IJPSR (2017), Volume 8, Issue 10 (Research Article)

INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES AND RESEARCH

Received on 26 February, 2017; received in revised form, 25 April, 2017; accepted, 12 May, 2017; published 01 October, 2017

COMPUTING SANSKRUTI INDEX OF TURC$_4$C$_8$(S) NANOTUBE

Y. Y. Gao [1], M. S. Sardar [2], S. M. Hosamani [3] and M. R. Farahani [* 4]

College of Pharmacy and Biological Engineering [1], Chengdu University, Chengdu - 610106, China.
University of Management and Technology (UMT) [2], Lahore, Pakistan.
Department of Mathematics [3], Rani Channamma University, Belgavi - 591156, Karnataka, India.
Department of Applied Mathematics [4], Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran.

Keywords:

Topological Index, Connectivity index, Sanskruti Index, TURC$_4$C$_8$(S), Nanotube

Correspondence to Author:
M. R. Farahani

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

E-mail: MrFarahani88@gmail.com

ABSTRACT: Among topological descriptors connectivity indices are very important and they have a prominent role in chemistry. One of them is Sanskruti index defined as $S(G)=\sum_{uv\in E(G)}\left(\frac{S_uS_v}{S_u+S_v-2}\right)^3$, where Su is the summation of degrees of all neighbours of vertex u in G. In this chapter we compute this new topological index for TURC$_4$C$_8$(S) nanotube.

INTRODUCTION: Let G be a simple connected graph in chemical graph theory. The vertices and edges of a graph also correspond to the atoms and bonds of the molecular graph, respectively. If e is an edge / bond of G, connecting the vertices /atoms u and v, then we write e = uv and say "u and v are adjacent". A simple graph is an un-weighted, undirected graph without loops or multiple edges. And also a connected graph is a graph such that there is a path between all pairs of vertices. Clearly, a molecular graph is a simple connected graph. A topological index is a numeric quantity from the structural graph of a molecule and is invariant on the automorphism of the graph.

QUICK RESPONSE CODE

DOI: 10.13040/IJPSR.0975-8232.8(10).4423-25

Article can be accessed online on: www.ijpsr.com

DOI link: http://dx.doi.org/10.13040/IJPSR.0975-8232.8 (10).4423-25

And computing topological indices of molecular graphs from chemical graph theory is an important branch of mathematical chemistry [1 - 3]. One of the best known and widely used is the Randić connectivity index and introduced in 1975 by Milan Randić [1], who has shown this index to reflect molecular branching.

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

The Sanskruti index S(G) of a graph G is defined in [25-28] as follows:

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

Where S_u is the summation of degrees of all neighbours of vertex u in G. The goal of this chapter is to study this new index and computing Sanskruti index of famous nano - structure

$TURC_4C_8(S)$ nanotubes. Our notation is standard and mainly taken from standard books of chemical graph theory [3]. One can see the references [4-11], for more details about topological and connectivity indices

Preliminaries: Consider the molecular graph G = $TURC_4C_8(S)$ nanotube and suppose that there are rs cycle C_8 and C_4 in its structure. Let us denote this graph simply by $TUC_4C_8[r; s]$. Obviously $TUC_4C_8[r; s]$ nanotube has 8rs + 2r vertices and 12rs + r edges. For further study and more detail of this nanotube, see the paper series [4-8, 10] and the general representation of this nano structure is shown in **Fig. 1** and **Fig. 2**.

The goal of this section is computing the Sanskruti index of a lattice of $TUC_4C_8[r; s]$, with r rows and s columns in following theorem.

Theorem 2.1: Let G be the 2 - Dimensional Lattice of $TURC_4C_8[r; s]$ nanotube (r; s > 1). Then the Sanskruti index of G is equal to:

$$S(G) = \frac{2187}{2} rs - \frac{36501941053}{86350888} r.$$

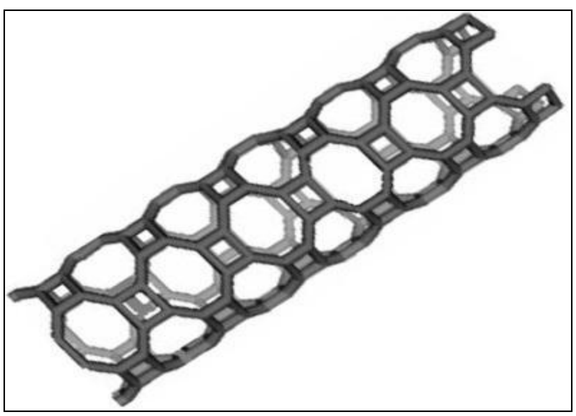

FIG. 1: THE 3 DIMENSIONAL LATTICE (OR CYLINDER) OF $TURC_4C_8(S)$ NANOTUBE [19]

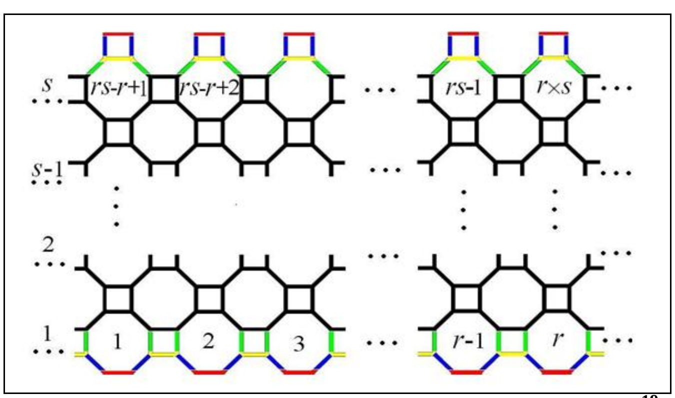

FIG. 2: DIMENSIONAL LATTICE OF $TUC_4C_8[R; S]$ [19]

Proof: Consider now 2 dimensional graph of lattice G = TUC4C8[r; s] (r; s > 1) depicted in **Fig. 1**. Summation of degrees of edge endpoints of this graph have ve types e(5;5); e(5;8); e(8;8); e(8;9) and e(9;9) that are shown in **Fig. 2** by red, blue, yellow, green and black colors. In other word for all edge e = uv of the types e(5;5); S(v)=S(u)=5 and for an edge f = vw of the types e(5;8); S(v)=5 and S(w)=8 and other types are analogous. Also the number of edges of the types e(5;5) and e(5;8) are equal to 2r and 22r, respectively and for other types see following table.

TABLE 1: SUMMATION OF DEGREES OF EDGE ENDPOINTS

Summation of degrees of edge endpoints	$^e(5;5)$	$^e(5;8)$	$^e(8;8)$	$^e(8;9)$	$^e(9;9)$
Number of edges of this type	2r	4r	2r	4r	12r-11r

$$S(TUC_4C_8[r,s]) = \sum_{uv\in E(G)} \left(\frac{S_u S_v}{S_u + S_v - 2} \right)^3 = \frac{2187}{2} rs - \frac{36501941053}{86350888} r.$$

CONCLUSION: In chemical graph theory, mathematical chemistry and mathematical physics, molecular descriptors, topological and connectivity indices are very important and useful and have more applications which characterize a molecular graph topology. In this work, a new connectivity topological index called "Sanskruti index" of $TURC_4C_8(S)$ nanotube was determined. Further works in this line are soon to be communicated [9-24].

ACKNOWLEDGEMENT: Nil.

CONFLICTS OF INTEREST: Nil.

REFERENCES:

1. M. Randic: On Characterization of Molecular Branching, J. Am. Chem. Soc. 1975; 97(23), 6609.
2. Todeschini R and Consonni V: Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.
3. Trinajsti N: Chemical Graph Theory, CRC Press, Boca Raton, FL 1992.
4. Arezoomand M: Energy and Laplacian Spectrum of $C_4C_8(S)$ Nanotori and Nanotube. Digest. J. Nanomater. Bios. 2009; 4(6): 899-905.
5. Asadpour J, Mojarad R and Safikhani L: Computing some topological indices of nano structure. Digest. J. Nanomater. Bios. 2011; 6(3): 937-941.
6. Ashrafi AR and Yousefi S: An Algebraic Method Computing Szeged index of $TUC_4C_8(R)$ Nanotori. Digest. J. Nanomater. Bios. 2009; 4(3): 407-410.

7. Ashrafi AR, Faghani M and Seyed Aliakbar SM: Some Upper Bounds for the Energy of $TUC_4C_8(S)$ Nanotori. Digest. J. Nanomater. Bios. 2009; 4(1): 59-64.
8. Ashrafi AR and Shabani H: The Hosoya Polynomial of $TUC_4C_8(S)$ Nanotubes. Digest. J. Nanomater. Bios. 2009; 4(3): 453-457.
9. Graovac A and Ghorbani M: A New Version of Atom-Bond Connectivity Index. Acta Chim. Slov. 2010; 57(3), 609.
10. Heydari A: On the Modified Schultz Index of $C_4C_8(S)$ Nanotori and Nanotube. Digest. J. Nanomater. Bios. 2010; 5(1): 51-56.
11. Furtula B, Graovac A and Vukicevic D: Atom-bond connectivity index of trees. Disc. Appl. Math. 2009; 157: 2828.
12. Ashrafi AR, Doslic T and Saheli M: The eccentric connectivity index of $TUC_4C_8(R)$ nanotubes. MATCH Commun. Math. Comput. Chem. 2011; 65: 221-230.
13. Alaeiyan M, Bahrami A and Farahani MR: Cyclically Domination Polynomial of Molecular Graph of Some Nanotubes. Digest Journal of Nanomaterials and Biostructures 2011; 6(1): 143-147.
14. Farahani MR: On the Higher Randic Indices of Nanotubes. Journal of Computational Methods in Molecular Design 2015; 5(3): 10-15.
15. Farahani MR, Imran M, Siddiqui MK, Afzal. Siddiqui MH and Baby S: The Second and Second-Sum-connectivity indices of $TUC_4C_8(S)$ Nanotubes. Journal of Optoelectronic and Biomedical Materials 2016; 8(2): 107-111.
16. Farahani MR: Multiplicative Versions of Zagreb indices of T $USC_4C_8(S)$. Journal of Chemistry and Materials Research 2015; 2(2): 67-70.
17. Farahani MR: Zagreb indices of T $UHRC_4(S)$ and T $USC_4C_8(S)$ Nanotubes. Journal of Advance in Mathematical Science 2015; 2(1): 98-105.
18. Farahani MR: Fifth Geometric-Arithmetic Index of $TURC_4C_8(S)$ Nanotubes. Journal of Chem-ica Acta. 2013; 2(1): 62-64.
19. Farahani MR: New Version of Atom-Bond Connectivity Index of $TURC_4C_8(S)$. International Journal of Chemical Modeling 2012; 4(4): 527-521.
20. Farahani MR: Domination polynomial of Nanotorus by using the 2-variables Generating Func-tion. Paci C Journal of Applied Mathematics 2014; 6(1): 79-95.
21. Farahani MR: Computing some connectivity indices of Nanotubes. Adv. Mater. Corrosion 2012; 1: 57-60.
22. Farahani MR: The Hyper-Zagreb Index of T $USC_4C_8(S)$ Nanotubes. International Journal of Engineering and Technology Research 2015; 3(1): 1-6.
23. Farahani MR: On Domination Polynomial of $TUC_4C_8(S)$ Nanotube. Paci c Journal of Applied Mathematics 2015; 7(2): 75-86.
24. Kulli VR: General Multiplicative Zagreb Indices of TUC_4C_8[m; n] and TUC_4[m; n] Nanotubes. Intern. J. Fuzzy Mathematical Archive 2016; 11(1): 39-43.
25. Hosamani SM: Computing Sanskruti index of certain nanostructures. Journal of Applied Math-ematics and Computing. In press.
26. Sardar MS, Zafar S and Farahani MR: Computing Sanskruti index of the Polycyclic Aromatic Hydrocarbons. Geology, Ecology, and Landscapes (TGEL) 2017; 1(1): 37-40.
27. Gao YY, Sardar MS, Zafar S and Farahani MR. Sanskruti index of Benzenoid molecular graphs. Applied Mathematics (scirp), 7403538. In press, 2017.
28. Y.Y. Gao, M.S. Sardar, S. Zafar, M.R. Farahani. Computing Sanskruti index of Dendrimer Nanostars. International Journal of Pure and Applied Mathematics. In press, 2017.

How to cite this article:
Gao YY, Sardar MS, Hosamani SM and Farahani MR: Computing sanskruti index of $TURC_4C_8(s)$ nanotube. Int J Pharm Sci Res 2017; 8(10): 4423-25.doi: 10.13040/IJPSR.0975-8232.8(10).4423-25.

All © 2013 are reserved by International Journal of Pharmaceutical Sciences and Research. This Journal licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 3.0 Unported License.

This article can be downloaded to **ANDROID OS** based mobile. Scan QR Code using Code/Bar Scanner from your mobile. (Scanners are available on Google Playstore)