Abstract: Among topological descriptors connectivity topological indices are very important and they have a prominent role in chemistry. One of them is Sanskruti index defined as $S(G) = \sum_{uv \in E(G)} \left( \frac{s_u s_v}{s_u + s_v - 2} \right)^3$ where $s_u$ is the summation of degrees of all neighbors of vertex $u$ in $G$. In this paper we compute this topological index for V-phenylenic nanotube and nanotori.

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1. Introduction and Preliminaries

Let $G = (V; E)$ be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge sets of it are represented by $V = V(G)$ and $E = E(G)$, respectively. In chemical graphs, the vertices correspond to the atoms of the molecule, and the edges represent to the chemical bonds. Also, if $e$ is an edge of $G$, connecting the vertices $u$ and $v$, then we write $e = uv$ and say $u$ and $v$ are adjacent.

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena ([1]-[5]). This theory had an important effect on the development of the chemical sciences.

Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry. In other words, if $G$ be the connected graph, then we can introduce many connectivity topological indices for it, by distinct and different definition. A connected graph is a graph such that there is a path between all pairs of vertices. One of the best known and widely used is the connectivity index, introduced in 1975 by Milan Randić [6], who has shown this index to reflect molecular branching and defined as follows:

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

The Sanskruti index $S(G)$ of a graph $G$ is defined as follows (see [7]-[11]):

$$S(G) = \sum_{uv \in E(G)} (S_u S_v / (S_u + S_v - 2))^3.$$  

where $S_u$ is the summation of degrees of all neighbors of vertex $u$ in $G$. In Refs [12]-[27] some topological indices of $V-$phenylenic nanotube and $V-$phenylenic nanotori are computed. In this paper, we continue this work to compute the Sanskruti index of molecular graphs related to $V-$phenylenic nanotube and nanotori. Our notation is standard and mainly taken from Refs. [1]-[5].

2. Main Results and Discussion

The goal of this section is to computing the Sanskruti index of $V-$phenylenic nanotube and nanotori. The novel phenylenic and naphthylenic lattices pro-
posed can be constructed from a square net embedded on the toroidal surface. Phenylenes are polycyclic conjugated molecules, composed of four membered ring (=square) and six-membered rings (=hexagons) such that every four membered ring (4-membered cycle) is adjacent to two 6-membered cycles, and no two six-membered rings are mutually adjacent. Each four-membered ring lies between two six-membered rings, and each hexagon is adjacent only two four-membered rings. Because of such structural features phenylenes are very interesting conjugated species [28]-[33]. The rapid development of the experimental study of phenylenes motivated a number of recent theoretical studies of thee conjugated \( \pi \)-electron systems [33].

Following M. V. Diudea [5] we denote a \( V \)-Phenylenic nanotube and \( V \)-Phenylenic nanotorus by \( G = V PHX[m, n] \) and \( H = V PHY[m, n] \), respectively. The general representation of these nano structures are shown in Figure 1 and Figure 2. For more information and background materials, refer to paper series [12]-[33] again. Now we have following theorems, immediately.

**Theorem 2.1.** \( \forall m, n \in \mathbb{N} \), the Sanskruti index \( S(G) \) of \( V \)- Phenylenic Nanotube \( V PHX[m, n] \) is equal to

\[
S(V PHX[m, n]) = -\frac{87714218531}{175616000} m + \frac{4782969}{4096} mn.
\]

**Figure 1:** The Molecular Graph of \( V \)-Phenylenic Nanotube \( V PHX[m, n] \).
Proof. Consider the $V-$phenylenic nanotube $G = VPHX[m, n]$ with $6mn$ vertices and $9mn - m$ edges (Figure 1). In $V-$phenylenic molecule, there are two partitions $V_2 = v \in V(G) | d_v = 2$ and $V_3 = v \in V(G) | d_v = 3$ of $V(VPHX[m, n])$, since the degree of an arbitrary vertex/atom of a molecular graph is equal to 2 or 3. Next, the two partitions of $E(G)$ are $E_5 = \{u, v \in V(G) | d_u = 3 & d_v = 2\}$ and $E_6 = \{u, v \in V(G) | d_u = d_v = 3\}$.

Also, two adjacent vertices $v_1, v_2$ of a vertex $v \in V_2$ have degree three, then $S_v = 2 \times 3 = 6$ and two edges $vv_1$ and $vv_2$ belong to $E_5$ (and $|E_5| = 2|V_2| = 4m$). Also, for all vertices $u$ in first and end row of $V-$phenylenic nanotube with degree three, $N(u) = v_1, v_2, v_3$ such that $v_1 \in V_2$ and $v_2, v_3 \in V_3 (uv_1 \in E_5$ and $uv_3, uv_2 \in E_6)$, thus $S_u = 2 \times 3 + 2 = 8$. Finally, for other vertices $S_w = 9$, because all other vertices and their edges belong to $V_3$ and $E_6$, respectively. So, the Sanskruti index $S(G)$ of $VPHX[m, n](m, n \geq 1)$ will be

$$S(VPHX[m, n]) = \sum_{uv \in E(G)} \left( \frac{S_u S_v}{S_u + S_v - 2} \right)^3$$

$$= 4m \left( \frac{6.8}{6 + 8 - 2} \right)^3 + 2m \left( \frac{8.8}{8 + 8 - 2} \right)^3 + 2m \left( \frac{8.9}{8 + 9 - 2} \right)^3$$

$$+ (9mn - 9m) \left( \frac{9.9}{9 + 9 - 2} \right)^3$$

$$= - \frac{87714218531}{175616000} m + \frac{4782969}{4096} mn. \quad \square$$

**Theorem 2.2.** $\forall m, n \in N$, the Sanskruti index $S(G)$ of $V-$Phenylenic Nanotori $H = VPHY[m, n]$ is equal to

$$S(VPHY[m, n]) = \frac{4782969}{4096} mn.$$

Proof. The proof is easily, since by considering the $V-$phenylenic nanotori $H = VPHY[m, n]$ with $6mn$ vertices and $9mn$ edges (Figure 2). We see that this nanotori is a Cubic graph and all vertices belong to $V_3$ and $\forall v \in V(VPHY[m, n])$ $S_v = 9$. This implies that all edges belong

$$S(VPHX[m, n]) = \sum_{uv \in E(G)} \left( \frac{S_u S_v}{S_u + S_v - 2} \right)^3$$

$$= (9mn) \left( \frac{9.9}{9 + 9 - 2} \right)^3 = \frac{4782969}{4096} mn. \quad \square$$
3. Conclusions

In this report, we study some properties of a new connectivity index of (molecular) graphs that called Sanskruti index. This connectivity index was defined as follows:

\[ S(G) = \sum_{uv \in E(G)} (\frac{S_u S_v}{S_u + S_v - 2})^3. \]

where \( S_u \) is the summation of degrees of all neighbors of vertex \( u \) in \( G \). In continue, closed analytical formulas for \( S(G) \) of a physico chemical structure of phenylenic nanotubes and nanotorus are given. These nano structures are \( V-\text{Phenylenic Nanotube } VPHX[m,n] \) and \( V\text{-phenylenic nanotorus } VPHY[m,n] \).

References


