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COMPUTING SOME CONNECTIVITY INDICES OF *V*-PHENYLENIC NANOTUBES AND NANOTORI

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Abstract

Let G be a simple connected graph in chemical graph theory and $e = uv$ be an edge of G. The Randić index $\chi(G)$ and sum-connectivity $X(G)$ of a nontrivial connected graph G are defined as the sum of the weights $\frac{1}{\sqrt{d_u d_v}}$ and $\frac{1}{\sqrt{d_u + d_v}}$ over all edges $e = uv$ of G, respectively. In this paper, we compute Randić $\chi(G)$ and sum-connectivity $X(G)$ indices of *V*-phenylenic nanotubes and nanotori.

Keywords: molecular graph, *V*-phenylenic nanotubes, *V*-phenylenic nanotori, Randić connectivity index, sum-connectivity index.

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1. Introduction

Let G be a simple connected graph in chemical graph theory. The vertex set and edge set of G denoted by $V(G)$ and $E(G)$, respectively, and its vertices correspond to the atoms and the edges correspond to the bonds [1-4].

There are many different kinds of topological indices or chemical indices. A chemical topological index is a numeric quantity from the structural graph of a molecule and is invariant on the automorphism of the graph. Some of them are distance based indices like *Wiener index*, some are degree based indices like the Randić index. The *Randić index* $\chi(G)$ of a graph G is defined as

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

It is also known as connectivity index or branching index. Randić in 1975 [5] proposed this index for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. There is also a good correlation between the Randić index and several physicochemical properties of alkanes: boiling points, surface areas, energy levels, etc.

In 2008, Zhou and Trinajstić introduced the sum-connectivity index $X(G)$ as

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

where d_u and d_v are the degrees of the vertices u and v, respectively.

For a comprehensive survey of its mathematical properties, see the book of Li and Gutman [6], or recent survey of Li and Shi [7]. See also the books of Kier and Hall [8, 9] for chemical properties of this index.

In this paper, we compute these connectivity topological indices of *V-phenylenic nanotubes* and *nanotori*.

2. Main Results and Discussion

In this section, Randić connectivity 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 V-phenylenic nanotubes and nanotori are computed. Before present the main results, we recall some useful definitions and notations.

Definition 1 ([10]). Consider an arbitrary vertex v with degree d_v of simple connected graph $G = (V(G); E(G))$ and we denoted the minimum degree with $\delta = \text{Min}\{d_v | v \in V(G)\}$ and the maximum degree with $\Delta = \text{Max}\{d_v | v \in V(G)\}$. By according to the vertices degree, we have several partitions of vertex set $V(G)$ and edge set $E(G)$ of graph G, as follow:

$$\forall k : \delta \le k \le \Delta, \quad V_k = \{v \in V(G) |\, d_v = k\},$$

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

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

Before going to calculate favourite connectivity indices, we divide the vertex set $V(VPHX[m, n])$ and the edge set $E(VPHX[m, n])$ of V-phenylenic nanotube in the following partitions:

$$V_3 = \{v \in V(VPHX[m, n]) | d_v = 3\},$$

$$V_2 = \{v \in V(VPHX[m, n]) | d_v = 2\},$$

$$E_5 = E_6{}^* = \{uv \in E(VPHX[m, n]) |\, d_u + d_v = 5 \,\&\, d_u \times d_v = 6\},$$

$$E_6 = E_9{}^* = \{uv \in E(VPHX[m, n]) |\, d_u + d_v = 6 \,\&\, d_u \times d_v = 9\}.$$

Molecular graphs V-phenylenic nanotubes and nanotorus are two families of nano-structures that their structure are consist of cycles with length four, six, and eight by different compound.

Professor Diudea denotes the V-phenylenic nanotubes and V-phenylenic nanotorus by $G = VPHX[m, n]$ and $H = VPHY[m, n]$, respectively [11]. Also, the general representations of these two kind of nano-structures are shown in Figure 1 and Figure 2. Readers can see the paper series [12-20], for a review historical details and further bibliography of V-phenylenic nanotubes and V-phenylenic nanotorus.

Theorem 1. *Consider V-phenylenic nanotubes* $G = VPHX[m, n]$ *for every* $m, n \in \mathbb{N} - \{1\}$. *Then*

The Randić connectivity index of G is equal to

$$\chi(VPHX[m, n]) = \left(3n + \frac{2\sqrt{6} - 5}{3}\right)m \approx (3n - 0.03367)m.$$

The sum-connectivity index of G is equal to

$$X(VPHX[m, n]) = \left(\frac{9\sqrt{6}n}{6} + \left(\frac{4\sqrt{5}}{5} - \frac{5\sqrt{6}}{6}\right)\right)m \approx (3.6742n - 0.2524)m.$$

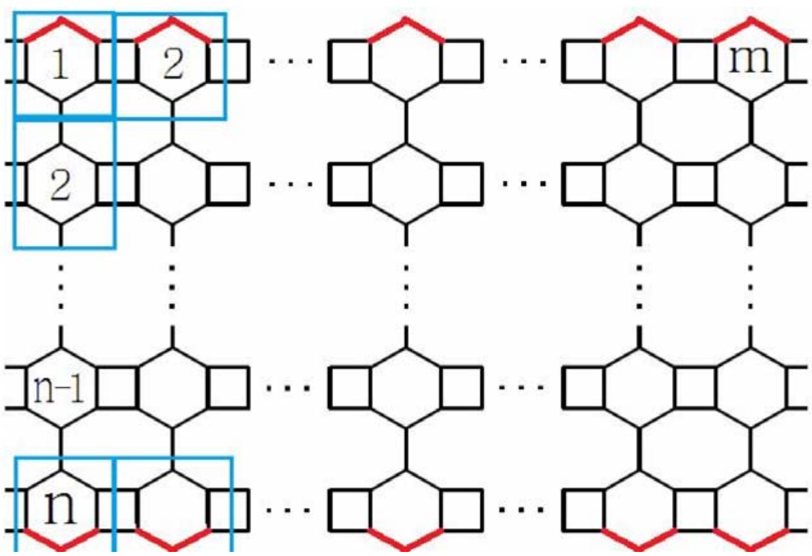

Figure 1. 2-D Lattice of the V-phenylenic nanotubes $G = VPHX[m, n]$.

Proof of Theorem 1. Consider V-phenylenic nanotube $G = VPHX[m, n]$ $(m, n > 1)$, since G consist of several adjacent hexagon (or cycle C_6), we denote the number of repetition of these C_6's in the first row/column by m and n, respectively.

Thus by look at the general case V-phenylenic nanotube $G = VPHX[m, n]$ in Figure 1, one can see that the number of vertices and edges in $G = VPHX[m, n]$ are equal to *6mn* and $9mn - m$, respectively. Since $|V_2| = m + m$ and $|V_3| = 6mn - 2m$. Then the number of edges of $G = VPHX[m, n]$ will be $|E(VPHX[m, n])| = \frac{1}{2}[2(2m) + 3(6mn - 2m)]$.

Now by according to Figure 2, we see that there exist the number of $2m + 2m$ members in the edge partition E_5 or $E_6{}^*$ (the red colour edges in Figure 1) and there are $9mn - 5m$ members in the edge partition E_6 or $E_9{}^*$ (the black colour edges in Figure 1).

Now, the Randić connectivity index, sum-connectivity index of V-phenylenic nanotube $G = VPHX[m, n]$ are equal, respectively, as

$$\chi(VPHX[m, n]) = \sum_{uv \in E(VPHX[m, n])} \frac{1}{\sqrt{d_u d_v}}$$

$$= \sum_{e=uv\in E_9^*} \frac{1}{\sqrt{d_u d_v}} + \sum_{e=uv\in E_6^*} \frac{1}{\sqrt{d_u d_v}}$$

$$= \frac{|E_9^*|}{\sqrt{9}} + \frac{|E_6^*|}{\sqrt{6}}$$

$$= \frac{9mn - 5m}{3} + \frac{4m\sqrt{6}}{6}$$

$$= \left(3n + \frac{2\sqrt{6} - 5}{3}\right)m,$$

and

$$X(VPHX[m,\ n]) = \sum_{uv \in E(VPHX[m,\ n])} \frac{1}{\sqrt{d_u + d_v}}$$

$$= \sum_{e=uv \in E_6} \frac{1}{\sqrt{d_u + d_v}} + \sum_{e=uv \in E_5} \frac{1}{\sqrt{d_u + d_v}}$$

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

$$= \left(\frac{9\sqrt{6}n}{6} + \left(\frac{4\sqrt{5}}{5} - \frac{5\sqrt{6}}{6}\right)\right)m. \qquad \square$$

Theorem 2. *Let G be the V-phenylenic nanotorus $H = VPHY[m,\ n]$, $\forall m,\ n > 1$. Then*

The Randić connectivity index of H is equal to $\chi(VPHY[m,\ n]) = 3mn$.

The sum-connectivity index of H is equal to $X(VPHY[m, n]) = \frac{3\sqrt{6}mn}{2}$

$= 3.6742mn$.

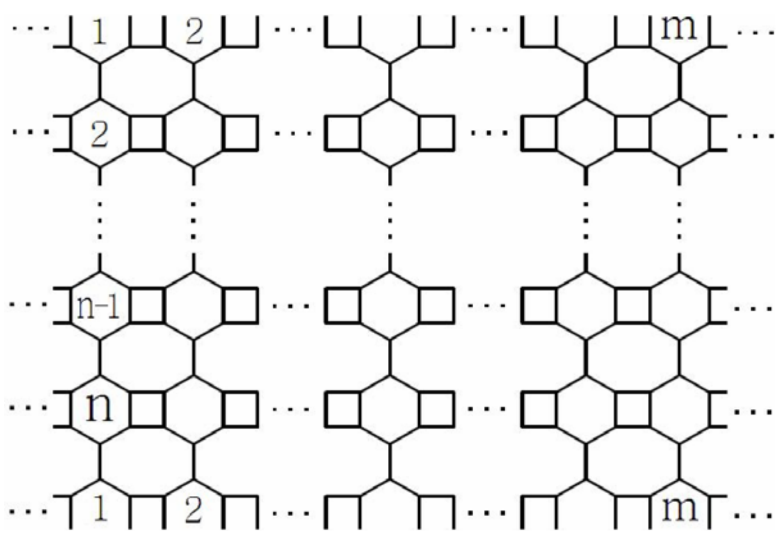

Figure 2. 2-D Lattice of the V-phenylenic nanotori $H = VPHY[m,\ n]$.

Proof of Theorem 2. Consider V-phenylenic nanotori $H = VPHY[m, n]$ $(\forall m, n > 1)$, where m and n be the number of hexagon in the first row and column in $H = VPHY[m, n]$. From the structure of V-phenylenic nanotori in Figure 2, it is easy to see that $VPHY[m, n]$ is a cubic graph (all its vertices have degree three).

Thus, the vertex partition V_3 is equal with $V(VPHY[m, n])$ and $|V_3| = |V(VPHY[m, n])| = 6mn$. Also, therefore the edge partitions E_6 or $E_9{}^*$ are equal with $E(VPHY[m, n])$ and $|E_6| = |E_9{}^*| = 9mn$.

And these imply that

$$\chi(VPHY[m, n]) = \sum_{uv \in E(VPHY[m, n])} \frac{1}{\sqrt{d_u d_v}} = \frac{|E|}{\sqrt{9}} = 3mn,$$

and

$$X(VPHY[m, n]) = \sum_{uv \in E(VPHY[m, n])} \frac{1}{\sqrt{d_u + d_v}} = \frac{|E|}{\sqrt{6}} = \frac{3\sqrt{6}mn}{2}.$$

Now, by computing Randić connectivity index $\chi(VPHY[m, n])$, sum-connectivity index $X(VPHY[m, n])$ for every $m, n \in \mathbb{N} - \{1\}$, the proof of Theorem 2 is completed. □

3. Conclusion

In this paper, we focus on the connected structure of two kind of nano-structures "V-phenylenic nanotubes $G = VPHX[m, n]$ and V-phenylenic nanotorus $H = VPHY[m, n]$". Also, we count some connectivity indices "Randić connectivity index and sum-connectivity index" of them.

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