FOUR VERTEX-DEGREE-BASED TOPOLOGICAL INDICES OF CERTAIN NANOTUBES

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Let G be a simple connected graph with vertex set V(G) and edge set E(G). The number of elements in V (G) is called the order of G, denoted as |V (G)|, and the number of elements in E(G) is called the size of G, denoted as |E(G)|. A topological index is a numerical descriptor of a molecular structure derived from the corresponding molecular graph. Recently, four vertex-degree based graph invariants, "reciprocal Randić (RR), reduced reciprocal Randić (RRR), reduced second Zagreb (RM_2) and forgotten (F) indices" was defined by I. Gutman. In this article, we compute these indices of $HC_5C_7[p;q]$ and $SC_5C_7[p;q]$ Nanotubes.

Keywords: Reciprocal Randić index, Reduced reciprocal Randić index, Reduced second Zagreb index, Forgotten index, $HC_5C_7[p;q]$ nanotube, $SC_5C_7[p;q]$ nanotube

1. Introduction

Let G(V(G),E(G)) be a simple connected graph, where V(G) and E(G) represents the vertex set and edge set, respectively. Number of elements in V(G) is called the order of G, denoted as |V(G)|, and the number of elements in E(G) is called the size of G, denoted as |E(G)|. For a vertex $u \in V(G)$, the degree of u in G, d(u), is the number of vertices adjacent with u in graph G.

A topological index is a numerical descriptor of the molecular structure derived from the corresponding molecular graph. Many topological indices are widely used for quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies. The concept of

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topological index came from work done by Harold Wiener in 1947 while he was working on boiling point of paraffin.
In chemical graph theory, several vertex-degree based topological indices have been and are currently considered and applied in QSPR=QSAR studies. Among them first Zagreb index M_1, the second Zagreb index M_2 are the oldest and most thoroughly investigated. Following are there definitions:

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

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

In addition, we mention some other vertex-degree based topological indices widely used in chemical literature. Randić index was proposed by the chemist Milan Randić [1] 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 [2] replaced $\frac{-1}{2}$ by any real number \alpha to generalize this index, which is known as the general Randić index.

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

The zeroth-order general Randić index, ${}^0R_\alpha(G)$ was defined in[3] as

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

Zhou et. al. in [4, 5] proposed the sum-connectivity index. The sum-connectivity index is obtained from Randić index by replacing d(u)d(v) by d(u)+d(v),

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

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

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

In 1980, Fajtlowicz defined an invariant of the Randić index called the harmonic index, defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}$$

For recent results on vertex-degree based topological indices, readers can see the paper series [6-18].

Recently, *Gutman et.al.* presented four vertex-degree based graph invariants, that earlier have been considered in the chemical and/or mathematical literature, but, that evaded the attention of most mathematical chemists. The new/old topological indices studied by *I. Gutman et. al.* are the following [19, 20]:
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

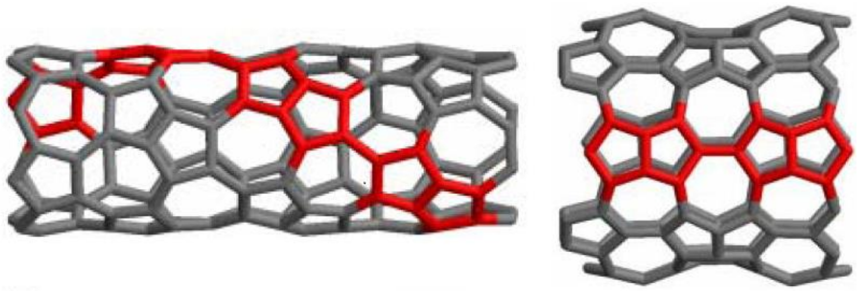
$$RM_2(G) = \sum_{uv\in E(G)} (d(u)-1)(d(v)-1)$$

In a study on the structure-dependency of the total π-electron energy, beside the first Zagreb index, it was indicated that another term on which this energy depends is of the form

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

Recently, this sum was named forgotten index, or shortly the F index.

Carbon nanotubes are types of nanostructure which are allotropes of carbon and having a cylindrical shape. Carbon nanotubes or molecular graphs ”$SC_5C_7[p,q]$” and ”$HC_5C_7[p,q]$” are two family of nanotubes, such that their structure are consist of cycles with length five and seven by different compound. In other words, a C_5C_7 net is a trivalent decoration made by alternating C_5 and C_7. It can cover either a cylinder or a torus. For a review, historical details and further bibliography see the 3-dimensional lattice of ”$VC_5C_7[p,q]$” and ”$HC_5C_7[p,q]$” nanotubes in Fig. 1 and their 2-dimensional lattice in Fig. 2 and Fig. 4, respectively. For further study reader can see [21-36].



(A) (B)

Fig. 1. The Molecular graph of SC_5C_7 (A) and HC_5C_7 (B) nanotubes

2. Main Results

In this section, we focus on the structures of two families of carbon nanotubes ”*$SC_5C_7[p,q]$*” and ”*$HC_5C_7[p,q]$*” are of nanotubes and we will compute the reciprocal Randić, reduced reciprocal Randić, reduced second Zagreb and forgotten indices of HC_5C_7 and SC_5C_7 nanotubes. To compute certain topological indices of thee nanotubes, we will partition the edge set based on degrees of end vertices of each edge of the graph.

2.1. Nanotube $HC_5C_7[p,q],(p,q>1)$

In this section, we calculate some topological indices of $HC_5C_7[p;q]$ nanotube. The two dimensional lattices of $HC_5C_7[p;q]$, in which p is the number of heptagons in first row and q is the number of periods in whole lattice. A period consist of four rows, a m^{th} period is shown in Fig.2. This nanotube is a C_5C_7 net and its 2-dimensional lattice is constructed by alternating C_5 and C_7 following the trivalent decoration as shown in Fig. 2 and Fig. 3. This type of pattern of C_5 and C_7 can either cover a cylinder or a torus. There are 16p vertices in one period of the lattice and 2p vertices are joined to the end of the graph, so $|V(HC_5C_7[p;q])|=16pq+2p$. Similarly, there are 24p edges in one period and 2p extra edges which are joined to the end of the graph in these nanotubes, so we have $|E(HC_5C_7[p;q])|=24pq-2p$.

Theorem 2. Consider the graph $HC_5C_7[p;q]$ nanotube, then

$$RR(HC_5C_7[p,q]) = (36q + 4\sqrt{6} - 15)2p \tag{5}$$

$$RRR(HC_5C_7[p,q]) = (12q + 2\sqrt{2} - 5)4p \tag{6}$$

$$RM_2(HC_5C_7[p,q]) = (4q - 1)24p \tag{7}$$

$$F(HC_5C_7[p,q]) = (108q - 19)4p \tag{8}$$

Proof. Consider the nanotube $G=HC_5C_7[p;q]$, where p is the number of heptagons in one row and q is the number of periods in whole lattice. To obtain the final results we partition the edge set based on degrees of end vertices of G. There are two partitions of edge set correspond to their degrees of end vertices which are

$$E_1 = \{uv \in E(G) \mid d(u) = 2 \, and \, d(v) = 3\}$$

$$E_2 = \{uv \in E(G) \mid d(u) = 3 \, and \, d(v) = 3\}$$

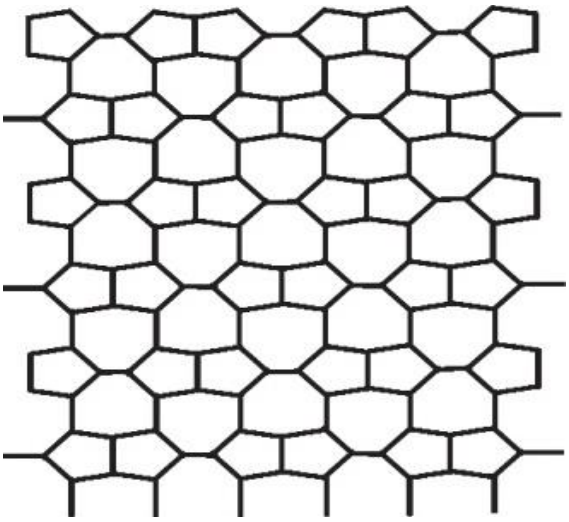


Fig. 2: The graph of $HC_5C_7[p;q]$ nanotube with p=3 and q=3

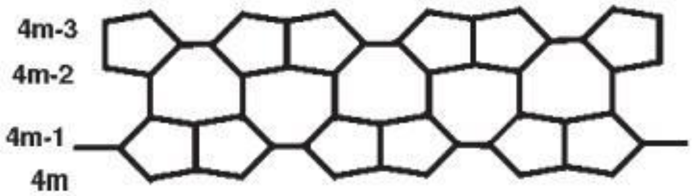


Fig. 3: The m[th] period of HC_5C_7 nanotube

The number of edges in E_1 and E_2 are 8p and 24pq-10p. Now, we can compute the RR; RRR; RM_2 and F to compute these indices for G. Since,

$$RR(G) = \sum_{uv \in E(G)} \sqrt{d(u)d(v)} = \sum_{uv \in E_1(G)} \sqrt{d(u)d(v)} + \sum_{uv \in E_2(G)} \sqrt{d(u)d(v)}$$

$$= 8p\sqrt{2 \cdot 3} + (24pq - 10p)\sqrt{3 \cdot 3}$$

$$= (36q + 4\sqrt{6} - 15)2p$$

which is the required (5) result.

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

$$= \sum_{uv \in E_1(G)} \sqrt{(d(u)-1)(d(v)-1)} + \sum_{uv \in E_2(G)} \sqrt{(d(u)-1)(d(v)-1)}$$

$$= 8p\sqrt{(2-1)(3-1)} + (24pq - 10p)\sqrt{(3-1)(3-1)}$$

$$= (12q + 2\sqrt{2} - 5)4p$$

which is the required (6) result.

$$RM_2(G)=\sum_{uv\in E(G)}(d(u)-1)(d(v)-1)$$
$$=\sum_{uv\in E_1(G)}(d(u)-1)(d(v)-1)+\sum_{uv\in E_2(G)}(d(u)-1)(d(v)-1)$$
$$=8p(2-1)(3-1)+(24pq-10p)(3-1)(3-1)$$
$$=(4q-1)24p$$

which is the required (7) result.

$$F(G)=\sum_{uv\in E(G)}(d(u)^2+d(v)^2)$$
$$=\sum_{uv\in E_1(G)}(d(u)^2+d(v)^2)+\sum_{uv\in E_2(G)}(d(u)^2+d(v)^2)$$
$$=8p(2^2+3^2)+(24pq-10p)(3^2+3^2)$$
$$=(108q-19)4p$$

which is the required (8) result, and the proof is complete.■

2.2. Nanotube SC_5C_7[p,q],(p,q>1)

In this section, we compute the certain vertex-degree based topological indices of SC_5C_7[p;q] nanotube. This nanotube is also C_5C_7 net is constructed by alternating C_5 and C_7 following the trivalent decoration as shown in Fig. 4 and Fig 5. This type of tiling can either cover a torus or cylinder too. The SC_5C_7[p;q], in which p is the number of heptagons in each row and q is the number of periods in whole lattice. A period consists of three rows as in Fig. 5 in which mth period is shown. There are 8p vertices in one period of the lattice so $|V(SC_5C_7[p;q])|=8pq$. Similarly, there are 12p edges in one period and 2p extra edges which are joined to the end of the graph so $|E(SC_5C_7[p;q])|=12pq\ 2p$.

Theorem 3. Consider the graph of SC_5C_7[p;q] nanotube, then

$$F(SC_5C_7[p,q])=(54q-19)4p \tag{9}$$
$$RM_2(SC_5C_7[p,q])=(48q-23)p \tag{10}$$
$$RRR(SC_5C_7[p,q])=(24q+6\sqrt{2}-17)p \tag{11}$$
$$RR(SC_5C_7[p,q])=(36q+6\sqrt{6}-25)p \tag{12}$$

Proof. Consider the nanotube G=SC_5C_7[p;q], where p is the number of heptagons in one row and q is the number of periods in whole lattice. To obtain the final results we partition the edge set based on degrees of end vertices of G. There are three partitions of edge set correspond to their degrees of end vertices which are

$$E_1 = \{uv \in E(G) \mid d(u) = 2 \text{ and } d(v) = 2\}$$
$$E_2 = \{uv \in E(G) \mid d(u) = 2 \text{ and } d(v) = 3\}$$
$$E_3 = \{uv \in E(G) \mid d(u) = 3 \text{ and } d(v) = 3\}$$

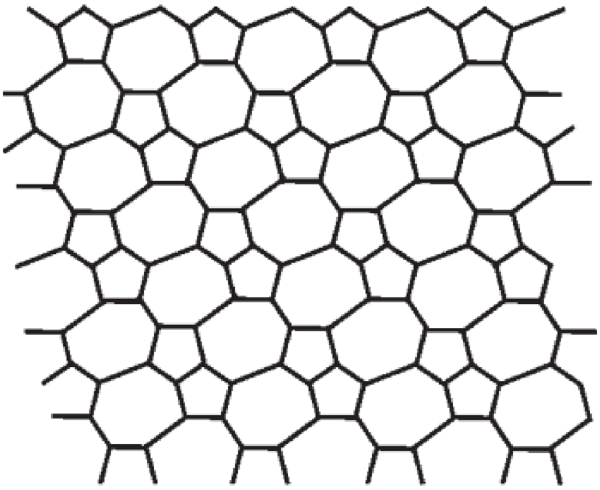


Fig. 4: The graph of $SC_5C_7[p;q]$ nanotube with p=4 and q=4.

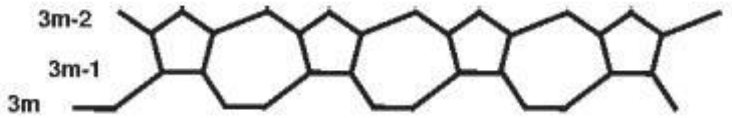


Fig. 5: The m[th] period of SC_5C_7 nanotube.

The number of edges in E_1; E_2 and E_3 are p; 6p and 12pq-9p. Now, we are able to apply the formula of RR; RRR; RM_2 and F to compute these indices for G. Since,

$$RR(G) = \sum_{uv \in E(G)} \sqrt{d(u)d(v)}$$
$$= \sum_{uv \in E_1(G)} \sqrt{d(u)d(v)} + \sum_{uv \in E_2(G)} \sqrt{d(u)d(v)} + \sum_{uv \in E_3(G)} \sqrt{d(u)d(v)}$$
$$= p\sqrt{2 \cdot 2} + 6p\sqrt{2 \cdot 3} + (12pq - 9p)\sqrt{3 \cdot 3}$$
$$= (36q + 6\sqrt{6} - 25)p$$

which is the required (9) result.

$$RRR(G) = \sum_{uv \in E(G)} \sqrt{(d(u)-1)(d(v)-1)}$$
$$= \sum_{uv \in E_1(G)} \sqrt{(d(u)-1)(d(v)-1)} + \sum_{uv \in E_2(G)} \sqrt{(d(u)-1)(d(v)-1)} + \sum_{uv \in E_3(G)} \sqrt{(d(u)-1)(d(v)-1)}$$
$$= p\sqrt{(2-1)(2-1)} + 6p\sqrt{(2-1)(3-1)} + (12pq-9p)\sqrt{(3-1)(3-1)}$$
$$= (24q + 6\sqrt{2} - 17)p$$

which is the required (10) result.

$$RM_2(G) = \sum_{uv \in E(G)} (d(u)-1)(d(v)-1)$$
$$= \sum_{uv \in E_1(G)} (d(u)-1)(d(v)-1) + \sum_{uv \in E_2(G)} (d(u)-1)(d(v)-1) + \sum_{uv \in E_3(G)} (d(u)-1)(d(v)-1)$$
$$= p(2-1)(2-1) + 6p(2-1)(3-1) + (12pq-9p)(3-1)(3-1)$$
$$= (48q - 23)p$$

which is the required (11) result.

$$F(G) = \sum_{uv \in E(G)} (d(u)^2 + d(v)^2)$$
$$= \sum_{uv \in E_1(G)} (d(u)^2 + d(v)^2) + \sum_{uv \in E_2(G)} (d(u)^2 + d(v)^2) + \sum_{uv \in E_3(G)} (d(u)^2 + d(v)^2)$$
$$= p(2^2 + 2^2) + 6p(2^2 + 3^2) + (12pq - 9p)(3^2 + 3^2)$$
$$= (54q - 19)4p$$

which is the required (12) result, and the proof is complete.■

3. Open Problems and Concluding Remarks

Recently, Gutman et. al. (re)introduced some new/old degree based topological indices and show that these topological indices have their own significance in the study of chemical graph theory. These indices are reciprocal Randić index, reduced reciprocal Randić index, reduced second Zagreb index and forgotten index. In this paper, we found these new/old topological indices of some nano-structure. These indices have not much studied up to now, so one can find the results for rest of nano-structures e.g. HAC_5C_7, $HAC_5C_6C_7$, and Dendrimers.

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