TWMS J. App. Eng. Math. V.8, N.2, 2018, pp. 477-482

COMPUTING SANSKRUTI INDEX OF CERTAIN NANOTUBES

V. SHIGEHALLI[1], R. KANABUR[1], §

Abstract. Recently, Hosamani [8], 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 octane isomers. In this paper we compute the Sanskruti index $S(G)$ of $NHPX[m, n]$ and $TUC_4[m, n]$ nanotubes.

Keywords: Molecular graph, H-Naphtalenic nanotube, $TUC_4[m, n]$ nanotube, Sanskruti index.

AMS Subject Classification: 05C90

1. Introduction

A molecular graph is a representation of a chemical compound having atoms as vertices and the bonds between atoms correspond to the edge of the graph. The collection of vertices of a graph, say G, is denoted by $V(G)$ and the set of edges is denoted by $E(G)$. The degree of a vertex v of a graph is the number of vertices of G adjacent to v, denoted by $d_G(v)$ or simply as d_v[2,3,14].

Topological invariant of a graph is a single number descriptor which is correlated to certain chemical, thermo-dynamical and biological behavior of the chemical compounds. Several topological indices have been defined over past decades which depend on degree of vertices.

Historically, the first vertex-degree-based structure descriptors were the graph invariants that now a days are called Zagreb indices [4].

$$M_1(G) = \sum_{u \epsilon V(G))} (d_G(u))^2 \qquad (1)$$

$$M_2(G) = \sum_{uv \epsilon E(G))} (d_G(u) d_G(v)) \qquad (2)$$

However,initially these were intended to be used for a completely different purpose and these were included among topological indices much later. The first genuine degree-based topological index was put-forward in 1975 by Milan Randić in his seminar paper on

[1] Department of Mathematics, Rani Channamma University, Belagavi - 591156, Karnataka, India.
e-mail: shigehallivs@yahoo.co.in; ORCID: https://orcid.org/0000-0002-9585-8899.
e-mail: rachukanabur@gmail.com; ORCID: https://orcid.org/0000-0001-7496-7503.

§ Manuscript received: January 3, 2017; accepted: February 3, 2017.
TWMS Journal of Applied and Engineering Mathematics, Vol.8, No.2

characterization of molecular branching [9] his index was defined as

$$R(G) = \sum_{uv\epsilon E(G))} \frac{1}{\sqrt{d_G(u)d_G(v)}} \tag{3}$$

Recently, Hosamani [8], studied a novel topological index, namely the Sanskruti index $S(G)$ of a molecular graph G.

$$S(G) = \sum_{uv\epsilon E(G))} \left(\frac{S_G(u)S_G(v)}{S_G(u) + S_G(v) - 2} \right)^3 \tag{4}$$

where $S_G(u)$ and $S_G(v)$ is the summation of degrees of all neighbours of vertices u and v in G.

$$S_G(u) = \sum_{u,v\epsilon E(G)} d_G(u)$$

and

$$N_G(u) = v\epsilon V(G)/uv\epsilon E(G)$$

The Sanskruti index shows good correlation with the entropy of octane isomers which is depicted in Figure 1.

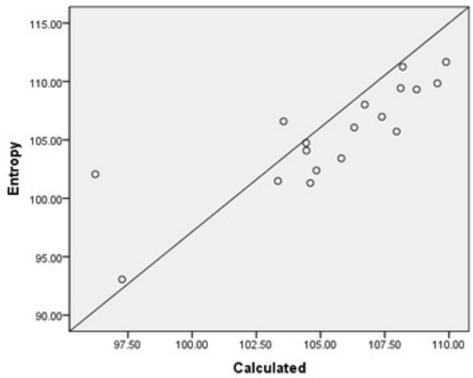

FIGURE 1. Correlations of S with entropy of octane isomers ($entropy = 1.7857S \pm 81.4286$).

In this paper, we continue the process of computing the Sanskruti index of some more nanotubes, which are $NHPX[m,n]$ and $TUC_4[m,n]$ nanotubes[1,6,7,10,11,12].

2. Main Results and Dissection

2.1. **H-Naphtalenic Nanotube.** In this section, we compute the certainC_6, C_6, C_4, C_6, C_6, C_4 in first row and a sequence of C_6,C_8, C_6, C_8 in other row. In other words, the whole lattice is a plane tiling can either cover a cylinder or a torus. These nanotube usually symbolized as $NPHX[m,n]$, in which m is the number of pair of hexagons in first row and n is the number of alternative hexagons in a column as depicted in Figure 2. Now

TABLE 1. Edge partition of graph of $NHPX[m,n]$ nanotube based on degree sum of vertices lying at unit distance from end vertices of each edge.

(S_a, S_b) where $u, v\epsilon E(H)$	(6,7)	(6,8)	(8,8)	(7,9)	(8,9)	(9,9)
Number of edges	$4m$	$4m$	$2m$	$2m$	$4m$	$15mn - 18m$

we compute important topological index Sanskruti index for 2D-lattice of $NHPX[m,n]$ nanotube. There are six types of edges in $NHPX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge as depicted in Figure 2 , in which different colours shows different partite sets of edge set of $NHPX[m,n]$ nanotube. In Figure 2, red colour shows the edges ab with $S_a = 6$ and $S_b = 7$, blue colour shows the type of edges ab with $S_a = 6$ and $S_b = 8$, green colour shows the type of edges ab with $S_a = S_b = 8$, yellow colour shows the type of edges ab with $S_a = 7$ and $S_b = 9$, brown colour shows the type of edges ab with $S_a = 8$ and $S_b = 9$ and black colour shows the partition having edges ab with $S_a = S_b = 9$.

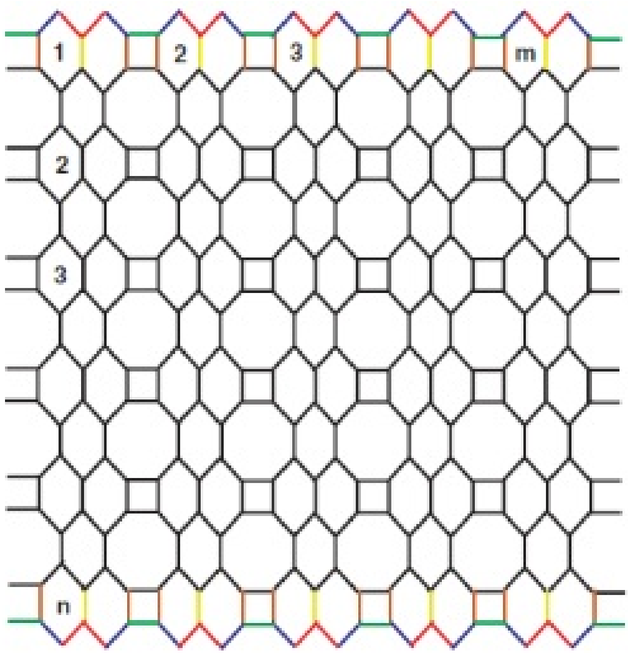

FIGURE 2. A graph of H-Naphtalenic nanotube $NPHX[m,n]$ showing different partite sets based on the degree sum of neighbors of end vertices of each edge.

In Table 1, cardinalities of such partite sets of edge set of graph of $NHPX[m,n]$ nanotube are shown. In the following theorem Sanskruti index of $NHPX[m,n]$ nanotube is computed.

Theorem 2.1. *Consider the graph of $NPHX[m,n]$ nanotubes, then its Sanskruti index is equal to*

$$S(NPHX[m,n]) = (1945.61n - 928.152)m$$

Proof. We use the edge partition of graph of $NPHX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge.
NOW by using the partition given in Table1 we can apply the formula of Sanskruti index to compute this index for $NPHX[m,n]$ nanotube.

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

$$\begin{aligned}
AG_2(NPHX(n)) &= (e_{6,7})\left(\frac{6\times 7}{6+7-2}\right)^3+(e_{6,8})\left(\frac{6\times 8}{6+8-2}\right)^3+(e_{8,8})\left(\frac{8\times 8}{8+8-2}\right)^3\\
&+ (e_{7,9})\left(\frac{7\times 9}{7+9-2}\right)^3+(e_{8,9})\left(\frac{8\times 9}{8+9-2}\right)^3+(e_{9,9})\left(\frac{9\times 9}{9+9-2}\right)^3\\
&= 4m\left(\frac{6\times 7}{6+7-2}\right)^3+4m\left(\frac{6\times 8}{6+8-2}\right)^3+2m\left(\frac{8\times 8}{8+8-2}\right)^3+2m\left(\frac{7\times 9}{7+9-2}\right)^3\\
&+ 4m\left(\frac{8\times 9}{8+9-2}\right)^3+(15mn-8m)\left(\frac{9\times 9}{9+9-2}\right)^3\\
&= 4m\left(\frac{42}{11}\right)^3+4m\left(\frac{48}{12}\right)^3+2m\left(\frac{64}{14}\right)^3+2m\left(\frac{63}{14}\right)^3+4m\left(\frac{72}{15}\right)^3\\
&+ (15mn-8m)\left(\frac{81}{16}\right)^3\\
&= \left(4\left(\frac{42}{11}\right)^3+4\left(\frac{48}{12}\right)^3+2\left(\frac{64}{14}\right)^3+2\left(\frac{63}{14}\right)^3+4\left(\frac{72}{15}\right)^3-18\left(\frac{81}{16}\right)^3\right)m\\
&+ \left(15\left(\frac{81}{16}\right)^3\right)mn\\
&= (1945.61n-928.152)m
\end{aligned}$$

2.2. **Nanotube Covered by C_4.** In this section, we compute certain topological indices of nanotube covered only by C_4. The 2D-lattice of this family of nanotube is a plane tiling of C_4. This tessellation of C_4 can either cover a cylinder or a torus. This family of nanotube is denoted by $TUC_4[m,n]$, in which m is the number of squares in a row and n is the number of squares in a column as shown in Figure 3.

Now we compute Sanskruti index for two dimensional lattice of $TUC_4[m,n]$ nanotube. There are five types of edges in the graph of $TUC_4[m,n]$ nanotube based on degree sum of vertices lying at unit distance from end vertices of each as shown in Figure 3 in which red coloured edges are the edge ab with $S_a = S_b = 7$, blue coloured edges are the edge ab with $S_a = 7$ and $S_b = 15$, green coloured edges are the edge ab with $S_a = S_b = 15$, yellow coloured edges are the edge ab with $S_a = 15$ and $S_b = 16$, black coloured edges are the edge ab with $S_a = S_b = 16$. Table2 shows the cardinalities of these partite sets.

Table 2. Edge partition of graph of $TUC_4[m,n]$ nanotube based on degree sum of vertices lying at unit distance from end vertices of each edge.

$(S_a,\, S_b)$ where $u, v\epsilon E(H)$	(7,7)	(7,15)	(15,15)	(15,16)	(16,16)
Number of edges	$(2m+2)$	$(2m+2)$	$(2m+2)$	$(2m+2)$	$(m+1)(2n-7)$

Theorem 2.2. *Let the graph of $TUC_4[m,n]$ nanotube with $(m \geq 1, n \geq 4)$, then its Sanskruti index is*

$$S(TUC_4[m,n]) = (1242.74n - 1752.65)(m+1)$$

Proof. We use the edge partition of graph of $TUC_4[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge.
Now by using the partition given in Table2 we can apply the formula of index to compute this index for $TUC_4[m,n]$ nanotube.

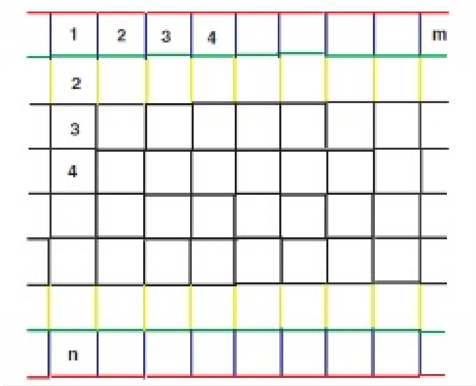

FIGURE 3. A graph of $TUC_4[m,n]$ nanotube showing the edge partition based on the degree sum of end vertices lying at unit distance from end vertices of each edge.

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

$$\begin{aligned}
S(TUC_4[m,n]) &= (e_{7,7})\left(\frac{7\times 7}{7+7-2}\right)^3 + (e_{7,15})\left(\frac{7\times 15}{7+15-2}\right)^3 \\
&+ (e_{15,15})\left(\frac{15\times 15}{15+15-2}\right)^3 + (e_{15,16})\left(\frac{15\times 16}{15+16-2}\right)^3 + (e_{16,16})\left(\frac{16\times 16}{16+16-2}\right)^3 \\
&= (2m+2)\left(\frac{7\times 7}{7+7-2}\right)^3 + (2m+2)\left(\frac{7\times 15}{7+15-2}\right)^3 \\
&+ (2m+2)\left(\frac{15\times 15}{15+15-2}\right)^3 + (2m+2)\left(\frac{15\times 16}{15+16-2}\right)^3 \\
&+ (m+1)\,(2n-7)\left(\frac{16\times 16}{16+16-2}\right)^3 \\
&= (2m+2)\left(\frac{49}{12}\right)^3 + (2m+2)\left(\frac{105}{20}\right)^3 + (2m+2)\left(\frac{225}{28}\right)^3 + (2m+2)\left(\frac{240}{29}\right)^3 \\
&+ (m+1)\,(2n-7)\left(\frac{256}{30}\right)^3 \\
&= \left(2\left(\frac{49}{12}\right)^3 + 2\left(\frac{105}{20}\right)^3 + 2\left(\frac{225}{28}\right)^3 + 2\left(\frac{240}{29}\right)^3 - 7\left(\frac{256}{30}\right)^3\right) m \\
&+ \left(\frac{256}{30}\right)^3 2mn + \left(\frac{240}{29}\right)^3 2n \\
&+ \left(2\left(\frac{49}{12}\right)^3 + 2\left(\frac{105}{20}\right)^3 + 2\left(\frac{225}{28}\right)^3 + 2\left(\frac{240}{29}\right)^3 - 7\left(\frac{256}{30}\right)^3\right) \\
&= (1242.74n - 1752.65)(m+1)
\end{aligned}$$

3. Conclusion

In this paper, we have computed the value of Sanskruti index for H-Naphtalenic nanotube and $TUC_4[m,n]$ nanotube without using computer.

References

[1] Bahramia,A and Yazdani,J , (2008), Padmakar-Ivan Index of H-Phenylinic Nanotubes and Nanotore, Digest Journal of Nanomaterials and Biostructures , 3 ,pp.265-267.
[2] Diudea.V.M, Gutman.I and J. Lorentz, (2001), Molecular Topology, Nova, Huntington.
[3] Gutman, I. and Trinajstic, N., (1972), Graph theory and molecular orbital. Total -electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17, pp.535-538.
[4] Gutman, I., (2013), Degree-based topological indices, Croat. Chem. Acta, 86, pp.251-361.
[5] Harary, F., (1969), Graph theory, Addison-Wesely, Reading mass.
[6] Hayat.S and Imarn.M, (2015), On Degree Based Topological Indices of Certain Nanotubes, Journal of Computational and Theoretical Nanoscience , 12, pp.1-7.
[7] Hosamani, S.M and Gutman,I., (2014), Zagreb indices of transformation graphs and total transformation graphs, Appl.Math.Comput. 247, pp.1156-1160.
[8] Hosamani, S.M., (2016), Computing Sanskrit index of certain nanostructures, J. Appl. Math. Comput.pp.1-9.
[9] Randic,M., (1975), On Characterization of Molecular Branching, J. Am. Chem. Soc., 97(23), pp.6609-6615.
[10] Shegehalli, V.S., and Kanabur, R., (2016), Computation of New Degree-Based Topological Indices of Graphene, Journal of Mathematics, pp.1-6.
[11] Shegehalli, V.S., and Kanabur, R., (2016), Computing Degree-Based Topological Indices of Polyhex Nanotubes, Journal of Mathematical Nanoscience, 6(1-2), pp.59- 68.
[12] Shegehalli, V.S., and Kanabur, R., (2016), New Version of Degree-Based Topological Indices of Certain nanotube, Journal of Mathematical Nano science, 6(1-2), pp.29-39.
[13] Todeschini, R., and Consonni,V., (2000), Handbook of Molecular Descriptors, Wiley-VCH, Weinheim.
[14] Trinajstic,N., (1992), Chemical Graph theory, CRC Press, Boca Raton.

Vijayalaxmi Shigehalli graduated from Karnatak University Dharwad. She is working as a professor in the Department of Mathematics at Rani Channamma University, Belagavi. She has successfully guided two Ph.D and two M.Phils, and published / presented some research articles in national and international conferences / journals.

Rachanna Kanabur is a research scholar in the Department of Mathematics, Rani Channamma University, Belagavi, Karnataka, India. He has published / presented few research papers in national and international conferences / journals.