Delta + 2\sqrt{\Delta - 1}$.
Proof: See [28].

Theorem 2.8: Among all trees, the maximum value of modified Randic index equals to $\frac{n-3}{2}$.
Proof: See [2].

Theorem 2.9: Let T be a tree with n vertices and algebraic connectivity a, the following ineqaulity holds:

$$R'.a < \frac{n-3}{2}(\Delta + 2\sqrt{\Delta - 1}).$$

Proof: Due to Theorem 2.7and 2.8, we have:

$$a < \Delta + 2\sqrt{\Delta - 1}\ ,\ R'(T) \leq \frac{n-3}{2},$$

so we have:

$$R'.a < \frac{n-3}{2}(\Delta + 2\sqrt{\Delta - 1})$$

Lemma 2.10 : Let G be a connected graph with n vertices and minimum degree $\delta \geq 2$. Then it follows that

$$D(G) \leq \frac{3n}{\delta+1} - 1.$$

Proof: see [6] for more details.

Theorem 2.11: Let G be a connected gaph with n verices and minimum degree $\delta \geq 2$. Then we get the following inequality:

$$\frac{R'}{D} \geq \frac{\delta\sqrt{(n-3)} - \frac{1}{2}}{3n}.$$

Proof: By the Inequality (1) and the above Lemma we have:

$$\frac{R'}{D} \geq \frac{\sqrt{2(n-3)} - \frac{1}{2}}{\frac{3n}{\delta+1} - 1} \geq \frac{(\delta+1)}{3n}\left(\sqrt{2(n-3)} - \frac{1}{2}\right) \geq \frac{\delta(\sqrt{n-3} - \frac{1}{2})}{3n}$$

.

Lemma 2.12: If G is a graph with n vertices and minimum degree δ, then we have:

$$\mu(G) \leq \frac{n}{\delta+1} + 2.$$

Proof: See [20] for more details.

Theorem 2.13: Let G be a connected graph with n vertices and minimum degree δ then it follows that

$$\frac{R'}{\mu} \geq \frac{\delta\left(\sqrt{(n-3)}-\frac{1}{2}\right)}{n+2(\delta+1)}.$$

Proof: By inequality (1) and the above Lemma we have

$$\frac{R'}{\mu} \geq \frac{\sqrt{2(n-3)}-\frac{1}{2}}{\frac{n}{\delta+1}+2} \geq \frac{(\delta+1)\sqrt{2(n-3)}}{n+2(\delta+1)} \geq \frac{\delta(\sqrt{n-3}-\frac{1}{2})}{n+2(\delta+1)}.$$

The proof is now complete.

Now, we obtain relations between the modified Randic index, Harmonic and ABC indices.

Theorem 2.14: let G be a nontrivial connected graph with n vertices and m edges then we have

$$H(G) \geq R'(G).$$

Proof: Let uv be an edge in G. Since $max(d_u, d_v) < d_u + d_v$, we have $\frac{1}{d_u+d_v} < \frac{1}{\max(d_u,d_v)}$. So clearly we obtain:

$$H(G) \geq R'(G).$$

Theorem 2.15: Let G be a nontrivial connected graph on n vertices and m edges, then we have:

$$H(G) \leq \frac{1}{2}(ABC)^2 + R'(G).$$

with equality if and only if $G \cong K_2$.

Proof: Let $f(x)=\frac{1}{x}$.It is obvious that $f(x)$ is a convex function. By Jensen's inequality, for each edge $uv \in E(G)$, we have

$$\frac{1}{\frac{1}{2}(d_u+d_v)} \leq \frac{1}{2}\left(\frac{1}{d_u}+\frac{1}{d_v}\right),$$

with equality if and only if $d_u = d_v$. Since $0 \leq \frac{1}{d_u}+\frac{1}{d_v}-\frac{2}{d_u d_v} < 1$, we have

$$\frac{2}{d_u+d_v} \leq \frac{1}{2}\left(\frac{1}{d_u}+\frac{1}{d_v}-\frac{2}{d_u d_v}\right)+\frac{1}{d_u+d_v}$$
$$\leq \frac{1}{2}\left(\frac{1}{d_u}+\frac{1}{d_v}-\frac{2}{d_u d_v}\right)+\frac{1}{\max(d_u,d_v)},$$

thus we have

$$\frac{1}{d_u+d_v} \leq \frac{1}{2}\left(\frac{1}{d_u}+\frac{1}{d_v}-\frac{2}{d_u d_v}\right)+\frac{1}{\max(d_u,d_v)} \leq \frac{d_u+d_v-2}{d_u d_v}+\frac{1}{\max(d_u,d_v)} = \frac{1}{2}(ABC)^2+R'(G).$$

The equality holds in the above inequality if and only if $d_u = d_v$.

Computation of the modified Randic index of $TUZC_6(p,q)$ nanotubes:

A carbon nanotube is forming from a graphite sheet that is rolled up so that it has a zigzag edge. In this paper, we computed the modified Randic index for some families of polyhex nanotubes, armchair, Phenylenic Nanotorus, Polycyclic Aromatic Hydrocarbons and polyomino chain (Figs. 2-8).

By considering the lattice of $TUZC_6$ [p,q], we denote the number of hexagon in the first row by p and the number of rows by q. In each row, there are 2p vertices and hence the number of vertices in this nanotube equals to 2pq. In [13] the authors obtained the hyper Wiener and Schultz indices of $TUZC_6$ [p,q] nanotube, in [14] the authors computed GA index for this nanotube and in [8], the author computed some connectivity index and Zagreb index of nanotube. Now in this section, we compute the modified index of $TUZC_6$ [p,q].

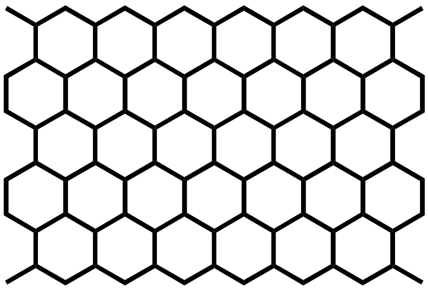

Fig. 2. The 2-Dimensional Lattice of $TUZC_6$[7,6]

Set $f_{m,n} = \{uv \mid uv \in E(G), d_v = m, d_u = n\}$, since in the graph of nanotube $TUZC_6$(p,q), all of edges uv are in $f_{2,3}$ or $f_{3,3}$, we need to obtain the number of $f_{2,3}$ and $f_{3,3}$.

Lemma 3.1: The number of $f_{2,3}$ equals to 4p and the number of $f_{3,3}$ equals to 3pq-5p.

Proof: Consider the $TUZC_6$[p,q] nanotube. At the first and last rows, there exist edges that every edge in these rows belong to $f_{2,3}$, hence the number of $f_{2,3}$ equals to 4p. At the other rows there exist p edges that belong to $f_{3,3}$ and the number of these edges are q-1, 2p edges that every edges belong to $f_{3,3}$ and the number of these edges are q-2, hence the number of $f_{3,3}$ equals to 3pq-5p.

Theorem 3.2 : The modified Randic index of $TUZC_6$[p,q] equals to $\frac{1}{3}(3pq - p)$.

Proof: By using the modified Randic index formula and the number of edges with their degrees we have:

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{max(d_u, d_v)} = \sum_{uv \in f_{2,3}} \frac{1}{max(d_u, d_v)} + \sum_{uv \in f_{3,3}} \frac{1}{max(d_u, d_v)}$$

$$= \frac{1}{3}\ (3pq - 5p + 4p) = \frac{1}{3}\ (3pq - p).$$

Now, we compute the modified Randic index of armchair $TUAC_6$[p,q] similar to previous section. The number of vertices in this armcheir equals to 2pq. The armchair's edges are in 3 types. The yellow edges belong to $f_{2,2}$, the red edges belong to $f_{2,3}$ and the other edges belong to $f_{3,3}$. The number of $f_{2,2}$, $f_{2,3}$ and $f_{3,3}$ are equal to p, 2p and 3pq-4p, respectively.

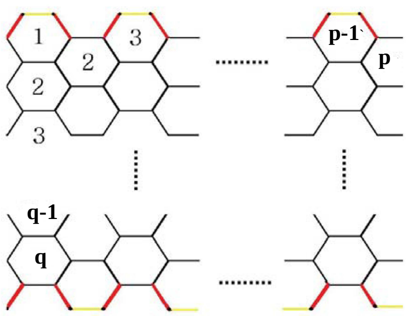

Fig. 3. The 2-Dimensional Lattice of $TUAC_6$[p,q]

Theorem 3.3: The modified Randic index of $TUAC_6[p,q]$ equals to $pq - \frac{p}{6}$.

Proof: Like the previous theorem we have:

$$R'(G) = \sum_{uv\in E(G)} \frac{1}{\max(d_u,d_v)} = \sum_{uv\in f_{2,2}} \frac{1}{\max(d_u,d_v)} + \sum_{uv\in f_{2,3}} \frac{1}{\max(d_u,d_v)} + \sum_{uv\in f_{3,3}} \frac{1}{\max(d_u,d_v)}$$

$$= \frac{p}{2} + \frac{2p}{3} + \frac{3pq-4p}{3} = pq - \frac{p}{6}$$

The next goal of this section is a computing a closed formula of the modified Randic index of $TUC_4C_8[p,q]$ nanotube. In the structure of this nanotube there are pq horizontal regular squar-octagone lattice with 8pq+2p vertices and 12pq+p edges (Fig. 4). For more results about this nanotube see [15-17, 24].

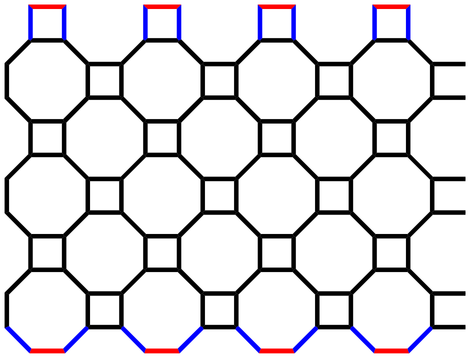

Fig. 4. 2-Dimensional Lattice of $TUC_4C_8[p,q]$ nanotube, with p=4 and q=3

Theorem 3.4: For $p, q \geq 1$, the modified Randic index of $TUC_4C_8[p,q]$ equals to $4pq + \frac{2p}{3}$.

Proof: Consider the Lattice of $TUC_4C_8[p,q]$ nanotube. In this nanotube we have three types of edges such that belong to $f_{2,2}$, $f_{2,3}$ and $f_{3,3}$ that are shown by red, blue and black colors such that $|f_{2,2}| = 2p$, $|f_{2,3}| = 4p$ and

$|f_{3,3}| = 12pq - 5p$. Thus we have

$$R'(G) = \sum_{uv\in E(G)} \frac{1}{\max(d_u,d_v)} = \sum_{uv\in f_{2,2}} \frac{1}{\max(d_u,d_v)} + \sum_{uv\in f_{2,3}} \frac{1}{\max(d_u,d_v)} + \sum_{uv\in f_{3,3}} \frac{1}{\max(d_u,d_v)}$$

$$= P + \frac{4p}{3} + \frac{12pq-5p}{3} = 4pq + \frac{2p}{3}$$

In continue, we obtain R'(G) of a physico chemical structure of Phenylenic Nanotorus. This nano structure is V-Phenylenic Nanotorus VPHY[p,q]. The structure of this nanotorus in terms of several $C_4C_6C_8$ net that composed of four and six membered rings such that every square is adjacent to two hexagones (Fig. 5).

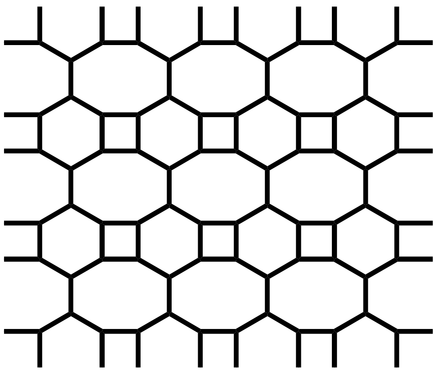

Fig. 5. The 2-Dimensional Lattice of VPHY[4,3]

Theorem 3.5: For $p, q \geq 1$, the modified Randic index of V-Phenylenic Nanotori VPHY[p,q] equals to $\frac{pq}{2}$.

Proof: Due to the general Figure of V-Phenylenic Nanotori VPHY[p,q], this nanotori has 6pq vertices, 9pq edges and all edges belong to $f_{3,3}$, this implies that

$$R'(G) = \sum_{uv\in E(G)} \frac{1}{\max(d_u,d_v)} = \sum_{uv\in f_{3,3}} \frac{1}{\max(d_u,d_v)} = \frac{pq}{2}$$

At the next goal, we calculate the modified Randic index of hydrocarbon structures *Polycyclic Aromatic Hydrocarbons (PAH$_n$)*. PAH_n are a complex group of chemicals containing two or more aromatic rings. PAH_ns are created when products like coal, oil, gas and garbage are burned but the burning process is not complete. The first member is *Benzene* (PAH_1) with six carbon and six hydrogen atoms and the second member is *coronene* (PAH_2) with 24 carbon and 12 hydrogen atoms (Fig. 6). By the Figure of the polycyclic aromatic hydrocarbon, it is easy to see that the general representation of has *PAH_n* $6n^2$ carbon and 6n hydrogen atoms.

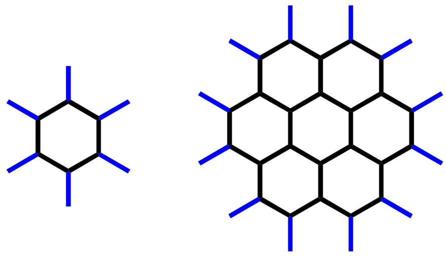

Fig. 6. The first and second member of polycyclic aromatic hydrocarbon PAH_n

Theorem 3.6: The modified Randic index of PAH_n equals to $n + 3n^2$.

Proof: Let PAH_n be the general representation of polycyclic aromatic hydrocarbon. The edge set of this graph can be dividing to two partitions, these partitions belong to $f_{1,3}$, $f_{3,3}$ and show that by blue and black color, respectively. All *Carbon* atoms have degree three and *Hydrogen* atoms have degree one, so we have $|f_{1,3}| = 6n$ and $|f_{3,3}| = 9n^2 - 3n$, so we have:

$$R'(G) = \sum_{uv\in E(G)} \frac{1}{\max(d_u,d_v)} = \sum_{uv\in f_{1,3}} \frac{1}{\max(d_u,d_v)} + \sum_{uv\in f_{3,3}} \frac{1}{\max(d_u,d_v)} = 2n + 3n^2 - n = n + 3n^2.$$

The modified Randic index of polyomino chain:

A polyomino system is a finite 2-connected plane graph such that each interior face is surrounded by a regular square of length one. A polyomino chain is a polyomino system, in which the joining of the centers of its adjacent regular forms a path $c_1c_2 \dots c_n$, where c_i is the center of the i-th square. Let B_n be the set of polyomino chains with n squares, the subgraph of B_n that induced by the vertices with degree 3 and n-2 squares, called a linear chain and denoted by L_n(Fig. 7). The subgraph of B_n induced by the vertices with degree bigger than 2 be a path with n-1 edges, called a zig-zag chain and denoted by Z_n (Fig. 8). In [31] the authors obtained Randic index of this graph.

A kink of a polyomino chain is any branched or angularly connected squares. A segment S of a polyomino chain is a maximal linear chain in the polyomino chains that include the kinks at its end. The number of squares in a segment denoted by $l(G)$.

A polyomino chains consist a sequence of segments $S_1,\dots,S_k$, $k \geq 1$, with $l(S_i) = l_i, i = 1, \dots, k$, where

$l_1+\dots+l_k = n + k - 1$ and n denote the number of squares of polyomino chain.

Fig. 7. The Linear chain

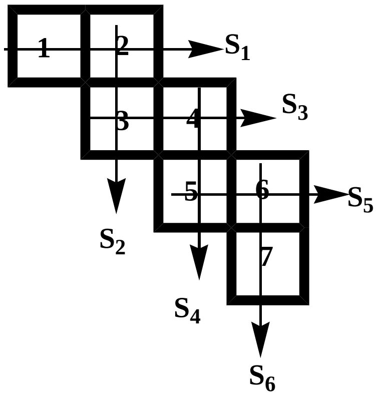

Fig. 8. The Zig-Zag chain

In the following, the aim is to calculate the Randic index of polyomino chains.

Theorem 4.1: Let L_n, Z_n be the polyomino chains then we have

$$R' \longrightarrow R'(L_n) = \begin{cases} 2, & n=1 \\ \frac{5}{3}, & n=2 \\ n+\frac{2}{3}, & n\geq 3 \end{cases} \quad , \quad R' \longrightarrow R'(Z_n) = \begin{cases} 2, & n=1 \\ \frac{5}{3}, & n=2 \\ \frac{9n-13}{12}, & n\geq 3 \end{cases}.$$

Proof: For $n \leq 2$ it is trivial, we assume that $n \geq 3$. By the general Figure of L_n, the number of $f_{2,2}$ equals to 2, the number of $f_{2,3}$ equals to 4 and the number of $f_{3,3}$ equals to $3n-5$. By the definition of modified Randic index, we have

$$R'(L_n) = \sum_{uv\in E(G)} \frac{1}{\max(d_u, d_v)} = \sum_{uv\in f_{2,2}} \frac{1}{\max(d_u, d_v)} + \sum_{uv\in f_{2,3}} \frac{1}{\max(d_u, d_v)} + \sum_{uv\in f_{3,3}} \frac{1}{\max(d_u, d_v)}$$

$$= 1 + \frac{4}{3} + \frac{3n-5}{3} = n + \frac{2}{3}.$$

The edge set of Z_n with *n* squares can be dividing to 5 partitions, these partitions belong to $f_{2,2}$, $f_{2,3}$, $f_{2,4}$, $f_{3,4}$ and $f_{4,4}$. Thus we have

$$R'(Z_n) = \sum_{uv\in E(G)} \frac{1}{\max(d_u, d_v)} = 1 + \frac{4}{3} + \frac{n-2}{2} + \frac{1}{2} + \frac{n-3}{4} = \frac{9n-13}{12}.$$

Theorem 4.2: Let B_n^1 be a polyomino chain with $n \geq 3$ squares and S_1, S_2 segments, such that $l_1 = 2, l_2 = n-1$. Then we have

$$R'(B_n^1) = \begin{cases} \frac{10}{3} & n=3, \\ n+\frac{1}{3} & n>3. \end{cases}$$

Proof: For $n = 3$ it is trivial, we assume that $n > 3$. By considering the general Figure of Z_n, we have

$$|f_{2,2}| = 2, |f_{2,3}| = 5, |f_{2,4}| = 1, |f_{3,4}| = 3 \text{ and } |f_{3,3}| = 3n-10.$$

So we have

$$R'(B_n^1) = \sum_{uv\in E(G)} \frac{1}{max(d_u,d_v)} = 1 + \frac{5}{3} + \frac{1}{4} + \frac{3}{4} + \frac{3n-10}{3} = n + \frac{1}{3}.$$

In following, we assume that $2 \le l(i) \le n-1$ such that $1 \le i \le k$.

Theorem 4.3: Let B_n^2 be a polyomino chain with $n \ge 4$ squares and $S_1, S_2, \dots, S_k$ $(k \ge 3)$ segments, such that $l_1 = l_k = 2, l_2, \dots, l_{k-1} \ge 3$. Then

$$R'(B_n^2) = \begin{cases} \frac{23}{6} & n = 4, \\ n - \frac{k}{3} + 1 & n > 4. \end{cases}$$

Proof: For $n = 4$ it is trivial. Therefore, we assume that $n > 4$. By considering the structure of B_n^2, we have $|f_{2,2}| = 2, |f_{2,3}| = 2k, |f_{2,4}| = 2, |f_{3,4}| = 4k - 6$ and $|f_{3,3}| = 3n + 1 - 2 - 2k - 2 - (4k - 6) = 3n - 6k + 3$.

Thus we have:

$$R'(B_n^2) = \sum_{uv\in E(G)} \frac{1}{max(d_u,d_v)} = 1 + \frac{2k}{3} + \frac{2}{4} + \frac{4k-6}{4} + \frac{3n-6k+3}{3} = n - \frac{k}{3} + 1 .$$

CONCLUSIONS

In this paper we achieved the lower and upper bounds for the modified Randic index in terms of girth, diameter and algebraic connectivity. Then we obtained a relation between this index with Harmonic and ABC indices. At the end of this paper we computed this index for some families of polyhex nanotubes $TUZC_6[p,q]$, $TUAC_6[p,q]$, $TUC_4C_8[p,q]$, VPHY[p,q] nanotorus, Polycyclic Aromatic Hydrocarbons and polyomino chains for the first time.

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