Received: 20 October 2020 | Revised: 26 November 2020 | Accepted: 10 December 2020
DOI: 10.22034/ecc.2021.120281

Eurasian Chemical Communications SAMI

FULL PAPER

Weighted entropies of Tuc_5c_8[P;Q] nanotube with the degree based topological indices as weights

Farkhanda Afzal[a] |Faiza Afzal[b] |Deeba Afzal[b,*] |Mohammad Reza Farahani[c] |Murat Cancan[d] |Süleyman Ediz[d]

[a]*MCS, National University of Sciences and Technology, Islamabad, Pakistan*

[b]*Department of Mathematics and Statistics, The University of Lahore, Lahore, 54000, Pakistan*

[c]*Department of Applied Mathematics, Iran University of Science and Technology, Tehran, Iran*

[d]*Faculty of Education, Van Yuzuncu Yıl University, Zeve Campus, Tuşba, 65080, Van, Turkey*

***Corresponding Author:**
Deeba Afzal
Email: deebafzal@gmail.com
Tel.: +923351572532

The entropy of a graph is a function depending both on the graph itself and on a probability distribution on its vertex set. This graph function originated in 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. In this article, we captured the symmetry present in the structure of molecular graph of nanotube. We computed entropies of TUC_5C_8[p;q] nanotube taking some degree-based topological indices as edge weights.

KEYWORDS

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

Introduction

The entropy of a graph is a function depending both on the graph itself and on a probability distribution on its vertex set. This graph function originated in the problem of source coding in information theory and was introduced by J. Korner 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. Chemical reaction network theory is an area of applied mathematics that attempts to model the behavior of real world chemical systems. Since its foundation in the 1960s, it has attracted a growing research community, mainly due to its applications in biochemistry and theoretical chemistry. It has also attracted interest of pure mathematicians due to the interesting problems that arise from the mathematical structures involved.

Topological indices are arithmetic numbers about a graph of the chemical molecules [1-13]. Each molecule is canonically represented by a set of topological indices. Topological descriptors are derived from hydrogen-suppressed molecular graphs. Here, we computed weighted entropies of TUC_5C_8[p;q] using some degree based topological indices.

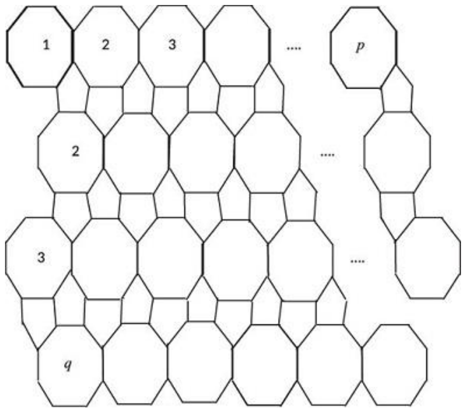

FIGURE 1 The 2-dimensional view of $TUC_5C_8[p;q]$ nanotube.

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

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

$TUC_5C_8[p;q]$ Nanotube

In the molecular graph of $TUC_5C_8[p;q]$ with G=(V,E) there are two types of vertices in the graph G; namely degrees 2 and 3 as seen from the Figure 1.

Let G=(V,E) be the $TUC_5C_8[p;q]$. Note that here p denotes the number of C_5C_8 nets horizontally and q denotes the tube levels. The 2D lattice graph of $TUC_5C_8[p;q]$ is shown in Figure 1.

There are 3 kinds of edges in $TUC_5C_8[p;q]$ as follows.

$E_1=\{uv \in E(TUC_5C_8)[p;q]: d_u=2; d_v=2\}$;

$E_2=\{uv \in E(TUC_5C_8)[p;q]: d_u=3; d_v=2\}$;

$E_3=\{uv \in E(TUC_5C_8)[p;q]): d_u=3; d_v=3\}$;

Such that $|E_1|=2p; |E_2|=4p; |E_3|=6pq-2p$.

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

Entropies of $TUC_5C_8[p;q]$ Nanotube

In this section we present our results.

Theorem 1. The entropy of $TUC_5C_8[p;q]$ with first Zagreb weight is

$$I(TUC_5C_8[p,q], M_1) = log(36pq+16p) - \frac{1}{36pq+16p}[168.08067008pq - 9.4580650].$$

Proof. By Definition 1, we have

$M_1(TUC_5C_8[p;q])=4p(9q+4)$;

$$I(TUC_5C_8[p,q], M_1) = log(36pq+16p)[|E_1|[(2+2)$$
$$\times \log(2+2)] + |E_2|[(2+3)\times\log(2+3)]$$
$$+|E_3[(3+3)\times\log(3+3)]$$
$$= log(36pq+16p) - \frac{1}{36pqq+16p}[(2p)[4\times log4]$$
$$+(4p)[5\times log5] + (6pq-2p)[6\times\log 6]$$
$$= log(36pq+16p) - \frac{1}{36pq+16p}[(2p)\times[4log4]$$
$$+(4p)[5log5] + (36pq)\times[6log6] - (2p)\times[6log6]$$
$$= log(36pq+16p) - \frac{1}{36pq+16p}$$
$$[168.08067008pq - 9.45806501p].$$

Theorem 2. The entropy of $TUC_5C_8[p;q]$ with second Zagreb weight is

$$PI(TUC_5C_8[p,q], M_2) = log(54pq+14p)$$
$$-\frac{1}{54pq+14p}[51.52909550pq - 7.6782692773p].$$

Proof. By Definition 1, we have

$M_2(TUC_5C_8[p;q])=2p(27q+7)$;

$$I(TUC_5C_8[p,q], M_2) = log(54pq+14p)$$
$$-\frac{1}{54pq+14}[|E_1|[(2.2)\times\log(2.2)] + |E_2|[(2.3)$$
$$\times\log(2.3)] + |E_3|[(3.3)\times\log(3.3)]]$$
$$= log(54pq+14p) - \frac{1}{54pq+14}[(2p)(4\times\log 4)$$
$$+(4p).(6\times\log 6) + (6pq-2p)(9\times\log 9)]$$
$$= log(54pq+14p) - \frac{1}{54pq+14}[2p(2.40823996)$$
$$+(4p)(4.6689075027)(6pq-2p)(8.588182585)]$$
$$= log(54pq+14p) - \frac{1}{54pq+14}[4.81647992p$$
$$+4.6689075027p + 51.52909551pq$$
$$-7.6782642773p]$$
$$= log(54pq+14p) - \frac{1}{54pq+14}$$
$$[51.52909551pq - 7.6782692773p].$$

Theorem 3. The entropy of $TUC_5C_8[p;q]$ with second Modified Zagreb weight is

$$I(TUC_5C_8[p,q],^m M_2) = log(0.24p + 1.6666pq)$$
$$-\frac{1}{0.24p+1.6666pq}[-0.63616167pq - 0.005683629p].$$

Proof. By Definition 1, we have

${}^mM(TUC_5C_8[p;q])=0:24p+1:6666pq$

$$I(TUC_5C_8[p,q],^m M) = log(0.24p + 1.6666pq)$$
$$-\frac{1}{0.24p+1.6666pq}[|E_1|[\frac{1}{2.2}\times\log\frac{1}{2.2}]$$
$$+|E_2|[\frac{1}{2.3}\times\log\frac{1}{2.3}] + |E_3|[\frac{1}{3.3}\times\log\frac{1}{3.3}]]$$

$$= log(0.24p+1.6666pq) - \frac{1}{0.24p+1.6666pq}$$
$$[(2p)(\frac{1}{4}\times\log\frac{1}{4})+(4p)(\frac{1}{6}\times\log\frac{1}{6})$$
$$+(6pq-2p)(\frac{1}{9}\times\log\frac{1}{9})]$$
$$= log(0.24p+1.6666pq) - \frac{1}{0.24p+1.6666pq}$$
$$[2p(-0.15051499783)+(4p)(-0.12969187506)$$
$$+(6pq-2p)(-0.10602694549)]$$
$$= log(0.24p+1.6666pq) - \frac{1}{0.24p+1.6666pq}$$
$$[-0.30102999p-0.518767500p$$
$$-0.63616167pq+0.21205389p]$$
$$= log(0.24p+1.6666pq) - \frac{1}{0.24p+1.6666pq}$$
$$[-0.63616167pq-0.005683629p].$$

Theorem 4. The entropy of *TUC5C8* with Augmented Zagreb weight is

$$I(TUC_5C_8, AZ) = log(25.781p+68.343pq)$$
$$-\frac{1}{25.781p+68.343pq}[2.98539765pq-16.3531868p].$$

Proof. By Definition 1, we have

AZ(TUC_{5}C_{8})=48p+22.78125p(3q-1),

$$I(TUC_5C_8, AZ) = log(25.781p+68.343pq)$$
$$-\frac{1}{25.781p+68.343pq}[|E_1|(\frac{2.2}{2+2-2^3})$$
$$\times\log(\frac{2.2}{2+2-2})^3]+[|E_2|(\frac{2.3}{2+3-2})^3$$
$$\times\log(\frac{2.3}{2+3-2})^3]+|E_3|[(\frac{3.3}{3+3-2})^3\times\log(\frac{3.3}{3+3-2})^3]$$
$$= log(25.781p+68.343pq) - \frac{1}{25.781p+68.343pq}$$
$$[(2p)(2^3\times\log 2^3)(4p)(2^3\times\log 2^3)$$
$$+(6pq-2p)(\frac{9}{4})^3\times\log(\frac{9}{4})^3]$$
$$= log(25.781p+68.343pq) - \frac{25.781p}{68.343pq}$$
$$[14.4494398p+28.898879p+2.98539765pq$$
$$-0.9965132p] = log(25.781p+68.343pq)$$
$$-\frac{1}{25.781p+68.343pq}[2.98539765pq-16.3531868p]$$

Theorem 5. The entropy of $TUC_5C_8[p;q]$ with Hyper second Zagreb weight is

$$I(TUC_5C_8[p,q], H_2) = log(486pq+14p)$$
$$-\frac{1}{486pq+14p}[927.5237pq-8.003334p].$$

Proof. By Definition 1, we have

$$H_2(TUC_5C_8[p,q]) = 486pq+14p,$$
$$I(TUC_5C_8[p,q], H_2) = \log(486pq+14p)$$
$$-\frac{1}{486pq+14p}[|E_1|[(2.2)^2\times\log(2.2)^2]$$
$$+[|E_2|[(2.3)^2\times\log(2.3)^2]+[|E_3|[(3.3)^2\times\log(3.3)^2]]$$
$$= \log(972pq-18p) - \frac{1}{972pq-18p}[(2p)\times 4^2\log 4^2$$
$$+(4p)\times 6^2\log 6^2+(6pq-2p)\times 9^2\log 9^2]$$
$$= log(486pq+14p) - \frac{1}{486pq+14p}[77.0636789p$$
$$+224.107560p+927.5237pq-309.174573p]$$
$$= log(486pq+14p) - \frac{1}{486pq+14p}$$
$$[927.5237pq-8.003334p].$$

Theorem 6. The entropy of $TUC_5C_8[p;q]$ with Redefined First Zagreb weight is

$$I(TUC_5C_8[p,q], ReZG_1) = log(216pq+60p)$$
$$-\frac{1}{216pq+60p}[-0.704365pq-0.029142p].$$

Proof. By Definition 1, we have

$$ReZG_1(TUC_5C_8[p,q]) = 216pq+60p,$$
$$I(TUC_5C_8[p,q], ReZG_1) = log(216pq+60p)$$
$$-\frac{1}{216pq+60p}[|E_1|[\frac{2+2}{2.2}\times\log\frac{2+2}{2.2}]$$
$$+[|E_2|[\frac{2+3}{2.3}\times\log\frac{2+3}{2.3}]+[|E_3|[\frac{3+3}{3.3}\times\log\frac{3+3}{3.3}]$$
$$= \log(216pq+60p) - \frac{1}{216pq+60p}[(2p).[\frac{4}{4}\times\log\frac{4}{4}]$$
$$+[(4p).[\frac{5}{6}\times\log\frac{5}{6}]+[(6pq-2p).[\frac{2}{3}\times\log\frac{2}{3}]$$
$$= \log(216pq+60p) - \frac{1}{216pq+60p}[-0.26393p$$
$$-0.704365pq+0.234788p]$$
$$= \log(216pq+60p) - \frac{1}{216pq+60p}$$
$$[-0.704365pq-0.029142p].$$

Theorem 7. The entropy of $TUC_5C_8[p;q]$ with Re-defined 2nd Zagreb weight is

$$I(TUC_5C_8[p,q], ReZG_2) = log(9pq-3.8p)$$
$$-\frac{1}{9pq-3.8p}[1.58482133pq-0.1482037p].$$

Proof. By Definition 1, we have

$ReZG_2(TUC_5C_8[p,q]) = 9pq - 3.8p,$

$I(TUC_5C_8[p,q], ReZG_2) = \log(9pq - 3.8p)$

$-\frac{1}{9pq-3.8p}[|E_1|[\frac{2.2}{2+2}\times\log\frac{2.2}{2+2}]$

$+[|E_2|[\frac{2.3}{2+3}\times\log\frac{2.3}{2+3}]+[|E_3|[\frac{3.3}{3+3}\times\log\frac{3.3}{3+3}]]$

$= \log(9pq-3.8p) - \frac{1}{9pq-3.8p}[(0).[\frac{4}{4}\times\log\frac{4}{4}]$

$+[(4p).[\frac{6}{5}\times\log\frac{6}{5}]+[(12pq-2p).[\frac{3}{2}\times\log\frac{3}{2}]]$

$= \log(9pq-3.8p) - \frac{1}{9pq-3.8p}[0.38006998p$

$+1.58482133pq - 0.52827377p]$

$= \log(9pq-3.8p) - \frac{1}{9pq-3.8p}$

$[1.58482133pq - 0.1482037p].$

Theorem 8. The entropy of $TUC_5C_8[p;q]$ with Re-defined 3rd Zagreb weight is

$I(TUC_5C_8[p,q], ReZG_3) = log(324pq + 44p)$

$-\frac{1}{324pq+44p}[561.2955pq + 28.687869p].$

Proof. By Definition 1, we have

$ReZG_3(TUC_5C_8[p,q]) = 324pq + 44p,$

$I(TUC_5C_8[p,q], ReZG_3) = \log(324pq + 44p)$

$-\frac{1}{324pq+44p}[|E_1|[(2.2)(2+2)\times\log(2.2)$

$(2+2)]+|E_2|[(2.3)(2+3)\times\log(2.3)(2+3)]$

$+[|E_3|[(3.3)(3+3)\times\log(3.3)(3+3)]]$

$= \log(324pq+44p) - \frac{1}{324pq+44p}$

$[(2p)\times 16\log 16 + (4p)\times 30\log 30$

$+(6pq-2p)\times 54\log 54]$

$= log(324pq+44p) - \frac{1}{324pq+44p}[38.531839p$

$+177.25455p - 561.2955pq - 187.09852p]$

$= log(324pq+44p) - \frac{1}{324pq+44p}$

$[561.2955pq + 28.687869p].$

Acknowledgments

The authors would like to thank the reviewers for their helpful suggestions and comments.

Orcid:

Farkhanda Afzal:
https://orcid.org/0000-0001-5396-7598
Deeba Afzal:
https://orcid.org/0000-0001-5268-7260
Mohammad Reza Farahani:
https://orcid.org/0000-0003-2969-4280
Murat Cancan:
https://orcid.org/0000-0002-8606-2274
Süleyman Ediz:
https://orcid.org/0000-0003-0625-3634

References

[1] F. Afzal, S. Hussain, D. Afzal, S. Razaq, *J. Inf. Opt. Sci.*, **2020**, *41*, 1061–1076.

[2] M. Cancan, S. Ediz, H. Mutee-Ur-Rehman, D. Afzal, *J. Inf. Opt. Sci.*, **2020**, *41*, 1117-1131.

[3] M. Cancan, S. Ediz, M.R. Farahani, *Eurasian Chem. Commun.*, **2020**, *2*, 641-645.

[4] A.Q. Baig, M. Naeem, W. Gao, J.B. Liu, *Eurasian Chem. Commun.*, **2020**, *2*, 634-640.

[5] F. Afzal, M.A. Razaq, D. Afzal, S. Hameed, *Eurasian Chem. Commun.*, **2020**, *2*, 652-662.

[6] M. Alaeiyan, C. Natarajan, G. Sathiamoorthy, M.R. Farahani, *Eurasian Chem. Commun.*, **2020**, *2*, 646-651.

[7] H. Yang, X. Zhang, *J. D. Math. Sci. and Cryp.*, **2018**, *21*, 1495-1507.

[8] M. Imran, S.A. Bokhary, S. Manzoor, M.K. Siddiqui, *Eurasian Chem. Communm.*, **2020**, *2*, 680-687.

[9] Z. Ahmad, M. Naseem, M.K. Jamil, Sh. Wang, M.F. Nadeem, *Eurasian Chem. Commun.*, **2020**, *2*, 712-721.

[10] Z. Ahmad, M. Naseem, M.K. Jamil, M.K. Siddiqui, M.F. Nadeem. *Eurasian Chem. Commun.*, **2020**, *2*, 663-671.

[11] M. Cancan, S. Ediz, M.R. Farahani, *Eurasian Chem. Commun.*, **2020**, *2*, 641-645.

[12] A.Q. Baig, M. Naeem, W. Gao, J.B. Liu, *Eurasian Chem. Commun.*, **2020**, *2*, 634-640.

[13] F. Afzal, M.A. Razaq, D. Afzal, S. Hameed, *Eurasian Chem. Commun.*, **2020**, *2*, 652-662.

[14] B.Y. Yang, Y.N. Yen, *Adv. Appl. Math.*, **1995**, *16*, 72-94.

[15] C.E. Shannon, *Bell. System Tech. J.*, **1948**, *27*, 379-423.
[16] C.E. Shannon, W. Weaver, *Univ. Illinois Press, Urbana.*, **1949**, *17,* 1-117.
[17] E. Trucco, *Bull. Math. Biol.*, **1965**, *18*, 129-135.
[18] K. Xu, K.C. Das, S. Balachandran, *MATCH Commun. Math. Comput. Chem.*, **2014**, *72*, 641-654.
[19] M.M. Dehmer, N.N. Barbarini, K.K. Varmuza, A.A. Graber, *BMC Structural Bio.*, **2010**, *10*, 18-34.
[20] N.P. Rao, P.A. Laxmi, *Appl. Sci.*, **2008**, *2*, 2443-2457.
[21] N. Rashevsky, *Bull. Math. Biophys.*, **1955**, *17*, 229-235.
[22] S. Ji, X. Li, B. Huo, *MATCH Commun. Math. Comput. Chem.*, **2014**, *72*, 723-732.

How to cite this article: Farkhanda Afzal, Faiza Afzal, Deeba Afzal*, Mohammad Reza Farahani, Murat Cancan, Süleyman Ediz. Weighted entropies of $Tuc_5c_8[P;Q]$ nanotube with the degree based topological indices as weights**.** *Eurasian Chemical Communications*, 2021, 3(1), 14-18. **Link:** http://www.echemcom.com/article_120281.html