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Degree-based entropy of molecular structure of HAC_5C_7[P,Q]

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This study aimed at using the calculated values of topological indices, degree weighted entropy of graph, the entropy measures are calculated viz., symmetric division index, inverse sum index atom-bond connectivity entropy and geometric arithmetic entropy for the nanotube HAC_5C_7[p,q].

KEYWORDS

Degree-based entropy; M-polynomial; topological indices; weighted entropy; molecular structure.

Introduction

Content of graphs and networks have been based on the profound and initial works of Shannon [1,2].

In order to measure the structural complexity of graphs and networks, the concept of graph entropy has been proposed [3,6]. Determining the complexity of the graphs has been used in various filed of sciences, including information theory, biology, chemistry and sociology.

Studying the entropy measurement of networks started after the groundbreaking work of Shannon [3]. Rashevsky used the concept of graph entropy to measure the structural complexity of the graph. Mowshowitz [7] introduced the entropy of the graph as information theory, which he interpreted as the structural information content of the graph.

We have various applications of graph entropy in economics. Mowshowitz [7] studied the mathematical properties of graph entropy and calculated in depth measurements of his particular application. We use the theory of graph entropy as a weighted graph, like previous studies [8-14].

In this report, we computed graph entropy for concatenated 5-cycles in one row and in two rows of various lengths by taking Zagreb indices, augmented Zagreb index, modified Zagreb indices and Randić index.

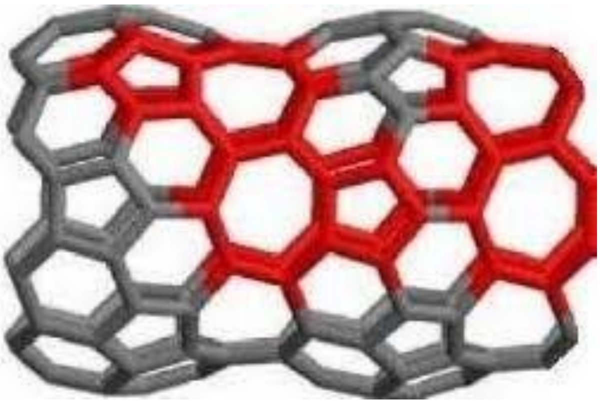

FIGURE 1 The cylinder lattice of HAC_5C_7[p,q] nanotube [15,16]

Entropy

Graph entropy associated with the graph was first considered by Korner and Mowshowitz [7]. Graph entropy has been used extensively to characterize the structure of graph-based systems in mathematical chemistry. In these applications the entropy of a graph is interpreted as its structural information content and serves as a complexity measure. Such a measure is associated with an equivalence relation defined on a finite graph. For example, it provides an equivalent definition for a graph to be perfect and it can also be applied to obtain lower bounds in graph covering problems.

It is also conjectured that the degree-based entropy can be used to measure network incongruity. Similar entopic measures which are based on vertex-degrees to detect network heterogeneity have been introduced by Sol and Valverde (2004) and Tan and Wu (2004).

Definition 1.1. (Entropy). Let the probability density function

$$P_{ij} = \frac{w(uv)}{\sum W(uv)}$$

then the entropy of graph G is defined as

$$I(G,w) = \sum P_{ij} \log P_{ij}.$$

$HAC_5C_7[p,q]$ Nanotube

The molecular graphs of carbon nanotube $HAC_5C_7[p,q]$ are given in Figure 1. For the structure, we refer to [17-37].

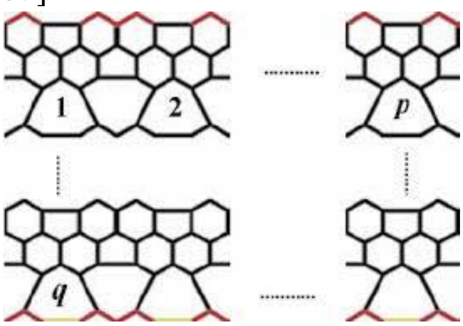

FIGURE 2 The 2-dimensional lattice of $HAC_5C_7[p,q]$ nanotube [15,16]

The edges of HAC_5C_7 can be partitioned into following cases:

$E_1 = \{xy \in E(HAC_5C_7)[p,q] : d_x=2, d_y=2\}$,

$E_2 = \{xy \in E(HAC_5C_7)[p,q] : d_x=3, d_y=2\}$,

$E_3 = \{xy \in E(HAC_5C_7[p,q]) : d_x=3, d_y=3\}$,

Where,

$|E_1|=0$,

$|E_2|=4p$,

$|E_3|=12pq-2p$,

Entropies of $HAC_5C_7[p,q]$ nanotube

Theorem 3.1. The entropy of $HAC_5C_7[p,q]$ with Symmetric division Index is:

$$I(HAC_5C_7[p,q], SSD) = log(24pq + 4.667p) - \frac{1}{24pq + 4.667p}[7.22471pq + 1.706078p].$$

Proof. By definition, we have

$SSD(HAC_5C_7[p,q]) = 24pq + 4.667p$.

$$I(SSD) = log(24pq + 4.667p) - \frac{1}{24pq + 4.667p}$$

$$\times\left[|E_1|[\frac{min(2,2)}{max(2,2)} + \frac{max(2,2)}{min(2,2)}] \times \log[\frac{min(2,2)}{max(2,2)} + \frac{max(2,2)}{min(2,2)}]\right]$$

$$+\left[|E_2|[\frac{min(3,2)}{max(3,2)} + \frac{max(3,2)}{min(3,2)}] \times log[\frac{min(3,2)}{max3,2} + \frac{max(3,2)}{min(3,2)}]\right]$$

$$+\left[|E_3|[\frac{min(3,3)}{max(3,3)} + \frac{max(3,3)}{min(3,3)}] \times log[\frac{min(3,3)}{max3,3} + \frac{max(3,3)}{min(3,3)}]\right]$$

$$= log(24pq + 4.667p) - \frac{1}{24pq + 4.667p}$$

$$\times\left[(0)(\frac{2}{2} + \frac{2}{2} \times log(\frac{2}{2} + \frac{2}{2})) + (4p)(\frac{2}{3} + \frac{3}{2}).log(\frac{2}{3} + \frac{3}{2})\right]$$

$$+(12pq - 2p)\left[(\frac{3}{3} + \frac{3}{3}) \times log(\frac{3}{3} + \frac{3}{3})\right]$$

$$= log(24pq + 4.667p) - \frac{1}{24pq + 4.667p}$$

$$\times[2.910198p + 7.22471pq - 1.204119p]$$

$$= log(24pq + 4.667p) - \frac{1}{24pq + 4.667p}[7.22471pq + 1.706078p] \blacksquare$$

Theorem 3.2. The Entropy of $HAC_5C_7[p,q]$ with inverse sum index weight is

$$I[HAC_5C_7[p,q], ISI] = log(18pq + 1.8p) - \frac{1}{18pq + 1.8p}[3.169642pq - 0.54666p].$$

Proof. By definition, we have

$ISI[HAC_5C_7[p,q]] = 18pq + 1.8p$,

$I[HAC_5C_7[p,q],ISI] = log[18pq + 1.8p]$
$-\frac{1}{18pq+1.8p}[+|E_1|[\frac{2.2}{2+2}\times log\frac{2.2}{2+2}]$
$+|E_2|[\frac{2.3}{2+3}\times log\frac{2.3}{2+3}]+|E_3|[\frac{3.3}{3+3}\times[\frac{3.3}{3+3}]$
$= log(18pq+1.8p) - \frac{1}{18pq+1.8p}[(0)(1\times log1)$
$+(4p)(\frac{5}{6}\times log\frac{5}{6})+(12pq-2p)(\frac{3}{2}\times log\frac{3}{2})]$
$= log(18pq+1.8p) - \frac{1}{18pq+1.8p}[-0.263937p$
$+3.169642pq+0.528273p]$
$= log(18pq+1.8p) - \frac{1}{18pq+1.8p}[3.169642pq-0.54666p]$

Theorem 3.3. The entropy of $HAC_5C_7[p,q]$ with Atom-Bond Connectivity is
$I(HAC_5C_7[p,q],ABC) = log(8pq+1.495093p)$
$-\frac{1}{8pq+1.495093p}[-0.19093235459p-1.408730072pq].$

Proof. By definition, we have
ABC(HAC₅C₇[p,q])=8pq+1.495093p,

$I(HAC_5C_7[p,q],ABC) = log(8pq+1.495093p)$
$-\frac{1}{8pq+1.495093p}[|E_1|\sqrt{\frac{2+2-2}{2.2}}\times log\sqrt{\frac{2+2-2}{2.2}}$
$+|E_2|\sqrt{\frac{3+2-2}{3.2}}\times log\sqrt{\frac{3+2-2}{3.2}}+|E_2|\sqrt{\frac{3+3-2}{3.3}}$
$\times log\sqrt{\frac{3+3-2}{3.3}}]$
$= log(8pq+1.495093p) - \frac{1}{8pq+1.495093p}[(0)(\sqrt{\frac{1}{2}}$
$\times log\sqrt{\frac{1}{2}})+(4p)(\sqrt{\frac{1}{2}}\times log\sqrt{\frac{1}{2}})[(12pq-2p)(\frac{2}{3}\times log\frac{2}{3})]$
$= log(8pq+1.495093p) - \frac{1}{8pq+1.495093p}$
$\times[-0.42572070p-1.408730072pq-0.234788345p]$
$= log(8pq+1.495093p) - \frac{1}{8pq+1.495093p}$
$\times[-0.19093235459p-1.408730072pq].$

Theorem 3.4. The entropy of $HAC_5C_7[p,q]$ with Geometric- Arithmetic Index is
$I(HAC_5C_7[p,q],GA) = log(12pq+3.5192p)$
$-\frac{1}{12pq+3.5192p}[-0.03474114p].$

Proof. By definition, we have
$GA(HAC_5C_7[p,q])=12pq+3.5192p$

$I(HAC_5C_7[p,q],GA)log(12pq+3.5192p)$
$-(\frac{1}{12pq+3.5192p})[|E_1|[2\frac{2(\sqrt{2.2})}{2+2}\times log2\frac{2(\sqrt{2.2})}{2+2}]$
$+|E_2|[2\frac{2(\sqrt{(3.2)}}{3+2}\times log2\frac{2(\sqrt{3.2})}{3+2}]+|E_3|[2\frac{2(\sqrt{3.3})}{3+3}$
$\times log2\frac{2(\sqrt{3.3})}{3+3}]$
$= log(12pq+3.5192p) - \frac{1}{12pq+3.5192p}$
$[(0)(1\times log1)(4p)(2\frac{\sqrt{6}}{5}\times log2\frac{\sqrt{6}}{5})+(12pq-2p)(1\times log1)]$
$= log(12pq+3.5192p) - \frac{1}{12pq+3.5192p}[-0.03474114p].$

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