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On the Randic and Sum-Connectivity Index of Nanotubes

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Abstract. *Milan Randić* proposed in 1975 a structural descriptor called the branching index that later became the well-known Randić connectivity index; it is defined on the ground of vertex degrees $\chi(G) = \sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$. In 2008, *B. Zhou* and *N. Trinajstić* proposed another connectivity index, named the Sum-connectivity index $X(G)$.In this paper, we focus on the structure of "$G = VC_5C_7[p,q]$" and "$H = HC_5C_7[p,q]$" nanotubes and counting *Randić* index $\chi(G) = \sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$ and sum-connectivity index $X(G) = \sum_{v_u v_v} \frac{1}{\sqrt{d_u + d_v}}$ of these nanotubes.

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1 Introduction

Let $G = (V; E)$ be a simple connected graph. The sets of vertices and edges of G are denoted by $V = V(G)$ and $E = E(G)$, respectively. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds.
In graph theory, we have many different connectivity topological index of an arbitrary graph G. A topological index is a numeric quantity from the structural graph of a molecule which is invariant under graph automorphisms.

The simplest topological indices are the number of vertices, the number of edges and degree of a vertex v of the graph G and we denoted by n, e and d_v, respectively. The degree of a vertex is equal to the number of its first neighbors. Also, $\forall u, v \in V(G)$, the distance $d(u, v)$ between u and v is defined as the length of any shortest path in G connecting u and v.
The connectivity index introduced in 1975 by *Milan Randić* [12], who has shown this index to reflect molecular branching. Randić index (First connectivity index) was defined as follows

$$\chi(G) = \sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u d_v}} \tag{1}$$

In general, the m-connectivity index of a graph G is defined as

$$^{m}\chi(G) = \sum_{v_{i_1} v_{i_2} \ldots v_{i_{m+1}}} \frac{1}{\sqrt{d_{i_1} d_{i_2} \ldots d_{i_{m+1}}}},$$

where $v_{i_1} v_{i_2} \ldots v_{i_{m+1}}$ runs over all paths of length m in G.
Recently, a closely related variant of the Randić connectivity index called the sum-connectivity index was introduced by *B. Zhou* and *N. Trinajstić* [13, 16] in 2008. For a connected graph G, its sum-connectivity index $X(G)$ is defined as the sum over all edges of the graph of the terms $\frac{1}{\sqrt{d_u + d_v}}$, that is,

$$X(G) = \sum_{v_u v_v} \frac{1}{\sqrt{d_u + d_v}} \tag{2}$$

where d_u and d_v are the degrees of the vertices u and v, respectively.
In this paper, we focus on the above connectivity indices "*Randić*" and "sum-connectivity" index and compute two indices for two types of nanotubes ("$G = VC_5C_7[p, q]$" and "$H = HC_5C_7[p, q]$"). Our notation is standard and for more information and background biography, refer to paper series [1-18].

2 Main Result

The aim of this section is to compute the *Randić* connectivity index and sum-connectivity index of $G = VC_5C_7[p, q]$ and $H = HC_5C_7[p, q]$ nanotubes. The structure of these nanotubes are consist of cycles with length five and seven (or C_5C_7 net) by different compound. 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

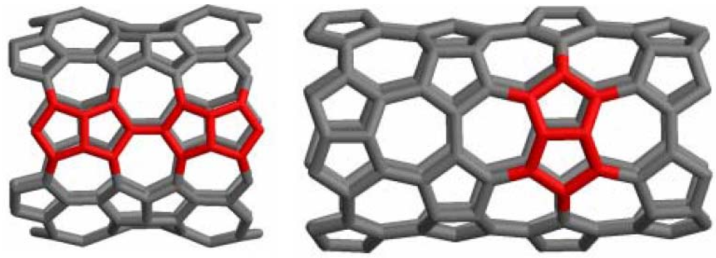

Figure 1: The Molecular graph of VC_5C_7 (A) and HC_5C_7 (B) nanotube.

lattice of $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ nanotubes in Figure 1 and their 2-dimensional lattice in Figure 2 and Figure 3, respectively.
Before presenting the main results, let us introduce some definitions. First, let us denote the number of pentagons in the first row of the 2D-lattice of G (Figure 2) and H (Figure 3) by p. In these nanotubes, the four first rows of vertices and edges are repeated alternatively, we denote the number of this repetition by q. $\forall p,q \in \mathbb{N}$ in each period of $G = VC_5C_7[p,q]$, there are $16p$ vertices and $6p$ vertices which are joined to the end of the graph. Thus the number of vertices in G is equal to

$$n = |V(VC_5C_7[p,q])| = 16pq + 6p.$$

Since $3p + 3p$ vertices have degree two and other have degree three ($16pq$), thus the number of edges in this nanotube is equal to

$$e = |E(VC_5C_7[p,q])| = \frac{2(6p) + 3(16pq)}{2} = 24pq + 6p.$$

Also, in each period of $H = HC_5C_7[p,q]$, there are $8p$ vertices. Hence

$$n = |V(HC_5C_7[p,q])| = 8pq + 5p,$$

$5p$ vertices which are joined to the end of H. And in each period there are $12p$ edges and we have q repetition and $5p$ addition edges, thus the number of edges in this nanotube is equal to $e = |E(HC_5C_7[p,q])| = 12pq + 5p$, $\forall p,q \in \mathbb{N}$. On the other hands $2p + 3p$ vertices have degree two and $8pq$ other vertices have degree three, and alternatively

$$e = \frac{2(5p) + 3(8pq)}{2} = 12pq + 5p$$

Definition 2.1. *Let $G = (V;E)$ be a simple connected graph and d_v is degree of vertex $v \in V(G)$ (Obviously $1 \le \delta \le d_v \le \Delta \le n-1$, such that*

$\delta = Min\{d_v | v \in V(G)\}$ and $\Delta = Max\{d_v | v \in V(G)\}$). We divide edge set $E(G)$ and vertex set $V(G)$ of graph G to several partitions, as follow:

$$\forall i,\ 2\delta \leq i \leq 2\Delta,\ E_i = \{e = uv \in E(G) | d_v + d_u = i\},$$

$$\forall j,\ \delta^2 \leq j \leq \Delta^2,\ E_j^* = \{e = uv \in E(G) | d_v \times d_u = j\}$$

and $$\forall k,\ \delta \leq k \leq \Delta,\ V_k = \{v \in V(G) | d_v = k\}.$$

Obviously, in nano science an atom (or a vertex v) of a nano structure G have at most four adjacent. In other words, d_v is equal to 1, 2, 3 and 4. Therefore, we have two partitions

- $V_3 = \{v \in V(G) | d_v = 3\}$
- $V_2 = \{v \in V(G) | d_v = 2\}$.

Note that hydrogen and single carbon atoms are often omitted. Also, the edge set of a molecular graph G can be dividing to three partitions, e.g. E_4, E_5 and E_6. In other words,

- For every $e = uv$ belong to E_4, $d_u = d_v = 2$.
- Similarly, for every $e = uv$ belong to E_6, $d_u = d_v = 3$.
- Finally, for every $e = uv$ belong to E_5, then $d_u = 2$ and $d_v = 3$.

Now, we have following theorems.

Theorem 2.2. *Let G be $VC_5C_7[p,q]$ nanotubes. Then:*

- *Randić connectivity index of G is equal to*

$$\chi(VC_5C_7[p,q]) = 8pq + 2(\sqrt{6} - 1)p. \qquad (3)$$

- *sum-connectivity index of G is equal to*

$$X(VC_5C_7[p,q]) = 4\sqrt{6}pq + (\frac{12\sqrt{5}}{5} - \sqrt{6})p. \qquad (4)$$

Proof. $\forall p, q \in \mathbb{N}$ consider nanotubes $G = VC_5C_7[p,q]$ with $16pq + 6p$ vertices and $24pq + 6p$ edges, such that $|V_2| = 6p$ and $|V_3| = 16pq$. So, we mark the edges of E_5, E_6^* by red color and the edges of E_6, E_9^* by black color (Figure 2). Thus, we have

- $|E_5| = |E_6^*| = 6p + 6p$
- $|E_6| = |E_9^*| = 24pq - 6p$.

Now, by according to definition of *Randić* connectivity index

$$\begin{aligned} {}^1\chi(VC_5C_7[p,q]) &= \sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u d_v}} = \sum_{e=uv\in E_9^*} \frac{1}{\sqrt{d_u d_v}} + \sum_{e=uv\in E_6^*} \frac{1}{\sqrt{d_u d_v}} \\ &= \frac{|E_9^*|}{\sqrt{9}} + \frac{|E_6^*|}{\sqrt{6}} \\ &= \frac{24pq-6p}{\sqrt{9}} + \frac{12p}{\sqrt{6}} \\ &= 8pq + 2(\sqrt{6}-1)p. \end{aligned} \tag{5}$$

Also, by according to the definition of sum-connectivity index, we have following equations:

$$\begin{aligned} {}^1X(VC_5C_7[p,q]) &= \sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}} = \sum_{e=uv\in E_6} \frac{1}{\sqrt{d_u + d_v}} + \sum_{e=uv\in E_5} \frac{1}{\sqrt{d_u + d_v}} \\ &= \frac{|E_6|}{\sqrt{6}} + \frac{|E_5|}{\sqrt{5}} \\ &= \frac{24pq-6p}{\sqrt{6}} + \frac{12p}{\sqrt{5}} \\ &= 4\sqrt{6}pq + (\frac{12\sqrt{5}}{5} - \sqrt{6})p. \end{aligned} \tag{6}$$

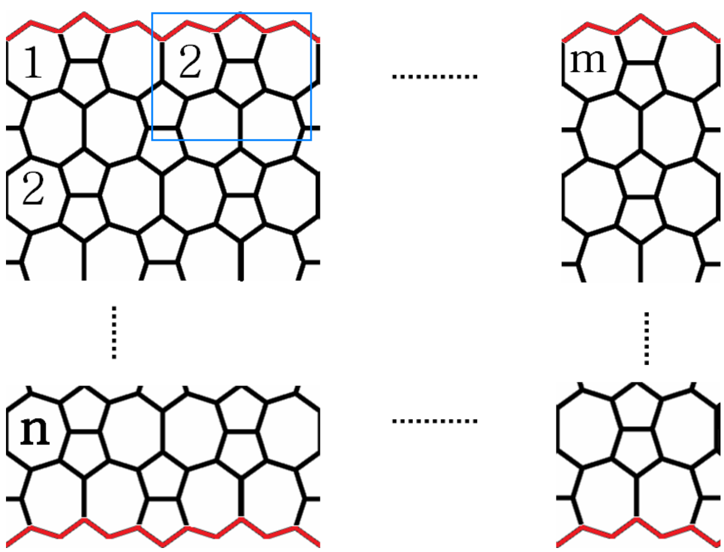

Figure 2: 2-Dimensional Lattice of $G = VC_5C_7[m,n]$.

Here, we complete the proof of Theorem 2.2. □

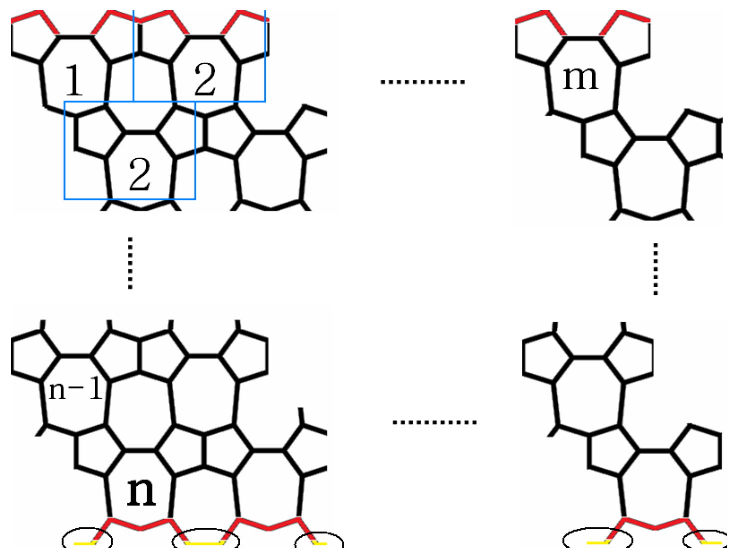

Figure 3: 2-Dimensional Lattice of $H = HC_5C_7[m,n]$.

Theorem 2.3. $\forall p, q \in \mathbb{N}$
- *Randić connectivity index of* $HC_5C_7[p,q]$ *nanotube is equal to*

$$\chi(HC_5C_7[p,q]) = 4pq + (\frac{8\sqrt{6}-5}{6})p. \tag{7}$$

- *Sum-connectivity index of* $HC_5C_7[p,q]$ *nanotube is equal to*

$$X(HC_5C_7[p,q]) = 2\sqrt{6}pq + (\frac{8\sqrt{5}}{5} - \frac{2\sqrt{6}}{3} + \frac{1}{2})p. \tag{8}$$

Proof. Consider nanotube $H = HC_5C_7[p,q]$, $\forall p, q \in \mathbb{N}$. Similar to $VC_5C_7[p,q]$ nanotube, H consists of heptagon and pentagon nets. But, in this nanotube there are $8pq + 5p$ atoms (vertices) and $12pq + 5p$ bonds (edges). Such that $|V_2| = 5p$ and $|V_3| = 8pq$, and alternatively • $|E_4| = |E_4^*| = p$
- $|E_5| = |E_6^*| = 4p + 4p$
- $|E_6| = |E_9^*| = 12pq - 4p$.

We mark all edge E_4, E_5 and E_6 by yellow, red and black color in Figure 3, respectively.

Thus, we have following equations for its connectivity indies.

$$\begin{aligned}
{}^1\chi(HC_5C_7[p,q]) &= \sum_{e=uv\in E(H)} \frac{1}{\sqrt{d_u d_v}} \\
&= \sum_{e=uv\in E_9^*} \frac{1}{\sqrt{d_u d_v}} + \sum_{e=uv\in E_6^*} \frac{1}{\sqrt{d_u d_v}} + \sum_{e=uv\in E_4^*} \frac{1}{\sqrt{d_u d_v}} \\
&= \frac{|E_9^*|}{\sqrt{9}} + \frac{|E_6^*|}{\sqrt{6}} + \frac{|E_4^*|}{\sqrt{4}} = \frac{12pq-4p}{3} + \frac{8\sqrt{6}p}{6} + \frac{p}{2} \\
&= 4pq + (\frac{8\sqrt{6}-5}{6})p. \qquad (9)
\end{aligned}$$

$$\begin{aligned}
{}^1X(HC_5C_7[p,q]) &= \sum_{e=uv\in E(H)} \frac{1}{\sqrt{d_u d_v}} \\
&= \sum_{e=uv\in E_6} \frac{1}{\sqrt{d_u d_v}} + \sum_{e=uv\in E_5} \frac{1}{\sqrt{d_u d_v}} + \sum_{e=uv\in E_4} \frac{1}{\sqrt{d_u d_v}} \\
&= \frac{|E_6|}{\sqrt{6}} + \frac{|E_5|}{\sqrt{5}} + \frac{|E_4|}{\sqrt{4}} = \frac{12pq-4p}{\sqrt{6}} + \frac{8p}{\sqrt{5}} + \frac{p}{2} \\
&= 2\sqrt{6}pq + (\frac{8\sqrt{5}}{5} - \frac{2\sqrt{6}}{3} + \frac{1}{2})p. \qquad (10)
\end{aligned}$$

And these complete the proof of Theorem 2.3. □

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