COMPUTATION OF SOME NEW/OLD VERTEX-DEGREE-BASED TOPOLOGICAL INDICES OF LINE GRAPH OF SUBDIVISION GRAPH OF SOME NANOSTRUCTURES

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A lot of topological indices have been introduced. Some topological indices that earlier have been considered in the mathematical chemistry, but failed to gain the attention of most mathematical chemists. Recently, some vertex-degree based topological indices "the reciprocal Randić index (RR), the reduced reciprocal Randić index (RRR), the reduced second Zagreb index (RM_2) and the forgotten index (F)" were reintroduced. In this paper, we computed these topological indices of line graphs of the subdivision graphs of Nanotube and Nanotorus of $TUC_4C_8[p;q]$.

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1. Introduction

In this article, we will consider only simple graphs without loops and multiple edges. Let G be simple graph with vertex set V (G) and edge set E(G). The degree of a vertex u, denoted by d(u) is the number of edges incident to u. The subdivision of an edge uv in a graph G is obtained by adding a new vertex w in V (G), and in edge set E(G) the edge uv is replaced by two new edges uw and wv. The subdivision graph S(G) is a graph resulting from the subdivision of all the edges of G. The line graph L(G) of a graph G is the graph whose vertices are the edges of G and two vertices of L(G) are adjacent if and only if their corresponding edges share a common endpoint in G. The L(S(G)) is the line graph of the subdivision graph of G.

A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix which represents the whole graph, and these representations are aimed to be uniquely defined for that graph. A topological index is a numeric quantity associated with a graph which characterizes the topology of the graph and is invariant under the graph automorphism. There are some major classes of topological indices such as distance based topological indices, degree based topological indices and counting related polynomials and indices of graphs. Among these classes degree based topological indices are of great importance and play a vital role in chemical graph theory and particularly in chemistry. The concept of topological index came from work done by Wiener [30] while he was working on boiling point of paraffin. He named this index as part number. Later on, the port number was renamed as Wiener index and then the theory of topological index started.

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Let G be a connected graph, then the Wiener index of G is defined as

$$W(G)=\frac{1}{2}\sum_{\{u,v\}\subset V(G)} d(u,v)$$

Where d (u; v) is the length of the shortest u-v path.

A large number of topological indices have been derived depending on vertex degrees. But only some of them found useful. Randić index was propo
sed by the chemist Milan Randić [26] in 1975. For a graph G it is defined as,

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

In 1998, Bollobas and Erdos [1] replaced $_2^1$ by any real number to generalize this index, which is known as the general Randić index.

$$R(G)=\sum_{uv\in E(G)}(d(u)d(v))^{\alpha}$$

The zeroth-order general Randić index, ^0R (G) was defined in [22] as

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

The first and second Zagreb indices are among the oldest and most famous topological indices, defines as follows

$$M_1(G)=\sum_{u\in V(G)} d(u)^2$$

$$M_2(G)=\sum_{uv\in E(G)} d(u)d(v)$$

Zhou et. al. in [31] proposed the sum-connectivity index as

$$\chi(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d}(u)+d(v)}$$

The concept of sum-connectivity index was extend to the general sum-connectivity index in [32]

$$\chi_{\alpha}(G)=\sum_{uv\in E(G)}(d(u)+d(v))^{\alpha}$$

For recent results on the vertex - degree based topological indices, we refer [2-16, 19, 23, 24, 27-29].

Recently, *I. Gutman et. al.* [17, 20] reinstates the neglected topological indices and showed that these topological indices have very promising applicative potential. The new/old topological indices studied by *I. Gutman et. al*. are the following: The reciprocal Randić index is defined as

$$RR(G)=\sum_{uv\in E(G)}\sqrt{d(u)d(v)}$$

The reduced reciprocal Randić index is defined as

$$RRR(G) = \sum_{uv \in E(G)} \sqrt{(d(u)-1)(d(v)-1)}$$

The reduced second Zagreb index is defined as

$$RM_2(G) = \sum_{uv \in E(G)} (d(u)-1)(d(v)-1)$$

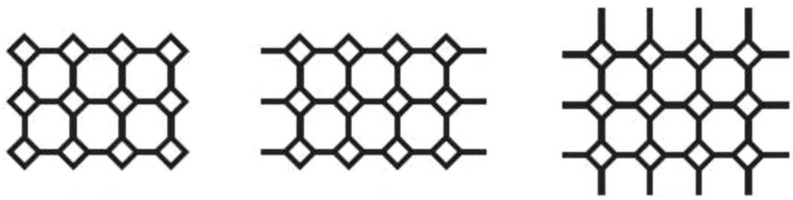
While studying the structure-dependency of the total-electron energy, it was indicated that other than Zagreb index, another term on which this energy depends is of the form

$$F(G) = \sum_{v \in V(G)} d(v)^3 = \sum_{uv \in E(G)} (d(u)^2 + d(v)^2)$$

Furtula et al. named this sum as forgotten index, or shortly the F index.

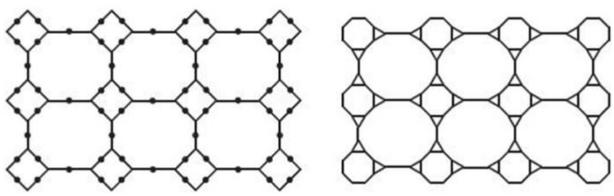
2. Topological indices of L(S(TUC$_4$C$_8$[p;q]))

In this paper, we computed the reciprocal Randić, reduced reciprocal Randić, reduced second Zagreb and forgotten indices of line graphs of the subdivision graphs of 2D-lattice, nanotube and nanotorus of TUC$_4$C$_8$[p;q], where p and q denote the number of squares in a row and number of rows of square respectively in 2D-latttice, nanotube and nanotorus of TUC$_4$C$_8$[p;q] [5-15, 25]. The number of vertices and edges of 2D-lattice, nanotube and nanotorus of TUC$_4$C$_8$[p;q] are given in Table 1. The graph of 2D-latttice, nanotube and nanotorus of TUC$_4$C$_8$[p;q] is shown in Fig. 1 (a), (b), (c) respectively. In order to compute certain topological indices of these nanotubes, we partitioned the edge set based on degrees of end vertices of each edge of the graph.



(a) (b) (c)

Fig. 1. (a) 2D-lattice of TUC$_4$C$_8$[p;q]; (b) TUC$_4$C$_8$[p;q] nanotube; (c) TUC$_4$C$_8$[p;q] nanotorus for p=4 and q=3.



(a) (b)

Fig. 2. (a) Subdivision of 2D-lattice of TUC$_4$C$_8$[p;q] for p=4 and q=3.; (b) line graph of the subdivision graph of 2D-lattice of TUC$_4$C$_8$[p;q] for p=4 and q=3

Table 1. Number of vertices and edges of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p;q]$

Graph	number of vertices	number of edges
2D lattice of TUC_4C_8[p;q]	4pq	6pq-p-q
TUC_4C_8[p;q] nanotube	4pq	6pq-p
TUC_4C_8[p;q] nanotorus	4pq	6pq

2.1. Topological indices of line graph of the subdivision graph of 2D-lattice of TUC_4C_8[p;q]

Theorem 1. Let G be line graph of the subdivision graph of 2D lattice of TUC_4C_8[p;q], then

$$RR(G) = (4\sqrt{6} - 29)(p+q) + 54pq + 20 - 8\sqrt{6}$$
$$RRR(G) = (4\sqrt{2} - 20)(p+q) + 36pq + 12 - 8\sqrt{6}$$
$$RM_2(G) = -34(p+q) + 72pq + 4$$
$$F(G) = -130(p+q) + 324pq$$

Proof. The subdivision graph of 2D-lattice of TUC_4C_8[p;q] and the line graph of the subdivision graph G are shown in the Fig. 2 (a) and (b), respectively. The graph G contains the vertices with degree 2 or 3 only. The total number of edges in G is 18pq 5p 5q. There are three types of edges in E(G) based on degrees of end vertices of each edge, i.e $E(G) = E_1(G) \cup E_2(G) \cup E_3(G).$ The edge partition E_1(G) contains 2p+2q+4 edges uv, where deg u=deg v=2, the edge partition E_2(G) contains 4p+4q 8 edges uv, where deg u=2 and deg v=3, and the edge partition E_3(G) contains 18pq-11p-11q+4 edges uv, where deg u=deg v=3.

With the help of this partition, we can nd the required results. We apply these to the formulas of RR; RRR; RM_2 and F to compute these indices for G. Since,

$$RR(G) = \sum_{uv \in E(G)} \sqrt{d(u)d(v)}$$
$$= \sum_{uv \in E_1(G)} \sqrt{d(u)d(v)} + \sum_{uv \in E_2(G)} \sqrt{d(u)d(v)} + \sum_{uv \in E_3(G)} \sqrt{d(u)d(v)}$$
$$= (2p+2q+4)\sqrt{2 \cdot 2} + (4p+4q-8)\sqrt{2 \cdot 3} + (18pq - 11p - 11q + 4)\sqrt{3 \cdot 3}$$
$$= (p+q)(4\sqrt{6} - 29) + 54pq + 20 - 8\sqrt{6}$$

which is the required (1) result.

$$RRR(G) = \sum_{uv \in E(G)} \sqrt{(d(u)-1)(d(v)-1)}$$
$$= \sum_{uv \in E_1(G)} \sqrt{(d(u)-1)(d(v)-1)} + \sum_{uv \in E_2(G)} \sqrt{(d(u)-1)(d(v)-1)} + \sum_{uv \in E_3(G)} \sqrt{(d(u)-1)(d(v)-1)}$$
$$= (2p+2q+4)\sqrt{(2-1)(2-1)} + (4p+4q-8)\sqrt{(2-1)(3-1)} + (18pq - 11p - 11q + 4)\sqrt{(3-1)(3-1)}$$
$$= (p+q)(4\sqrt{2} - 20) + 36pq + 12 - 8\sqrt{2}$$

which is the required (2) result.

$$RM_2(G) = \sum_{uv \in E(G)} (d(u)-1)(d(v)-1)$$
$$= \sum_{uv \in E_1(G)} (d(u)-1)(d(v)-1) + \sum_{uv \in E_2(G)} (d(u)-1)(d(v)-1) + \sum_{uv \in E_3(G)} (d(u)-1)(d(v)-1)$$
$$= (2p+2q+4)(2-1)(2-1) + (4p+4q-8)(2-1)(3-1) + (18pq-11p-11q+4)(3-1)(3-1)$$
$$= 72pq - 34(p+q) + 4$$

which is the required (3) result.

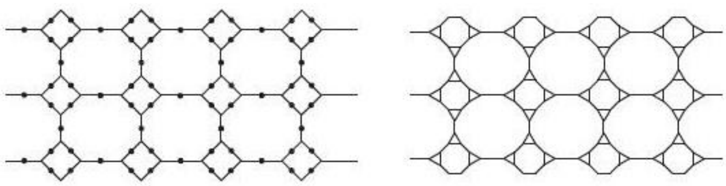
$$F(G) = \sum_{uv \in E(G)} (d(u)^2 + d(v)^2)$$
$$= \sum_{uv \in E_1(G)} (d(u)^2 + d(v)^2) + \sum_{uv \in E_2(G)} (d(u)^2 + d(v)^2) + \sum_{uv \in E_3(G)} (d(u)^2 + d(v)^2)$$
$$= (2p+2q+4)(2^2+2^2) + (4p+4q-8)(2^2+3^2) + (18pq-11p-11q+4)(3^2+3^2)$$
$$= 324pq - 130(p+q)$$

which is the required (4) result, and the proof is complete.

2.2. Topological indices of line graph of the subdivision graph of $TUC_4C_8[p;q]$ Nanotube

Theorem 2. Let H be line graph of the subdivision graph of $TUC_4C_8[p;q]$ nanotube, then:

$$RR(H) = p(4\sqrt{6} - 29 + 54q)$$
$$RRR(H) = p(4\sqrt{2} - 20 + 36q)$$
$$RM_2(H) = p(-34 + 72q)$$
$$F(H) = p(-138 + 324q)$$



(a) (b)

Fig. 3. (a) subdivision of $TUC_4C_8[p;q]$ nanotube for p=4 and q=3.; (b) line graph of subdivision of $TUC_4C_8[p;q]$ for p=4 and q=3. Nanotube

Proof. The subdivision graph of $TUC_4C_8[p;q]$ nanotube and the graph H are shown in the Fig. 3 respectively. The graph H contains 12pq-2p vertices among which 4p are vertices of degree 2 and remaining all vertices are of degree 3. The total number of edges of G is 18pq-5p. There are three type of edges in E(H) based on degrees of end vertices of each edge, i.e $E(H) = E_1(H) \cup E_2(H) \cup E_3(H)$. The edge partition $E_1(H)$ contain 2q edges uv, where deg u=deg v=2, the edge partition $E_2(H)$ contain 4p edges uv, where deg u=2 and deg v=3, and the edge partition $E_3(H)$ contain 18pq-11p edges uv, where deg u=deg v=3.

With the help of this partition we can easily and the required results. We apply these to the formulas of RR; RRR; RM_2 and F compute these indices for H. Since,

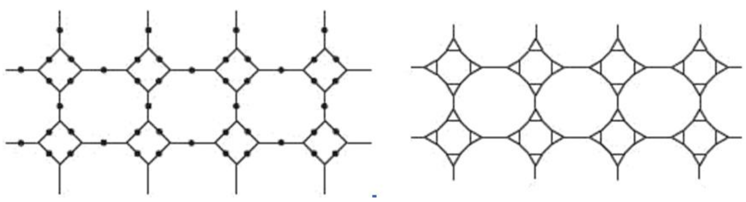
$$RR(H)=\sum_{uv\in E(H)}\sqrt{d(u)d(v)}$$
$$=\sum_{uv\in E_1(H)}\sqrt{d(u)d(v)}+\sum_{uv\in E_2(H)}\sqrt{d(u)d(v)}+\sum_{uv\in E_3(H)}\sqrt{d(u)d(v)}$$
$$=2p\sqrt{2\cdot 2}+4p\sqrt{2\cdot 3}+(18pq-11p)\sqrt{3\cdot 3}$$
$$=p(-138+324q)$$
which is the required 1

$$RRR(H)=\sum_{uv\in E(H)}\sqrt{(d(u)-1)(d(v)-1)}$$
$$=\sum_{uv\in E_1(H)}\sqrt{(d(u)-1)(d(v)-1)}+\sum_{uv\in E_2(H)}\sqrt{(d(u)-1)(d(v)-1)}+\sum_{uv\in E_3(H)}\sqrt{(d(u)-1)(d(v)-1)}$$
$$=2p\sqrt{(2-1)(2-1)}+4p\sqrt{;}2(2-1)(3-1)+(18pq-11p)\sqrt{(3-1)(3-1)}$$
$$=p(4\sqrt{2}-20+36q)$$
which is the required 2 result.
$$RM_2(H)=\sum_{uv\in E(H)}(d(u)-1)(d(v)-1)$$
$$=\sum_{uv\in E_1(H)}(d(u)-1)(d(v)-1)+\sum_{uv\in E_2(H)}(d(u)-1)(d(v)-1)+\sum_{uv\in E_3(H)}(d(u)-1)(d(v)-1)$$
$$=2p(2-1)(2-1)+4p(2-1)(3-1)+(18pq-11p)(3-1)(3-1)$$
$$=p(-34+72q)$$
which is the required 3 result.
$$F(H)=\sum_{uv\in E(H)}(d(u)^2+d(v)^2)$$
$$=\sum_{uv\in E_1(H)}(d(u)^2+d(v)^2)+\sum_{uv\in E_2(H)}(d(u)^2+d(v)^2)+\sum_{uv\in E_3(H)}(d(u)^2+d(v)^2)$$
$$=2p(2^2+2^2)+4p(2^2+3^2)+(18pq-11p)(3^2+3^2)$$
$$=p(4\sqrt{6}-29+54q)$$
which is the required 4 result, and the proof is complete.

2.3. Topological indices of line graph of the subdivision graph of TUC_4C_8[p;q] Nanotorus

Theorem 3. Let K be line graph of the subdivision graph of TUC_4C_8[p;q] nanotorus, then:

1. *RR(K)=54pq*
2. *RRR(K)=36pq*
3. *RM_2(K)=72pq*
4. *F (K)=162pq*



(a) (b)

Fig. 4. (a) Subdivision of TUC_4C_8 [p;q] nanotorus for p=4 and q=2.; (b) line graph of subdivision of TUC_4C_8[p;q] for p=4 and q=2. nanotorus

Proof. The subdivision graph of $TUC_4C_8[p;q]$ nanotorus and the graph K are shown in the Fig 4, respectively. We can see that K is a cubic graph of order 12pq and size 18pq. We apply the formulas of RR; RRR; RM_2 and F to compute these indices for K. Since,

$$RR(K)=\sum_{uv\in E(K)}\sqrt{d(u)d(v)}=18pq\sqrt{3\cdot 3}=54pq$$

which is the required 1 result.

$$RRR(K)=\sum_{uv\in E(K)}\sqrt{(d(u)-1)(d(v)-1)}=18pq\sqrt{(3-1)(3-1)}=36$$

which is the required 2 result.

$$RM_2(K)=\sum_{uv\in E(K)}(d(u)-1)(d(v)-1)=18pq(3-1)(3-1)=72pq$$

which is the required 3 result.

$$F(K)=\sum_{uv\in E(K)}(d(u)^2+d(v)^2)=18pq(3^2+3^2)=324pq.$$

which is the required 4 result, and the proof is complete.

Conclusion

In this report, we present some properties of vertex-degree based topological indices of molecular graphs, called “the reciprocal Randić index (RR), the reduced reciprocal Randić index (RRR), the reduced second Zagreb index (RM_2) and the forgotten index (F)” and we computed a closed formulas of these topological indices of line graphs of the subdivision graphs of Nanotube and Nanotorus of $TUC_4C_8[p;q]$.

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