

On Sanskruti Index of the Line Graphs of Certain Nanostructures

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Abstract: In QSAR/QSPR study, topological indices are utilized to guess the bioactivity of chemical compounds. Hosamani [11], has studied a novel topological index, namely the Sanskruti index $S(G)$ of a molecular graph G . The Sanskruti index $S(G)$ shows good correlation with entropy of an octane isomers. In this paper we compute the Sanskruti index $S(G)$ of line graphs of V-Phenylenic nanotubes, V-Phenylenic nanotorus, H-Naphtalenic nanotubes and H-Naphtalenic nanotorus.

Keywords: Sanskruti index, topological index, molecular graph, Nanotubes, Nanotorus

1. Introduction

Let G be a simple graph. The order of a graph is $|V(G)|$ its number of vertices denoted by p . The size of a graph is $|E(G)|$, its number of edges denoted by q . The degree of a vertex, denoted by $d_G(v)$. The line graph $L(G)$ of a graph is the graph derived from G in such a way that the edges in G are replaced by vertices in $L(G)$ and two vertices in $L(G)$ are connected whenever the corresponding edges in G are adjacent [24]. For any number d , we define $V_d = \{u \in V(G) \mid S_G(u) = d\}$, in which $S_G(u) = \sum_{v \in N_G(u)} d_G(v)$ and $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$.

Topological indices are the mathematical measures which correspond to the structures of any simple finite graph. They are invariant under the graph isomorphism. The interest of study of topological indices is mainly associated with its applications in QSAR/QSPR. The applications of line graphs in chemistry was originated from structural chemistry. The first edge version molecular descriptors were introduced in 1981 the advanced theory of molecular branching and complexity. For several molecular descriptors based on the line graph of molecular graph, more about its applications and edge version of other molecular structures and nanotubes referred to the articles [1 – 10]. One of the best known and widely used is the connectivity index, introduced in 1975 by Milan Randić [9], who has shown this index to reflect molecular branching and defined as $R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$.

The Sanskruti index $S(G)$ of a graph G is defined as follows [11 – 15]; $S(G) = \sum_{uv \in E(G)} \left(\frac{S_u S_v}{S_u + S_v - 2} \right)^3$ where S_u is the summation of degrees of all neighbours of vertex u in G .

In 2018, V. Shigehalli, R. Kanabur calculated the Sanskruti index of H-Naphtalenic Nanotube and Nanotori [16]. In 2017, Muhammad Shoaib Sardar, Mohammad Raza

Farahani studied the Sanskruti index of Titania Nanotubes [17]. In 2017, Gao, Y. Farahani, M. R., Sardar, M. S., and Zafars., computed Sanskruti index of circumcoronene series of Benzenoid [18] and the dendrimer nanostars [14]. In 2017, Jiang, H., Sardar, M. S., Farahani, M. R., Rezaei and Siddiqu, M. K., calculated the Sanskruti index of V-Phenylenic nanotubes and nanotori [19]. Motivated by the results of [23], we computed the Sanskruti index of line of graph of V-Phenylenic nanotubes, V-Phenylenic nanotorus, H-Naphtalenic nanotubes and H-Naphtalenic nanotorus.

2. Main Results and Discussion

Following M.V. Diudea [22] we denote a V-Phenylenic nanotube and V-Phenylenic nanotorus by $VPHX[m, n]$ and $VPHY[m, n]$ respectively, where m denotes the number of hexagons in a row and n denotes the alternative hexagons in a column. H-Naphtalenic nanotube and H-Naphtalenic nanotorus usually symbolized as $NPHX[m, n]$ and $NPHY[m, n]$, in which m is the number of pair of hexagons in first row and n is the number of alternative hexagons in a column.

Lemma 2.1 [21]

Let G be a (p, q) graph whose points have degree d_i , then $L(G)$ has q points and q_L lines, where $q_L = \frac{1}{2} \sum d_i^2 - q$.

Theorem 2.2

Let G be a line graph of 2D-lattice of V-Phenylenic nanotube $VPHX[m, n]$ ($m, n > 1$). Then $S(G) = 11184.81mn - 6795.89m$.

Proof:

The graph of 2D-lattice of V-Phenylenic nanotube $VPHX[m, n]$ and the graph G are shown in Figure 1 and Figure 2 respectively. The 2D-lattice of $VPHX[m, n]$ is a graph of order $6mn$ and size $9mn - m$. Then by Lemma 2.1, the line graph of 2D-lattice of $VPHX[m, n]$ is of order of $9mn -$

mand size $18mn - 4m$. Further note that the vertices of G are either of degree 3 or 4. From Figure 1 and 2, it can be easily verified that in $G, |V_{11}| = 4m, |V_{14}| = 2m, |V_{15}| = 4m$ and $|V_{16}| = 9mn - 11m$. Thus the edge partition based on the degree sum of neighbour vertices of each vertex is obtained, as shown in Table 1.

Table 1: Edge partition of G , when $m > 1$ and $n > 1$.

$(S_G(u), S_G(v))$ where $uv \in E(G)$	Number of edges
(11, 11)	$2m$
(11, 14)	$4m$
(11, 15)	$4m$
(14, 15)	$4m$
(15, 16)	$8m$
(16, 16)	$(18mn - 26m)$

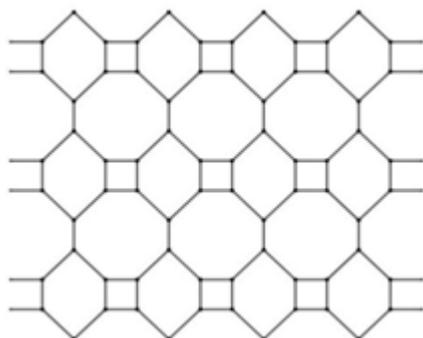


Figure 1: Graph of 2D-lattice of V-Phenylene VPHX[4, 3] nanotube.

Now,
 $S(G) =$

$$\begin{aligned} & \sum_{uv \in E(G)} \left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2} \right)^3 \\ &= 2m \left(\frac{11 \times 11}{11 + 11 - 2} \right)^3 + 4m \left(\frac{11 \times 14}{11 + 14 - 2} \right)^3 \\ & \quad + 4m \left(\frac{11 \times 15}{11 + 15 - 2} \right)^3 \\ & \quad + 4m \left(\frac{14 \times 15}{14 + 15 - 2} \right)^3 \\ & \quad + 8m \left(\frac{15 \times 16}{15 + 16 - 2} \right)^3 \\ & \quad + (18mn - 26m) \left(\frac{16 \times 16}{16 + 16 - 2} \right)^3 \\ &= 11184.8106mn - 6795.8978m. \end{aligned}$$

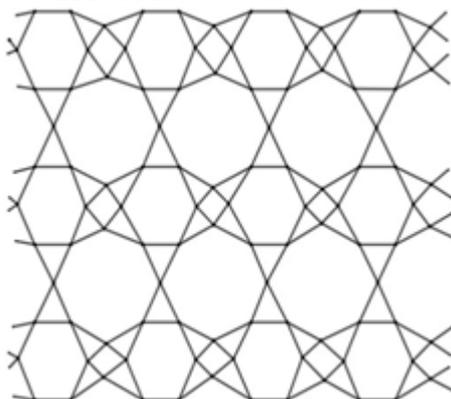


Figure 2: Line Graph of 2D-lattice of V-Phenylene VPHX[4, 3] nanotube.

Theorem 2.3

Let G be a line graph of 2D-lattice of V-Phenylene nanotorus $VPHY[m, n]$ ($m, n > 1$). Then $S(G) = 11184.8106mn$.

Proof:

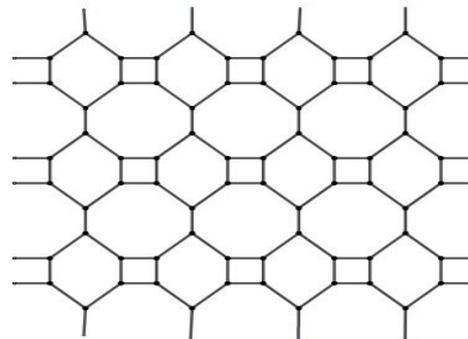


Figure 3: Graph of 2D-lattice of V-Phenylene VPHY [4, 3] nanotorus.

The graph of 2D-lattice of V-Phenylene nanotorus $VPHY[m, n]$ and the graph G are shown in Figure 3 and 4 respectively. The 2D lattice of $VPHY[m, n]$ is a graph of order $6mn$ and size $9mn$. Then by Lemma 2.1, the line graph of 2D-lattice of $VPHY[m, n]$ is a order of $9mn$ and size $18mn$. Further note that the degree of each vertex is 4 in G . From Figure 3 and 4, it can be easily verified that in $G, |V_{16}| = 9mn$ and we have trivial edge partition based on the degree sum of neighbour vertices of each vertex is obtained, as shown in Table 2.

Table 2. Edge partition of G , when $m > 1$ and $n > 1$.

$(S_G(u), S_G(v))$ where $uv \in E(G)$	Number of edges
(16, 16)	$18mn$

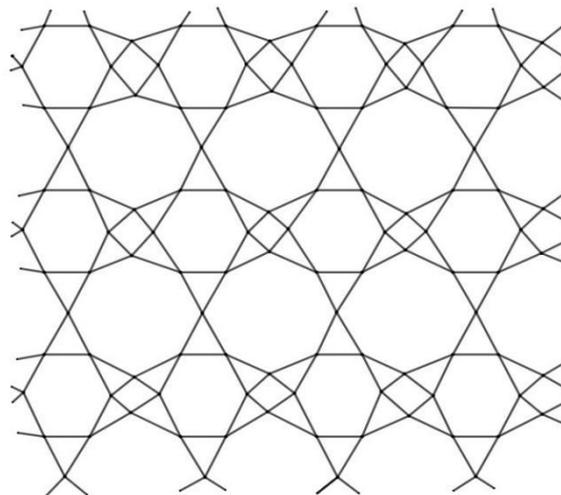


Figure 4: Line Graph of 2D-lattice of V-Phenylene VPHY [4, 3] nanotorus.

$$\begin{aligned} \text{Now, } S(G) &= \sum_{uv \in E(G)} \left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2} \right)^3 \\ &= (18mn) \left(\frac{16 \times 16}{16 + 16 - 2} \right)^3 \\ &= 11184.8106mn. \end{aligned}$$

Theorem 2.4

Let G be a line graph of 2D-lattice of H -Naphthalenic nanotube $NPHX[m, n]$ ($m, n > 1$). Then $S(G) = 18641.3511mn - 12982.8961m$.

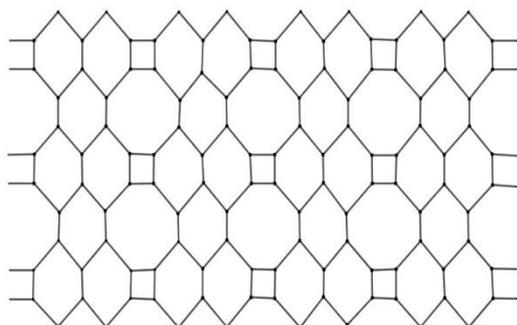


Figure 5: Graph of 2D-lattice of H-Naphtalenic NPHX[4, 3] nanotube

Proof:

The graph of 2D-lattice of H -Naphthalenic nanotube $NPHX[m, n]$ and the graph G are shown in Figure 5 and 6 respectively. The 2D lattice of $NPHX[m, n]$ is a graph of order $10mn$ and size $15mn - 2m$. Then by Lemma 2.1, the line graph of 2D-lattice of $NPHX[m, n]$ is of order $15mn - 2m$ and size $30mn - 8m$. Further note that the vertices of G are either of degree 3 or 4. From Figure 5 and 6, it can be easily verified that in $G, |V_{10}| = 4m, |V_{11}| = 4m, |V_{14}| = 4m, |V_{15}| = 4mn$ and $|V_{16}| = 15mn - 18m$. Thus the edge partition based on the degree sum of neighbour vertices of each vertex is obtained, as shown in Table 4.

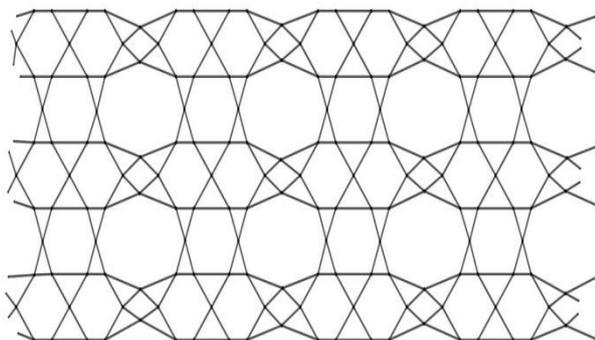


Figure 6: Line Graph of 2D-lattice of H-Naphtalenic NPHX[4, 3] nanotube

$$\text{Now, } S(G) = \sum_{uv \in E(G)} \left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2} \right)^3$$

$$\begin{aligned} &= 2m \left(\frac{10 \times 10}{10 + 10 - 2} \right)^3 + 4m \left(\frac{10 \times 11}{10 + 11 - 2} \right)^3 \\ &\quad + 4m \left(\frac{10 \times 14}{10 + 14 - 2} \right)^3 \\ &\quad + 4m \left(\frac{11 \times 14}{11 + 14 - 2} \right)^3 \\ &\quad + 4m \left(\frac{11 \times 15}{11 + 15 - 2} \right)^3 \\ &\quad + 4m \left(\frac{14 \times 15}{14 + 15 - 2} \right)^3 \\ &\quad + 4m \left(\frac{14 \times 16}{14 + 16 - 2} \right)^3 \\ &\quad + 8m \left(\frac{15 \times 16}{15 + 16 - 2} \right)^3 \\ &\quad + (30mn - 42m) \left(\frac{16 \times 16}{16 + 16 - 2} \right)^3 \\ &= 18641.3511mn - 12982.8961m. \end{aligned}$$

Table 3: Edge partition of G , when $m > 1$ and $n > 1$.

$(S_G(u), S_G(v))$ where $uv \in E(G)$	Number of edges
(10, 10)	2m
(10, 11)	4m
(10, 14)	4m
(11, 14)	4m
(11, 15)	4m
(14, 15)	4m
(14, 16)	4m
(15, 16)	8m
(16, 16)	$(30mn - 42m)$

Theorem 2.5

Let G be a line graph of 2D-lattice of H -Naphthalenic nanotube $NPHY[m, n]$ ($m, n > 1$). Then $S(G) = 18641.3511mn$.

Proof:

The graph of 2D-lattice of H -Naphthalenic nanotube $NPHY[m, n]$ and the graph G are shown in Figure 7 and 8 respectively. The 2D lattice of $NPHY[m, n]$ is a graph of order $10mn$ and size $15mn$. Then by Lemma 2.1, the line graph of 2D-lattice of $NPHY[m, n]$ is of order $15mn$ and size $30mn$. Further note that the degree of each vertex is 4 in G . From Figure 7 and 8, it can be easily verified that in $G, |V_{16}| = 15mn$ and we have the trivial edge partition based on the degree sum of neighbour vertices of each vertex is obtained, as shown in Table 4.

$$\begin{aligned} \text{Now, } S(G) &= \sum_{uv \in E(G)} \left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2} \right)^3 \\ &= (30mn) \left(\frac{16 \times 16}{16 + 16 - 2} \right)^3 \\ &= 18641.3511mn. \end{aligned}$$

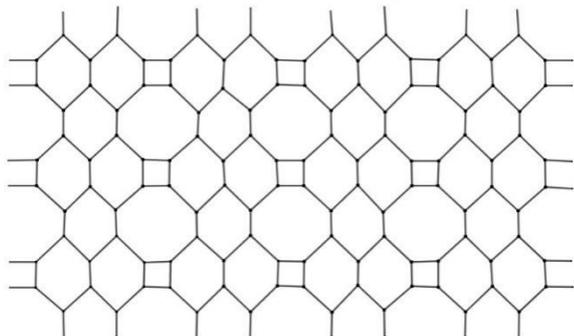


Figure 7: Graph of 2D-lattice of H-Naphtalenic NPHY [4, 3] nanotorus.

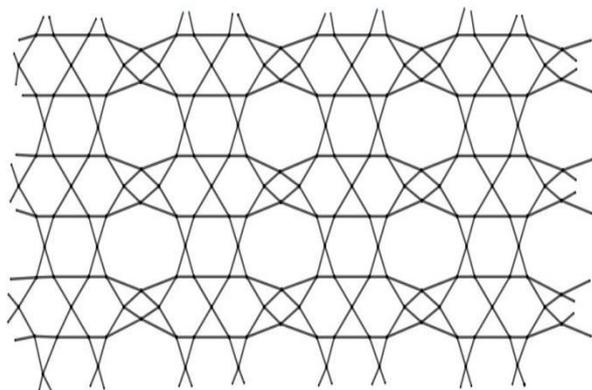


Figure 8: Line Graph of 2D-lattice of H-Naphtalenic NPHY [4, 3] nanotorus

Table 4: Edge partition of G, when $m > 1$ and $n > 1$.

$(SG(u), SG(v))$ where $uv \in E(G)$	Number of edges
(16, 16)	30mn

3. Conclusions

In this paper, we have computed the value of Sanskruti Index of line graph of V-Phenylenic nanotube, V-Phenylenic nanotorus, H-Naphtalenic nanotube and H-Naphtalenic nanotorus.

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