COMPUTING SANSKRUTI INDEX OF V-PHENYLENIC NANOTUBES AND NANOTORI

H. Jiang¹, M.S. Sardar², M.R. Farahani^{3 §},
M. Rezaei⁴, M.K. Siddiqui⁵

¹School of Information Science and Engineering
Chengdu University
Chengdu, 610106, P.R. CHINA

²University of Management and Technology (UMT)
Lahore, PAKISTAN

³Department of Applied Mathematics
Iran University of Science and Technology (IUST)
Narmak, Tehran, 16844, IRAN

⁴Department of Mathematics
Buein Zahra Technical University
Buein Zahra, Qazvin, IRAN

Department of Mathematics
⁵Comsats Institute of Information Technology
Sahiwal, PAKISTAN

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 $S(G) = \sum_{uv \in E(G)} (\frac{S_u S_v}{S_u + S_v - 2})^3$ where S_u is the summation of degrees of all neighbors of vertex u in G . In this paper we compute this topological index for V-phenylenic nanotube and nanotori.

AMS Subject Classification: 05C90, 05C35, 05C12

Key Words: molecular graph, benzenoid, Capra operation, topological index, Sanskruti index

Received: May 4, 2017

Revised: July 10, 2017

Published: August 9, 2017

© 2017 Academic Publications, Ltd.

url: www.acadpubl.eu

[§]Correspondence author

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]):

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

where S_u is the summation of degrees of all neighbors of vertex u in G . In 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 these conjugated π -electron systems [33].

Following M. V. Diudea [5] we denote a V -Phenylenic nanotube and V -Phenylenic nanotorus by $G = VPHX[m, n]$ and $H = VPHY[m, n]$, 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. $\forall m, n \in N$, the Sanskruti index $S(G)$ of V -Phenylenic Nanotube $VPHX[m, n]$ is equal to

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

Figure 1: The Molecular Graph of V -Phenylenic Nanotube $VPHX[m, n]$.

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 $E_5 = \{uv \in E(G) | d_u = 3 \& d_v = 2\}$ and $E_6 = \{uv \in E(G) | d_u = d_v = 3\}$.

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 $uv_2, uv_3 \in E_6$), 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

$$\begin{aligned} S(VPHX[m, n]) &= \sum_{uv \in E(G)} \left(\frac{S_u S_v}{S_u + S_v - 2} \right)^3 \\ &= 4m \cdot \left(\frac{6 \cdot 8}{6 + 8 - 2} \right)^3 + 2m \cdot \left(\frac{8 \cdot 8}{8 + 8 - 2} \right)^3 + 2m \cdot \left(\frac{8 \cdot 9}{8 + 9 - 2} \right)^3 \\ &\quad + (9mn - 9m) \cdot \left(\frac{9 \cdot 9}{9 + 9 - 2} \right)^3 \\ &= -\frac{87714218531}{175616000}m + \frac{4782969}{4096}mn. \end{aligned} \quad \square$$

Theorem 2.2. $\forall m, n \in \mathbb{N}$, 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

$$\begin{aligned} S(VPHX[m, n]) &= \sum_{uv \in E(G)} \left(\frac{S_u S_v}{S_u + S_v - 2} \right)^3 \\ &= (9mn) \cdot \left(\frac{9 \cdot 9}{9 + 9 - 2} \right)^3 = \frac{4782969}{4096}mn. \end{aligned} \quad \square$$

Figure 2: The Molecular Graph of V-Phenylenic Nanotorus $VPHY[m, n]$.

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:

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

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

References

- [1] R. TODESCHINI AND V. CONSONNI: Handbook of Molecular Descriptors, Wiley-TUACH, Weinheim (2000).
- [2] N. TRINAJSTIC: Chemical Graph Theory, 2nd ed. CRC Press; Boca Raton, FL: (1992); 20-75.
- [3] I. GUTMAN, N. TRINAJSTIC: Graph theory and molecular orbitals. Total f-electron energy of alternant hydrocarbons. Chem. Phys. Lett. 17(4), (1972), 535-538. [https://doi.org/10.1016/0009-2614\(72\)85099-1](https://doi.org/10.1016/0009-2614(72)85099-1)
- [4] P. J. CAMERON: Cambridge University Press, Cambridge, (1994).
- [5] M. V. DIUDEA: Fuller. Nanotub. Carbon Nanostruct, (2002), 10, 273-292.

- [6] M. RANDIC: Characterization of molecular branching. J. Amer. Chem. Soc. **97**, (1975) 6609-6615. DOI: 10.1021/ja00856a001
- [7] S. M. HOSAMANI: S. M. HOSAMANI: Computing Sanskruti index of certain nanostructures. Journal of Applied Mathematics and Computing. In press, 2017. DOI 10.1007/s12190-016-1016-9.
- [8] M.S. SARDAR, S. ZAFAR, M.R. FARAHANI. Computing Sanskruti index of the Polycyclic Aromatic Hydrocarbons. Geology, Ecology, and Landscapes. In press, (2017), [http : //dx.doi.org/10.1080/24749508.2017.1301056](http://dx.doi.org/10.1080/24749508.2017.1301056)
- [9] Y.Y. GAO, M.R. FARAHANI, M.S. SARDAR, S. ZAFAR. On the Sanskruti Index of Circumcoronene Series of Benzenoid. Applied Mathematics. **8** (4), (2017), 520-524. doi:10.4236/am.2017.84041
- [10] Y.Y. GAO, M.S. SARDAR, S.M. HOSAMANI, M.R. FARAHANI. Computing sanskruti index of $TURC_4C_8(s)$ nanotube. International Journal of Pharmaceutical Sciences and Research. **8** (10), (2017), 1000-03. doi: 10.13040/IJPSR.0975-8232.8(10).1000-03.
- [11] Y.Y. GAO, M.S. SARDAR, S. ZAFAR, M.R. FARAHANI. Computing Sanskruti index of dendrimer nanostars. International Journal of Pure and Applied Mathematics. **115**(2), In press, (2017), [http : //ijpam.eu/contents/index.php](http://ijpam.eu/contents/index.php)
- [12] V. ALAMIAN, A. BAHRAMI AND B. EDALATZADEH: PI Polynomial of V-Phenylenic Nanotubes and Nanotori. Int. J. Mol. Sci., 9(3), (2008), 229-234; doi:10.3390/ijms9030229
- [13] M. ALAEIYAN, A. BAHRAMI AND M. R. FARAHANI: Cyclically Domination Polynomial of Molecular Graph of Some Nanotubes. Digest. J. Nanomater. Bios. 6(1), (2011), 143-147.
- [14] J. ASADPOUR: Some topological polynomial indices of nanostructures, Optoelectron. Adv. Mater.-Rapid Commun. 5(7), (2011), 769-772.
- [15] A. BAHRAMI AND J. YAZDANI: Vertex PI Index of V-Phenylenic Nanotubes and Nanotori. Digest Journal of Nanomaterials and Biostructures, 4(1), (2009), 141-144.
- [16] M. DAVOUDI MOHFARED, A. BAHRAMI AND J. YAZDANI: PI Polynomial of V-Phenylenic Nanotubes. Digest Journal of Nanomaterials and Biostructures, 5(2), (2010), 441-445.
- [17] M. R. FARAHANI: Computing GA_5 index of V-Phenylenic Nanotubes and Nanotori. Int. J. Chem Model. 5(4), (2013), 479-484.
- [18] M. R. FARAHANI: Computing fourth atom-bond connectivity index of V-Phenylenic Nanotubes and Nanotori. Acta Chimica Slovenica. 60(2), (2013), 429-432.
- [19] M. R. FARAHANI: omputing Theta Polynomial and Theta Index of V-phenylenic Planar, Nanotubes and Nanotoris. Int. J. Theoretical Chemistry. 1(1), (2013), 01-09.
- [20] M.R. FARAHANI, M.R. RAJESH KANNA: The Generalized Zagreb Index of V-Phenylenic Nanotubes and Nanotorus. Journal of Chemical and Pharmaceutical Research. 7(11), (2015), 241-245.
- [21] M. GHORBANI, H. MESGARANI, S. SHAKERANEH: Computing GA index and ABC index of V-phenylenic nanotube. Optoelectron. Adv. Mater.-Rapid Commun. 5(3), (2011), 324-326.
- [22] A. D. MANIKPURI, S. AZIZ, E. JOHN, P.V. KHADIKAR: Computation of the Sadhana (Sd) Index of Linear Phenylenes and Corresponding Hexagonal Sequences. Iranian J. Math. Chem, 1(1), (2010), 79-90.

- [23] P.E. JOHN, S. AZIZ, P.V. KHADIKAR: Use of Structure Codes (Counts) for Computing Topological Indices of Carbon Nanotubes: Sadhana (Sd) Index of Phenylenes and its Hexagonal Squeezes. *Iranian J. Math. Chem*, 1(1), (2010), 91-94.
- [24] Z. YARAHMADI: A Note on the First Geometric-Arithmetic Index of Hexagonal Systems and Phenylenes. *Iranian J. Math. Chem*, 2(2), (2011), 101-108.
- [25] S. MORADI, S. BABARAHIMI AND M. GHORBANI: Two Types of Geometric-Arithmetic index of V-phenylenic Nanotube. *Iranian J. Math. Chem*, 2(2), (2011), 109-117.
- [26] M. GHORBANI, H. MESGARANI, S. SHAKERANEH: Optoelectron. *Adv. Mater. Rapid Commun.* 2011, 5(3), 324-326.
- [27] N. PRABHAKARA RAO AND K. L. LAKSHMI: Eccentricity Connectivity Index of V-Phenylenic Nanotubes. *Digest Journal of Nanomaterials and Biostructures*, 6(1), (2010), 81-87.
- [28] S.C. BASAK, Q. ZHU AND D. MILLS: Prediction of Anticancer Activity of 2-phenylindoles: Comparative Molecular Field Analysis Versus Ridge Regression using Mathematical Molecular Descriptors. *Acta Chim. Slov.* 57, (2010), 541-550.
- [29] S. J. CYVIN AND I. GUTMAN: *Lecture Note in Chemistry*, Springer-Verlag, Berlin, (1988), 46.
- [30] I. GUTMAN AND S. J. CYVIN: The number of Kekul, structures in long benzenoid chains. *J. Chem. Phys.* 1988, 147(1), 121-125. [https://doi.org/10.1016/0009-2614\(88\)80235-5](https://doi.org/10.1016/0009-2614(88)80235-5)
- [31] I. GUTMAN AND S. J. CYVIN: Counting Kekule structures in some conjugated systems with repeating units. *J. Serb. Chem. Soc.* 1990, 55, 555-561.
- [32] I. GUTMAN, S. MARKOVIC, V. LUKOVIC, V. RADIVOJEVIC AND S. RANDIĆ *Coll. Sci. Papers Fac. Sci. Kragujevac*, (1987), 8, 15-34.
- [33] I. GUTMAN, P. PETKOVIC AND P. V. KHADIKAR: Bounds for the total π -electron energy of phenylenes. *Revue Roumaine de Chimie*. 41, (1996), 637-643.