NanoNEXT

Review Article

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Entropy Measures of Some Nanotubes Using Sombor Index

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Abstract: In (QSAR)/(QSPR) studies, topological indices play an essential role, as a molecular descriptor. For measuring the structural information of chemical graphs and complex networks, the graph entropies with topological indices take the help of Shannon's entropy concept, which now become the information-theoretic quantities. In discrete mathematics, biology, and chemistry, the graph entropy measures play an essential role. In this paper, we study the Boron Nanotube and we compute entropies of these structures by making relation of newly defined degree based topological indices, called Sombor index with the help of the information function, which is the number of vertices of different degrees together with the number of edges among the various vertices. Further, the numerical and graphical comparison are also studied.

Keywords: Entropy, Sombor Index, Molecular Graph, Nanotubes

1. Introduction

A significant role in the chemical graph theory, is predicting the chemical properties of non-materials without going into labs. Chem-informatics is a new discipline, used to calculate the biological activities and characteristics of non-materials in quantitative structure-activity (QSAR) and structure-property (QSPR) connections [1, 2]. A new subject known as, Chem-informatics which have the combination of chemistry, mathematics, and information science, which helps in the bio-activity and physiochemical properties of chemical compounds.

In Shannon's renowned paper entitled *"The entropy of a probability distribution is known as a measure of the unpredictability of information content or a measure of the uncertainty of a system"* the concept of entropy was introduced. Later, entropy was found to be useful in graphs and chemical networks. It was developed for measuring the structural information of graphs and chemical networks. The idea of graph entropy based on the classifications of vertex orbits was introduced by Rashevsky [3]. Now a day, graph entropies are broadly used in various fields like chemistry, biology, ecology, and sociology. The graph entropy measures the relative probability distributions with elements (like vertices, edges, etc.) of a graph that can be classified as intrinsic and extrinsic measures. There are more than a few types of such graph entropy measures (See [4]). The degree powers are extremely important invariants and are studied extensively in graph theory, and network science, and they are used as the information functional to investigate the networks (See [5-7]). In this paper, we measure the entropy of some molecular graphs using the Sombor index and study them with the help of graph.

2. Preliminaries

Here, some of the definitions are discussed and those are used in our work. Let G be a simple graph with vertex set $V = V(G)$ an edge set, $E = E(G)$ and ζ denotes a meaningful information function. The number of edges of G that a connected to a vertex v and its degree $\chi(v)$. The graph entropy (Shannon's) of a graph G is given by:

$$ENT_{\zeta}(G) = -\sum_{i=1}^{n} \frac{\zeta(v_i)}{\sum_{j=1}^{n}\zeta(v_j)}\left[\frac{\log\zeta(v_i)}{\sum_{j=1}^{n}\zeta(v_j)}\right] \quad (1)$$

Now, if $v_i \in V$ and information function $\zeta(v_i)$ denotes the degree of the vertex v_i, which means $\zeta(vi) = \chi(vi)$, then equation (1) with fundamental theorem in graph theory becomes,

$$ENT_{\zeta}(G) = \log(2p) - \frac{1}{2p}\log\left[\prod_{i=1}^{n}\chi(v_i)^{\chi(v_i)}\right] \quad (2)$$

In [8], edge weighted graph entropy have defined and given by,

$$\mathrm{ENT}_{\zeta}(G) = -\sum_{v_1v_2\in E(G)} \frac{\zeta(v_1v_2)}{\sum_{v_1v_2\in E(G)}\zeta(v_1v_2)} \log\left[\frac{\zeta(v_1v_2)}{\sum_{v_1v_2\in E(G)}\zeta(v_1v_2)}\right] \quad (3)$$

In [9] Gutman defined new degree based topological index called Sombor index, denoted by $SO(G)$ and defined as,

$$\mathrm{SO}(G) = \sum_{vu\in E} \sqrt{d_u^2 + d_v^2} \quad (4)$$

By reducing equation (3), we get Sombor entropy as follow,

$$\mathrm{ENT}_{SO}(G) = \log\big(\mathrm{SO}(G)\big) - \frac{1}{\mathrm{SO}(G)} \log\left[\prod_{v_1v_2\in E(G)}^{n} \sqrt{\chi(v_1)^2+\chi(v_2)^2}^{\sqrt{\chi(v_1)^2+\chi(v_2)^2}}\right] \quad (5)$$

3. Application of Degree Based Entropies

In 1946, Shannon's paper become the initial view of the modern information theory. There are many applications in the field of biology and chemistry found in [10, 12]. The applications of Shannon's entropy formulas are found in [13, 14]. In the various fields (biology, chemistry) the entropy measures of graphs are applied and found in [15]. Generally, the entopic network measures are used to explore the biological or chemical properties of molecular graphs. In this paper, we have introduced new degree-based entropy that can be used to measure network heterogeneity. The entopic measures are studied with the help of vertex-degrees topological indices to detect network heterogeneity are found in [16,17].

4. Results on Boron Triangular Nanotubes

Nanoscience has developed into the heart of the current age because of its rising applications. There are top four sections namely, nanowires, nanotubes, nanocrystals, and nanomaterials. Nanowires and nanotubes are one-dimensional sections. After the 1990s, the importance of one-dimensional nanomaterials developed unexpectedly, and many works are done on this. The molecular structure is a graph in which vertices as atoms, and edges, as chemical bonds. Due to the unique quality of Boron nanotubes, such as electronic structure, work function, structural stability, and transport qualities, it is wildly studied [18]. The significance of the two structural classes of boron nanotubes can't be showy. One of them is generated from a triangular sheet, and the other one is generated from a sheet. Both the nanotubes are more conductive than each other, in spite of their structure or chirality. In theoretical chemistry, we use the mathematical technique to learn molecular structures [19, 20]. Figure 1 shows the perceptions of boron triangular and boron-nanotube. For more on entropy see [21-23].

We compute the Sombor entropy of Boron Triangular Nanotubes with the help of Equation (5) and Table 1. For Boron Triangular Nanotubes, the Sombor index is as followes:

$$\mathrm{SO}(G) = 18mn\sqrt{2} + 12\sqrt{13}\,n - 60\sqrt{2}\,n$$

Now use equation (3) (with Table 1) we get,

$$ENT_{SO}(G) = \log\left(18mn\sqrt{2} + 12\sqrt{13}\,n - 60\sqrt{2}\,n\right) - \frac{\log\left(\left[4\sqrt{2}\right]^{4\sqrt{2}} 3n\right)}{18mn\sqrt{2} + 12\sqrt{13}\,n - 60\sqrt{2}\,n} - \frac{\log\left(\left[2\sqrt{13}\right]^{2\sqrt{13}} 6n\right)}{18mn\sqrt{2} + 12\sqrt{13}\,n - 60\sqrt{2}\,n} - \frac{\log\left(\left[6\sqrt{2}\right]^{6\sqrt{2}} 3n(3m-2)/2\right)}{18mn\sqrt{2} + 12\sqrt{13}\,n - 60\sqrt{2}\,n}$$

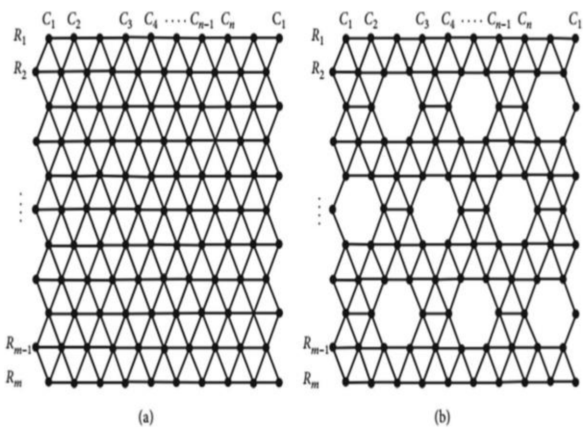


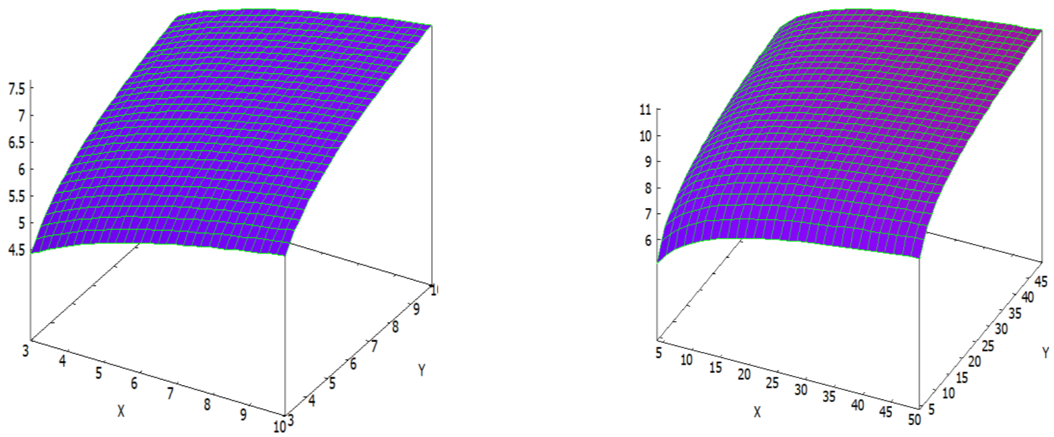
Figure 1. 2D Molecular Structure of (a) Boron Nanotubes and (b) Alpha boron Nanotubes

Table 1. Edge partition of Boron Triangular Nanotubes based on degrees of each edge and vetex

$(\chi(v_1), \chi(v_2))$	Frequency	Set of edges
(4,4)	$3n$	E_1
(4,6)	$6n$	E_2
(6,6)	$\frac{3n(3m-8)}{2}$	E_3

Table 2. Edge partition of Alpha Boron Triangular Nanotubes based on degrees of each edge and vetex

$(\chi(v_1), \chi(v_2))$	Frequency	Set of edges
(4,4)	$3n$	E_1
(4,5)	$4n$	E_2
(4,6)	$\frac{3n(3m-8)}{2}$	E_3
(5,5)	$\frac{n(3m-8)}{2}$	E_4
(6,6)	$2n(m-3)$	E_5



(a) Sombor entropy of Alpha Boron Triangular Nanotube

(b) Sombor entropy of Alpha Boron Triangular

Figure 2. Sombor entropy of nonotubes

5. Results on Alpha Boron Triangular Nanotubes

The edge partition of the Alpha Boron Triangular Nanotubes is given in Table 2. We compute Sombor entropy of this Nanotubes with the help of Equation (5) and Table 2.

The Sombor index for this Nanotubes is as follows:

$$SO(G) = \left(4\sqrt{41} - 4\sqrt{13} - 6\sqrt{61} - 8\sqrt{2}\right)n + \left(2\sqrt{61} + \frac{15\sqrt{2}}{2}\right) mn \quad (7)$$

Now equation (4) (with Table 2) can be written as:

$$ENT_{SO}(G) = \log\left(\left(4\sqrt{41} - 4\sqrt{13} - 6\sqrt{61} - 8\sqrt{2}\right)n + \left(2\sqrt{61} + \frac{15\sqrt{2}}{2}\right)mn\right) - \frac{\log\left(\left[\sqrt{32}\right]^{\sqrt{32}} 3n\right)}{\left(4\sqrt{41}-4\sqrt{13}-6\sqrt{61}-8\sqrt{2}\right)n+\left(2\sqrt{61}+\frac{15\sqrt{2}}{2}\right)mn} - \frac{\log\left(\left[\sqrt{41}\right]^{\sqrt{41}} 4n\right)}{\left(4\sqrt{41}-4\sqrt{13}-6\sqrt{61}-8\sqrt{2}\right)n+\left(2\sqrt{61}+\frac{15\sqrt{2}}{2}\right)mn} - \frac{\log\left(\left[\sqrt{52}\right]^{\sqrt{52}} 2n\right)}{\left(4\sqrt{41}-4\sqrt{13}-6\sqrt{61}-8\sqrt{2}\right)n+\left(2\sqrt{61}+\frac{15\sqrt{2}}{2}\right)mn} - \frac{\log\left(\left[\sqrt{50}\right]^{\sqrt{50}} \frac{n(3m-8)}{2}\right)}{\left(4\sqrt{41}-4\sqrt{13}-6\sqrt{61}-8\sqrt{2}\right)n+\left(2\sqrt{61}+\frac{15\sqrt{2}}{2}\right)mn} - \frac{\log\left(\left[\sqrt{61}\right]^{\sqrt{61}} 2n(m-3)\right)}{\left(4\sqrt{41}-4\sqrt{13}-6\sqrt{61}-8\sqrt{2}\right)n+\left(2\sqrt{61}+\frac{15\sqrt{2}}{2}\right)mn} \quad (8)$$

Table 3. Numerical values of Sombor Entropies for Nanotubes[n].

[n]	$ENT_{SO(G)}$ (Boron Triangular Nanotub)	$ENT_{SO(G)}$ (Alpha Boron Trian- gular Nanotub)
[4]	5.373101608188483	5.11170727047355
[5]	5.994648295072788	5.852654213370223
[6]	6.459153310272955	6.372815336653734
[7]	6.831922264919784	6.776536235432427
[8]	7.144019651128448	7.107845028033726
[9]	7.412809515743534	7.389491370867745
[10]	7.6490430547951	7.634814760617512
[11]	7.859865238824556	7.852339088328805
[12]	8.050277923414857	8.04785971107262

6. Comparisons and Discussion

In view of the fact that, degree-based entropy has a broad range of applications in science. Scientists are benefited from the numerical and graphical representation of these predictable outcomes. In this paper, we have found Sombor entropies for Boron Triangular Nanotubes and Alpha Boron Triangular Nanotubes with different values of n,a newly defined degreebased topological index called Sombor index. In small values forn, we created Table 3 for the numerical comparison of various entropy. And as observed in Table 3, the values of entropy are in rising order, as n rising. The graphical representations of results can be seen in the Figures 2 for definite values of n.

7. Conclusion

In this article, we examine the graph entropies connected with a new information function using Shannon's entropy and Chen et al.'s entropy definitions in this research. We have created a connection among the newly defined degree-based topological indices, the Sombor index with degree-based entropies. We calculated the Sombor entropies for the Boron Triangular Nanotubes and Alpha Boron Triangular Nanotubes. Next, the numerical values of these entropies are tabulated.

References

[1] E. Deutsch S. Klavzar, M-Polynomial and Degree-Based Topological Indices, Iranian Journal of Mathematical Chemistry 6 (2015) 93-102. [DOI]

[2] D. Stover, D. Normile, Buckytubes, Popular Science, 240 (1992) 31.

[3] N. Rashevsky, Life, information theory, and topology, The bulletin of mathematical biophysics, 17 (1955) 229-235. [DOI]

[4] A.Mowshowitz, M. Dehmer, Entropy and the complexity of graphs revisited, Entropy 14 (2012) 559-570. [DOI]

[5] S. Manzoor, M.K. Siddiqui, S. Ahmad, On Entropy Measures of Molecular Graphs Using Topological Indices, Arabian Journal of Chemistry, 13 (2020) 6285-6298. [DOI]

[6] S. Cao, M. Dehmer, Degree-based entropies of networks revisited, Applied Mathematics and Computation, 261 (2015) 141-147. [DOI]

[7] S. Cao, M. Dehmer, Y. Shi, Extremality of degree-based graph entropies, Information Sciences, 278 (2014) 22-33. [DOI]

[8] Z. Chen, M. Dehmer, Y. Shi, A Note on Distance-Based Graph Entroprodes, Entropy 16 (2014) 5416-5427. [DOI]

[9] I. Gutman, Geometric approach to degree-based topological indices: Sombor indices, MATCH Communications in Mathematical and in Computer Chemistry, 86 (2021) 11-16.

[10] C.E. Shannon, A mathematical theory of communication, The Bell System Technical Journal, 27 (1948) 379-423. [DOI]

[11] H. Morowitz, Some order-disorder considerations in living systems, The bulletin of mathematical biophysics, 17 (1953) 81-86. [DOI]

[12] H.Quastler, Information theory in biology, The bulletin of mathematical biophysics, 16 (1954) 183-185.[DOI]

[13] N. Rashevsky, Life, information theory, and topology, The bulletin of mathematical biophysics, 17 (1955) 229-235. [DOI]

[14] E.Trucco, A note on the information content of graphs, The bulletin of mathematical biophysics, 18 (1956) 129-135. [DOI]

[15] M. Dehmer, A. Mowshowitz, A history of graph entropy measures, Information Sciences, 181 (2011) 57-78. [DOI]

[16] R.V. Sol, S.I. Valverde, Information theory of complex networks: on evolution andarchitectural constraints, Complex Networks. Lecture Notes in Physics, 650 (2004) 189-207. [DOI]

[17] Y.J. Tan, J. Wu, Network structure entropy and its application to scale-free networks, Syst. Eng.-Theory Pract, 6 (2004) 1-3.

[18] V. Bezugly, J. Kunstmann, B. Grundkotter-Stock, T. Frauenheim, T. Niehaus, G. Cuniberti, Highly Con-ductive Boron Nanotubes: Transport Properties, Work Functions, and Structural Stabilities, ACS Nano, 5 (2011) 4997-5005. [DOI]

[19] S. J. Cyvin, I. Gutman, (1988) Lecture Notes in Chemistry, Springer-Verlag, Berlin.

[20] N. Trinajstic, I. Gutman, Mathematical Chemistry, Croatica Chemica Acta, 75 (2002). 329-356.

[21] Y.C. Kwun, H.M.ur. Rehman, M. Yousaf, W. Nazeer, S.M. Kang, The Entropy of Weighted Graphs with Atomic Bond Connectivity Edge Weights, Discrete Dynamics in Nature and Society 2018 (2018) 1-10. [DOI]

[22] S. Manzoor, M.K. Siddiqui, S. Ahmad, On Entropy Measures of Polycyclic Hydroxychloroquine Used for Novel Coronavirus (COVID-19) Treatment, Polycyclic Aromatic Compounds, (2020) 1-26. [DOI]

[23] S. Manzoor, M.K. Siddiqui, S. Ahmad, On Physical Analysis of Degree-Based Entropy Measures for Metal-Organic Superlattices, The European Physical Journal Plus, 136, (2021) 1-22. [DOI]

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