On the Randic and Sum-Connectivity Index of Nanotubes

Mohammad Reza Farahani

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 $G = V C_5 C_7[p, q]$ and $H = H C_5 C_7[p, q]$ nanotubes and counting Randić index $\chi(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$ and sum-connectivity index $X(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$ 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

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

(1)

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

$$m\chi(G) = \sum_{v_1v_2...v_{m+1}} \frac{1}{\sqrt{d_{i_1}d_{i_2}...d_{i_{m+1}}}},$$

where $v_{i_1}v_{i_2}...v_{i_{m+1}}$ 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,

$$X(G) = \sum_{uv} \frac{1}{\sqrt{d_u + d_v}}$$

(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 (“$G = V C_5 C_7[p, q]$” and “$H = H C_5 C_7[p, q]$”). 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 $G = V C_5 C_7[p, q]$ and $H = H C_5 C_7[p, q]$ nanotubes. The structure of these nanotubes are consist of cycles with length five and seven (or $C_5 C_7$ net) by different compound. A $C_5 C_7$ 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 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 16$p$ vertices and 6$p$ 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 8$p$ vertices. Hence

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

5$p$ vertices which are joined to the end of $H$. And in each period there are 12$p$ edges and we have $q$ repetition and 5$p$ 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 $1 \leq \delta \leq d_v \leq \Delta \leq n - 1$, such that
\[ \delta = \text{Min}\{d_v | v \in V(G)\} \text{ and } \Delta = \text{Max}\{d_v | v \in V(G)\} \]. 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

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

- Sum-connectivity index of \(G\) is equal to

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

\[ 1 \chi(VC_5C_7[p, q]) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} = \sum_{e=uv \in E_6} \frac{1}{\sqrt{d_u d_v}} + \sum_{e=uv \in E_5} \frac{1}{\sqrt{d_u d_v}} \]

\[ = \frac{|E_6^*|}{\sqrt{9}} + \frac{|E_5^*|}{\sqrt{6}} \]

\[ = \frac{24pq - 6p}{\sqrt{9}} + \frac{12p}{\sqrt{6}} \]

\[ = 8pq + 2(\sqrt{6} - 1)p. \quad (5) \]

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

\[ 1 X(VC_5C_7[p, q]) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} = \sum_{e=uv \in E_6} \frac{1}{\sqrt{d_u + d_v}} + \sum_{e=uv \in E_5} \frac{1}{\sqrt{d_u + d_v}} \]

\[ = \frac{|E_6|}{\sqrt{6}} + \frac{|E_5|}{\sqrt{5}} \]

\[ = \frac{24pq - 6p}{\sqrt{6}} + \frac{12p}{\sqrt{5}} \]

\[ = 4\sqrt{6}pq + \left( \frac{12\sqrt{5}}{5} - \sqrt{6} \right)p. \quad (6) \]

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

Here, we complete the proof of Theorem 2.2. \( \square \)
Theorem 2.3. $\forall p, q \in \mathbb{N}$

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

$$\chi(HC_5C_7[p, q]) = 4pq + \left( \frac{8\sqrt{6} - 5}{6} \right)p.$$  \hspace{1cm} (7)

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

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

- $|E_4| = |E_4^*| = 4p + 4p$
- $|E_5| = |E_5^*| = 4p + 4p$
- $|E_6| = |E_6^*| = 12pq - 4p$.

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 indices.

\[ 1\chi(HC_5C_7[p, q]) = \sum_{e=uv \in E(H)} \frac{1}{\sqrt{d_u d_v}} \]

\[ = \sum_{e=uv \in E^*_6} \frac{1}{\sqrt{d_u d_v}} + \sum_{e=uv \in E^*_5} \frac{1}{\sqrt{d_u d_v}} + \sum_{e=uv \in E^*_4} \frac{1}{\sqrt{d_u d_v}} \]

\[ = \frac{|E^*_6|}{\sqrt{6}} + \frac{|E^*_5|}{\sqrt{5}} + \frac{|E^*_4|}{\sqrt{4}} = \frac{12pq - 4p}{3} + \frac{8\sqrt{6}p}{6} + \frac{p}{2} \]

\[ = 4pq + \left(\frac{8\sqrt{6} - 5}{6}\right)p. \quad (9) \]

\[ 1X(HC_5C_7[p, q]) = \sum_{e=uv \in E(H)} \frac{1}{\sqrt{d_u d_v}} \]

\[ = \sum_{e=uv \in E^*_6} \frac{1}{\sqrt{d_u d_v}} + \sum_{e=uv \in E^*_5} \frac{1}{\sqrt{d_u d_v}} + \sum_{e=uv \in E^*_4} \frac{1}{\sqrt{d_u d_v}} \]

\[ = \frac{|E^*_6|}{\sqrt{6}} + \frac{|E^*_5|}{\sqrt{5}} + \frac{|E^*_4|}{\sqrt{4}} = \frac{12pq - 4p}{\sqrt{6}} + \frac{8p}{\sqrt{5}} + \frac{p}{2} \]

\[ = 2\sqrt{6}pq + \left(\frac{8\sqrt{5}}{5} - \frac{2\sqrt{6}}{3} + \frac{1}{2}\right)p. \quad (10) \]

And these complete the proof of Theorem 2.3. \( \square \)

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Mohammad Reza Farahani
Department of Applied Mathematics,
Iran University of Science and Technology (IUST),
Narmak, Tehran 16844, Iran
E-mail: MR_Farahani@mathdep.iust.ac.ir & MRFarahani88@gmail.com

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