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FULL PAPER

# Weighted entropies of $HAC_5C_7[p;q]$ nanotube

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The aim of this article was to compute weighted entropy of some well-known nanostructure $HAC_5C_7[p;q]$. We applied probability density function to formulate entropy by taking different topological indices as edge weights for example Zagreb indices, modified Zagreb indices, augmented Zagreb index and Randić index. Using edge division of nanotube, we computed the stated entropies.

**KEYWORDS**

Nanotube; topological indices; weighted entropy; Zagreb indices; Randić index.

## Introduction

Chemical graph theory is the branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena. In chemical graph theory, a molecular graph is a simple graph in which atoms and chemical bonds between them are represented by vertices and edges respectively.

Over 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 [8]. And determining the complexity of the graphs has been used in various fields of sciences, including information theory, biology, chemistry and sociology.

We have different applications of graph entropy in communications and economics. The concept of graph entropy has been used as a weighted graph to solve the problem of weighted chemical graph entropy by using a special information functional [6]. Some degree-based indices are characterized by investigating the extremes of the entropy of certain class of graphs [9] and [5]. In this paper, we computed 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 Randić 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 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 it can also be applied to obtain lower bounds in graph covering problems.

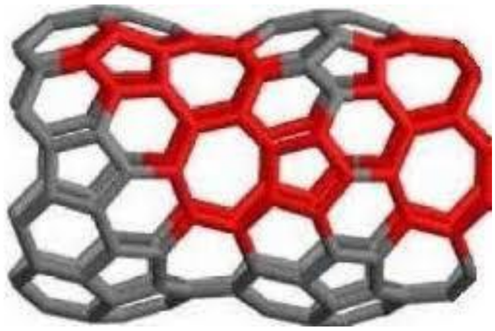

**FIGURE 1** The cylinder lattice of $HAC_5C_7[p;q]$ nanotube [10-22]

**Definition 1.** (Entropy). Let the probability density function

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

then the entropy of graph G is defined as

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

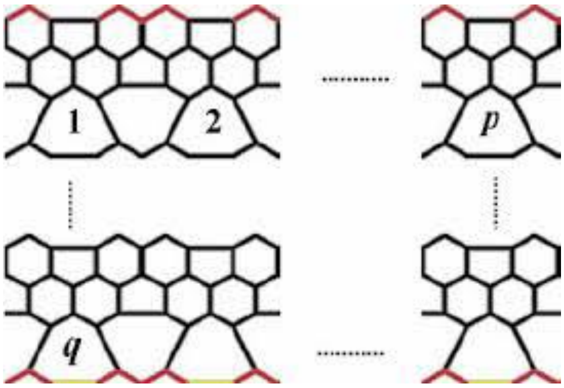


**FIGURE 2** The 2-dimensional lattice of $HAC_5C_7[p;q]$ nanotube [10-22]

## $HAC_5C_7[p;q]$ Nanotube

The molecular graphs of carbon nanotube $HAC_5C_7[p;q]$ are shown in Figure 1. The structures of this nanotube consist of cycles $C_5$ and $C_7$ ($C_5C_7$) net, which is a trivalent decoration constructed by alternating $C_5$ and $C_7$ by different compound. It can cover either a cylinder or a torus.

This nanotube consists of heptagon and pentagon nets. Since there are pq heptagons ($C_7$) in H and the size of all $C_5C_7$ nets is 8, the size of vertex set of $HAC_5C_7[p;q]$ nanotube (p,q) is equal to $n=V(HAC_5C_7[p;q])=8pq+2p$. On the other hand, there exist p numbers of vertices as degree 2 in the first row of H and p numbers of vertices in the end row of H.

It can be observed from Figure2 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.

## Entropies of $HAC_5C_7[p;q]$ Nanotube

**Theorem 1.** The entropy of $HAC_5C_7[p;q]$ with first Zagreb weight is

$$I(HAC_5C_7, M_1) = log(72pq+8p) - \frac{1}{72pq+8p}[56.0268900pq + 4.641584p]$$

**Proof.** By definition, we have

$M_1(HAC_5C_7[p;q])=72pq+8p;$

$$I(HAC_5C_7[p,q], M1) = \log(72pq+8p) - \frac{1}{72pq+8p}[|E_1|(2+2)\times log(2+2)]$$
$$+[|E_2|(2+3)\times log(2+3)] + |E_3|(3+3)\times log(3+3)]$$
$$= log(72pq+8p)\frac{1}{72pq+8p}[(0)(4\times log4)$$
$$+(4p)(5\times log5) + (12pq-2p)(6\times log6)]$$
$$= log(72pq+8p) - \frac{1}{72pq+8p}[13.979400p$$
$$+56.0268900pq - 9.337815p]$$
$$= log(72pq+8p) - \frac{1}{72pq+8p}[56.0268900pq + 4.641584p].$$

**Theorem 2.** The entropy of $HAC_5C_7[p;q]$ with second Zagreb weight is

$$I(HAC_5C_7[p,q], M_2) = log(108pq+6p) - \frac{1}{108pq+6p}[103.058191pq + 1.49926648p].$$

**Proof.** By definition, we have

$M_2(HAC_5C_7[p;q])=108pq+6p;$

$$I(HAC_5C_7[p,q], M_2) = log(108pq+6p) - \frac{1}{108pq+6p}[|E_1|(2.2)\times log(2.2) + |E_2|(3.2)$$
$$\times log(3.2)] + |E_3|(3.3)\times log(3.3)]$$

$$= log(108pq+6p) - \frac{1}{108pq+6p}[(0)(4log4)$$
$$+(4p)(6log6)+(12pq-2p)(9log9)]$$
$$= log(108pq+6p) - \frac{1}{108pq+6p}[18.67563p$$
$$+103.058191pq+17.176365p]$$
$$= log(108pq+6p) - \frac{1}{108pq+6p}[103.058191pq+1.49926648p].$$

**Theorem 3.** The entropy of HAC5C7[p;q] with Modified Second Zagreb index is

$$I(HAC_5C_7[p,q],^m M_2) = log(1.333pq+0.4444p)$$
$$-\frac{1}{1.333pq+0.4444p}[-1.272323pq-0.3067135p].$$

**Proof.** By definition, we have

$$I(HAC_5C_7[p,q],^m M_2) = 1.333pq+0.4444p.$$
$$I(HAC_5C_7[p,q],^m M_2) = log(1.333pq+0.4444p)$$
$$-\frac{1}{1.333pq+0.4444p}|E_1|(\frac{1}{2.2}\times log\frac{1}{2.2})$$
$$+|E_2|(\frac{1}{2.3}\times log\frac{1}{3.3})+(|E_3|(\frac{1}{3.3}\times log(\frac{1}{3.3})]$$
$$= log(1.333pq+0.4444p) - \frac{1}{1.333pq+0.4444p}$$
$$[(0)(\frac{1}{4})\times log\frac{1}{4}][(4p)\frac{1}{6}(\times log(\frac{1}{6}))+(12pq-2p)(\frac{1}{9})$$
$$\times log(\frac{1}{9}))] = log(1.333pq+0.4444p)$$
$$-\frac{1}{1.333pq+0.4444p}[-0.5187675p$$
$$-1.272323pq+0.212054p]$$
$$= log(1.333pq+0.4444p) - \frac{1}{1.333pq+0.4444p}$$
$$[-1.272323pq-0.3067135p].$$

**Theorem 4.** The entropy of $HAC_5C_7$[p;q] with Augmented Zagreb Index is

$$I[HAC_5C_7[p,q],A] = log(136.6875pq-20.609375p)$$
$$-\frac{1}{136.6875pq-20.609375p}[5.9707953pq-27.90379644p].$$

**Proof.** By definition, we have

$$A[HAC_5C_7[p,q]] = 136.6875pq-20.609375p$$
$$= log(136.6875pq-20.609375p)$$
$$-\frac{1}{136.6875pq-20.609375p}|E_1|[\frac{2.2}{2+2-2}]^3$$
$$\times log[\frac{2.2}{2+2-2^3}]]+[|E_2|[\frac{2.3}{2+3-2}]^3$$
$$\times log[\frac{2.3}{2+3-2^3}]+|E_3|[\frac{3.3}{3+3-2}]^3\times log(\frac{3.3}{3+3-2}]^3].$$
$$= log(136.6875pq-20.609375p)$$
$$-\frac{1}{136.6875pq-20.609375p}[(0)(2^3\times log2^3)$$
$$+(4p)[2^3\times log2^3]+(12pq-2p)[\frac{9}{4}]^3\times log[\frac{9}{4}]^3]$$
$$= log(136.6875pq-20.609375p)$$
$$-\frac{1}{136.6875pq-20.609375p}[28.898879p$$
$$+5.9707953pq-0.99513255p]$$
$$= log(136.6875pq-20.609375p)$$
$$-\frac{1}{136.6875pq-20.609375p}[5.9707953pq-27.90379644p]$$

**Theorem 5.** The entropy of $HAC_5C_7$[p;q] with Redefined First Zagreb weight is

$$I(HAC_5C_7, ReZG_1) = \log(432pq+28p)$$
$$-\frac{1}{432pq+28p}[-1.4087300pq-0.029142p].$$

**Proof.** By definition, we have

$$ReZG_1(HC_5C_7[p,q]) = 432pq+28p,$$
$$I(HAC_5C_7[p,q], ReZG_1) = \log(432pq+28p)$$
$$-\frac{1}{432pq+28p}[|E_1|[\frac{2+2}{2.2}\times\log\frac{2+2}{2.2}]$$
$$+[|E_2|[\frac{2+3}{2.3}\times\log\frac{2+3}{2.3}]+[|E_3|[\frac{3+3}{3.3}\times\log\frac{3+3}{3.3}]$$
$$= \log(432pq+28p) - \frac{1}{432pq+28p}[(0).[\frac{4}{4}\times\log\frac{4}{4}]$$
$$+[(4p).[\frac{5}{6}\times\log\frac{5}{6}]+[(12pq-2p).[\frac{2}{3}\times\log\frac{2}{3}]$$
$$= \log(432pq+28p) - \frac{1}{432pq+28p}[-0.26393p$$
$$-1.4087300pq+0.234788p]$$
$$= \log(432pq+28p) - \frac{1}{432pq+28p}$$
$$[-1.4087300pq-0.029142p].$$

**Theorem 6.** The entropy of $HAC_5C_7$[p;q] with Re-defined 2nd Zagreb weight is

$$I(HAC_5C_7, ReZG_2) = \log(18pq-1.8p)$$
$$-\frac{1}{18pq-1.8p}[3.16964266pq-0.1482037887p].$$

**Proof.** By definition, we have

$$ReZG_2(HC_5C_7[p,q]) = 18pq-1.8p,$$
$$I(HAC_5C_7[p,q], ReZG_2) = \log(18pq-1.8p)$$
$$-\frac{1}{18pq-1.8p}[|E_1|[\frac{2.2}{2+2}\times\log\frac{2.2}{2+2}]$$
$$+[|E_2|[\frac{2.3}{2+3}\times\log\frac{2.3}{2+3}]+[|E_3|[\frac{3.3}{3+3}\times\log\frac{3.3}{3+3}]]$$

$$= \log(18pq-1.8p)-\frac{1}{18pq-1.8p}[(0).[\frac{4}{4}\times\log\frac{4}{4}]$$
$$+[(4p).[\frac{6}{5}\times\log\frac{6}{5}]+[(12pq-2p).[\frac{3}{2}\times\log\frac{3}{2}]]$$
$$= \log(18pq-1.8p)-\frac{1}{18pq-1.8p}[0.38006998p$$
$$+3.16964266pq-0.52827377p]$$
$$= \log(18pq-1.8p)-\frac{1}{18pq-1.8p}$$
$$[3.16964266pq-0.1482037887p].$$

**Theorem 7.** The entropy of $HAC_5C_7[p;q]$ with Re-defined 3rd Zagreb weight is

$$I(HAC_5C_7[p,q],ReZG_3)=\log(648pq+12p)$$
$$-\frac{1}{648pq+12p}[1122.591156pq-9.84397606088p].$$

**Proof.** By definition, we have

$$ReZG_3(HAC_5C_7[p,q])=648pq+12p,$$
$$I(HAC_5C_7[p,q],ReZG_3)=\log(648pq+12p)$$
$$-\frac{1}{648pq+12p}[|E_1|[(2.2)(2+2)\times\log(2.2)(2+2)]$$
$$+|E_2|[(2.3)(2+3)\times\log(2.3)(2+3)]$$
$$+[|E_3|[(3.3)(3+3)\times\log(3.3)(3+3)]]$$
$$= \log(648pq+12p)-\frac{1}{648pq+12p}[(0)\times16\log16$$
$$+(4p)\times30\log30+(12pq-2p)\times54\log54]$$
$$= log(648pq+12p)-\frac{1}{648pq+12p}[177.25455p$$
$$+1122.591156pq-187.09852606p]$$
$$= log(648pq+12p)-\frac{1}{648pq+12p}$$
$$[1122.591156pq-9.84397606088p].$$

**Theorem 8.** For the straight chain of pentagons, the weighted entropy with Randić index weight is

$$I(G,R)=\log(1.4831632476n+1)+0.5525899692$$
$$+\frac{0.0842380208}{n}+0.63575975n.$$

Proof. Using the definition of Randić index we have

$$R(G(n,S))=1.48316324276n+1I(G,R(n,S))$$
$$=\log(R)-\frac{1}{R}\sum_{gh\in E(G)}(\frac{1}{\sqrt{d_g.d_h}}\log\frac{1}{\sqrt{d_g.d_h}})$$
$$=\log(1.48316324276n+1)-\frac{1}{1.4831632476n+1}$$
$$(4.(\frac{1}{\sqrt{2.2}}\log\frac{1}{\sqrt{2.2}})+2n.(\frac{1}{\sqrt{2.3}}\log\frac{1}{\sqrt{2.3}})$$
$$+(2n-3).(\frac{1}{\sqrt{3.3}}\log\frac{1}{\sqrt{3.3}}))$$
$$=\log(1.48316324276n+1)-(1+\frac{0.6742346142}{n})$$
$$(-0.6020599913-0.3176789177n$$
$$-0.3180808365n+0.4771212548)$$
$$=\log(1.48316324276n+1)-(-0.6357597542n$$
$$-0.1249387365-0.4286512326-\frac{0.0842380208}{n})$$
$$=\log(1.48316324276n+1)+0.5535899692$$
$$+\frac{0.0842380208}{n}+0.6357597542n.$$

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