Degree-based entropy of molecular structure of $HAC_5C_7[p,q]$

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Abstract

The graph entropy measures take part in various problem domains such as graph theory, biology and chemistry. 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: `Topological indices, weighted entropy.`

1. Introduction

In the last fifty years, the investigations into the information content of graphs and networks have been based on the profound and initial works due to Shannon [2] and [3]. In order to measure the structural complexity of graphs and networks, the concept of graph entropy has been proposed [9] and [4]. Determining the complexity of the graphs has been used in various filed of sciences, including information theory, biology, chemistry and sociology.

We have different applications of graph entropy in communications and economics. We use the concept of graph entropy as a weighted graph, as in [7] who solved the problem of weighted chemical graph entropy by using a special information functional. Some degree-based indices are characterized by investigating the extremes of the entropy of certain class of graphs[10] and [6]. In this paper, we compute graph entropy for concatenated 5-cycles in one rows and in two rows of various lengths by taking Zagreb indices, augmented Zagreb index, modified Zagreb indices and Randic index.

Entropy

The entropy of a graph is a functional depending both on the graph itself and on a probability distribution on its vertex set. This graph functional originated from the problem of source coding in information theory and was introduced by J. Krner in 1973. Although the notion of graph entropy has its roots in information theory, it was proved to be closely related to some classical and frequently studied graph theoretic concepts. For example, it provides an equivalent definition for a graph to be perfect and

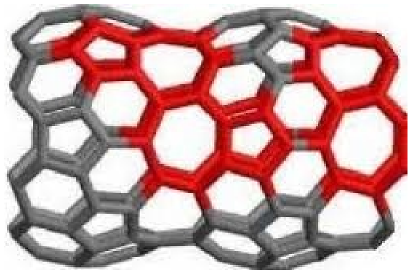

Figure 2.1: The cylinder lattice of $HAC_5C_7[p,q]$ nanotube.

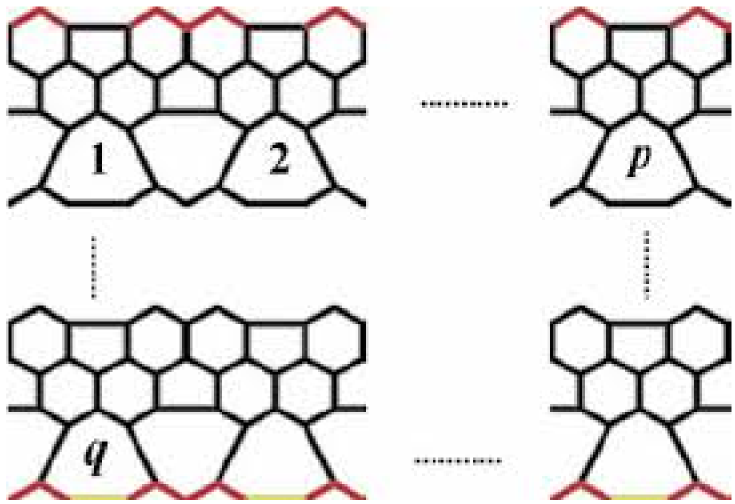

Figure 2.2: The 2-dimensional lattice of $HAC_5C_7[p,q]$ nanotube.

it can also be applied to obtain lower bounds in graph covering problems.

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

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

2. $HAC_5C_7[p,q]$ Nanotube

The molecular graphs of carbon nanotube $HAC_5C_7[p,q]$ are shown in Figure 1. For structure we refer [5].

It can be observed from figure 2 that the edge set of HAC_5C_7 can be divided into following classes

$$E_1 = \{uv \in E(HAC_5C_7)[p,q] : d_u = 2, d_v = 2\},$$

$$E_2 = \{uv \in E(HAC_5C_7)[p,q] : d_u = 3, d_v = 2\},$$

$$E_3 = \{uv \in E(HAC_5C_7[p,q]) : d_u = 3, d_v = 3\},$$

Such that

$$|E_1| = 0,$$

$$|E_2| = 4p,$$

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

Now from this edge partition, we can have following results immediately.

3. Entropies of $HAC_5C_7[p,q]$ Nanotube

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

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

Proof. By definition, we have

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

$$
\begin{aligned}
I(SSD) &= log(24pq+4.667p) - \frac{1}{24pq+4.667p} \\
&\left[|E_1|[\frac{min(2,2)}{max(2,2)} + \frac{max(2,2)}{min(2,2)}] \times \log[\frac{min(2,2)}{max(2,2)} + \frac{max(2,2)}{min(2,2)}]\right] + \\
&\left[|E_2|[\frac{min(3,2)}{max(3,2)} + \frac{max(3,2)}{min(3,2)}] \times log[\frac{min(3,2)}{max3,2} + \frac{max(3,2)}{min(3,2)}]\right] + \\
&\left[|E_3|[\frac{min(3,3)}{max(3,3)} + \frac{max(3,3)}{min(3,3)}] \times log[\frac{min(3,3)}{max3,3} + \frac{max(3,3)}{min(3,3)}]\right] \\
&= log(24pq+4.667p) - \frac{1}{24pq+4.667p} \\
&\left[(0)(\frac{2}{2} + \frac{2}{2} \times log(\frac{2}{2} + \frac{2}{2})) + (4p)(\frac{2}{3} + \frac{3}{2}).log(\frac{2}{3} + \frac{3}{2})\right] \\
&+(12pq-2p)\left[(\frac{3}{3} + \frac{3}{3}) \times log(\frac{3}{3} + \frac{3}{3})\right] \\
&= log(24pq+4.667p) - \frac{1}{24pq+4.667p} \\
&[2.910198p + 7.22471pq - 1.204119p] \\
&= log(24pq+4.667p) - \frac{1}{24pq+4.667p} \\
&[7.22471pq + 1.706078p].
\end{aligned}
$$

□

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

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

Proof. By definition, we have

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

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

□

Theorem 3.3. *The entropy of $HAC_5C_7[p,q]$ with Aotm Bond Connectivity is*

$$
\begin{aligned}
I(HAC_5C_7[p,q],ABC) &= log(8pq+1.495093p)-\frac{1}{8pq+1.495093p} \\
&[-0.19093235459p-1.408730072pq].
\end{aligned}
$$

Proof. By definition, we have

$$
ABC(HAC_5C_7[p,q]) = 8pq+1.495093p,
$$

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

□

Theorem 3.4. *The entropy of $HAC_5C_7[p,q]$ with Geometric Arthmetic 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

$$GA(HAC_5C_7[p,q]) = 12pq + 3.5192p$$

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

□

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