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

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

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

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

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 $X(G) = \sum_{\nu \neq \nu' \in V(G)} \frac{1}{\sqrt{d_\nu + d_{\nu'}}}$ 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 $\nu$ with degree $d_\nu$ of simple connected graph $G = (V(G); E(G))$ and we denoted the minimum degree with $\delta = \text{Min}\{d_\nu | \nu \in V(G)\}$ and the maximum degree with $\Delta = \text{Max}\{d_\nu | \nu \in V(G)\}$. 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:

$$\forall k : \delta \leq k \leq \Delta, \quad V_k = \{\nu \in V(G) | d_\nu = k\},$$

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

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

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:

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

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

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

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

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

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

![Figure 1. 2-D Lattice of the $V$-phenylenic nanotubes $G = VPHX[m, n]$.](image_url)
Proof of Theorem 1. Consider $V$-phenylenic nanotube $G = \text{VPHX}[m, n]$ \((m, n > 1)\), 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 $G = \text{VPHX}[m, n]$ in Figure 1, one can see that the number of vertices and edges in $G = \text{VPHX}[m, n]$ are equal to $6mn$ and $9mn - m$, respectively. Since $|V_2| = m + m$ and $|V_3| = 6mn - 2m$. Then the number of edges of $G = \text{VPHX}[m, n]$ will be $|E(\text{VPHX}[m, n])| = \frac{1}{2} [2(2m) + 3(6mn - 2m)]$.

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 $G = \text{VPHX}[m, n]$ are equal, respectively, as

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

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

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

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

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

\[
X(VPHX[m, n]) = \sum_{u,v \in E(VPHX[m, n])} \frac{1}{\sqrt{d_u + d_v}} \\
= \sum_{e=uv \in E_6} \frac{1}{\sqrt{d_u + d_v}} + \sum_{e=uv \in E_5} \frac{1}{\sqrt{d_u + d_v}} \\
= \frac{|E_6|}{\sqrt{6}} + \frac{|E_5|}{\sqrt{5}} \\
= \left( \frac{9\sqrt{6}n}{6} + \left( \frac{4\sqrt{5}}{5} - \frac{5\sqrt{6}}{6} \right) \right) m. \quad \blacksquare
\]

**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 \( X(VPHY[m, n]) = \frac{3\sqrt{6}mn}{2} \)

\( = 3.6742mn. \)

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**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

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

and

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

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. $\square$

3. Conclusion

In this paper, we focus on the connected structure of two kind of nanostructures “$V$-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.
References

