Harmonic Temperature Index of Certain Nanostructures

Kishori P. Narayankar.[#1], Afework Teka Kahsay[*2], Dickson Selvan.[+3]

[#]Assistant Professor, Department of Mathematics, Mangalore University
[*,+]Research Scholars, Department of Mathematics, Mangalore University
Mangalagangothri – 574199, India

Abstract −*In the study of $QSPR/QSAR$, topological indices such as Zagreb index, Harmonic index, atom-bond connectivity index are exploited to estimate the bioactivity of chemical compounds. Inspired by many degree based topological indices, we propose here a new topological index, called the Harmonic temperature index $HTI(G)$ of a molecular graph G, which shows good correlation with entropy, acentric factor, enthalpy of vaporization and standard enthalpy of vaporization of an octane isomers. In this paper we compute the Harmonic temperature index $HTI(G)$ of line graphs of subdivision graphs of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.*

Keywords− *Temperature of a vertex, HarmonicTemperature index, nanostructures.*

I. Introduction

Molecular descriptors are playing significant role in chemistry, pharmacology, etc.Among them, topological indices have a prominent place [1]. There are numerousof topological descriptors that have found some applications in theoretical chemistry, especially in QSPR/QSAR research [2,3,4]. Within all topological indices, those of the most investigated are the descriptors based on the valences of atoms in molecules (in graph-theoretical notions degrees *of vertices of graph*).

Topological indices are numerical parameters of a graph which are invariant undergraph isomorphism.For a collection of recent results on topological indices, interested readers can refer the articles [5,6,7].

Let G be a connected graph of order n and size m. Let $V(G)$ and $E(G)$ be its vertex and edge sets, respectively. The edge joining the vertices u and v is denoted by uv. The *degree* of a vertex u in a graph G is the number of edges incidence to u and is denoted by d_u or $d(u)$.

The temperature of a vertex u of a connected graph G is defined by SiemionFajtlowiczas [8].

$$T(u) = \frac{d_u}{n - d_u}$$

where d_u is the degree of a vertex u, and n is order of graph G.

Harmonic index is defined for the first time by S. Fajtlowicz in [11]. The Harmonic index of a graph G is defined as:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}$$

Recently, Kishori P. N. and Dickson S. has introduced temperature index of a graph in [10] and is defined as $\sum_{uv \in E(G)} [T_u + T_v]$ and we extend this study for Harmonic temperature index.Inspired by the work on degree based topological indices and Harmonic index, we now define the Harmonic temperature index $HTI(G)$ of a molecular graph G as follows.

$$HTI(G) = \sum_{uv \in E(G)} \frac{2}{T_u + T_v}$$

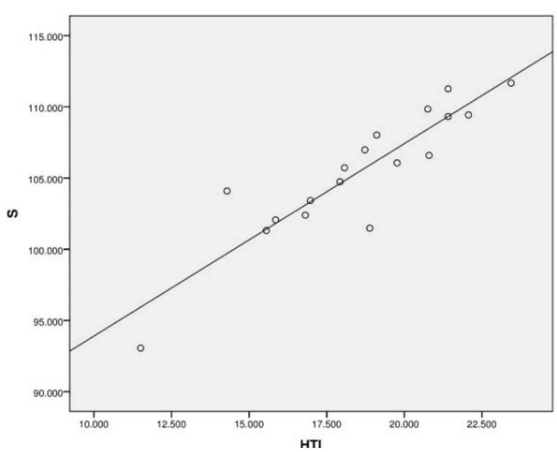
where T_u and T_v are the temperature of the vertex u and v, respectively.

II. On Chemical Applicability of the Harmonic Temperature Index

In this section we will discuss the regression analysis of entropy (S), acentric factor (AcentFac), enthalpy of vaporization (HVAP) and standard enthalpy of vaporization (DHVAP) of an octane isomers on the Harmonic temperature index of the corresponding molecular graph. The productivity of HTI was tested using a dataset of octane isomers, found at http://www.moleculardescriptors.eu/dataset.htm. It is shown that the HarmonicT-index has a good correlation with the entropy $(\mathrm{R} = 0.902)$, acentric factor$(\mathrm{R} = 0.941)$, standard enthalpy of vaporization $(\mathrm{R} = 0.902)$ and enthalpy of vaporization $(\mathrm{R} = 0.962)$ of octane isomers.

Table I: Experimental Values of the Entropy, Acentric Factor, Enthalpy of Vaporization, Standard Enthalpy of Vaporization and the Corresponding Values of Harmonic Temperature Index of Octane Isomers.

Alkane	S	AcentFac	HVAP	DHVAP	HTI
n-octane	111.67	0.397898	73.19	9.915	23.436
2-methyl-heptane	109.84	0.377916	70.3	9.484	20.753
3-methyl-heptane	111.26	0.371002	71.3	9.521	21.409
4-methyl-heptane	109.32	0.371504	70.91	9.483	21.409
3-ethyl-hexane	109.43	0.362472	71.7	9.476	22.065
2,2-dimethyl-hexane	103.42	0.339426	67.7	8.951	16.970
2,3-dimethyl-hexane	108.02	0.348247	70.2	9.272	19.110
2,4-dimethyl-hexane	106.98	0.344223	68.5	9.029	18.727
2,5-dimethyl-hexane	105.72	0.35683	68.6	9.051	18.071
3,3-dimethyl-hexane	104.74	0.322596	68.5	8.973	17.927
3,4-dimethyl-hexane	106.59	0.340345	70.2	9.316	20.794
2-methyl-3-ethyl-pentane	106.06	0.332433	69.7	9.209	19.765
3-methyl-3-ethyl-pentane	101.48	0.306899	69.3	9.081	18.884
2,2,3-trimethyl-pentane	101.31	0.300816	67.3	8.826	15.553
2,2,4-trimethyl-pentane	104.09	0.30537	64.87	8.402	14.288
2,3,3-trimethyl-pentane	102.06	0.293177	68.1	8.897	15.854
2,3,4-trimethyl-pentane	102.39	0.317422	68.37	9.014	16.810
2,2,3,3-tetramethylbutane	93.06	0.255294	66.2	8.410	11.507



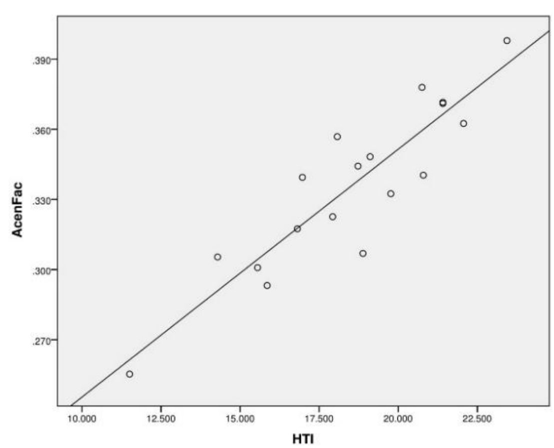
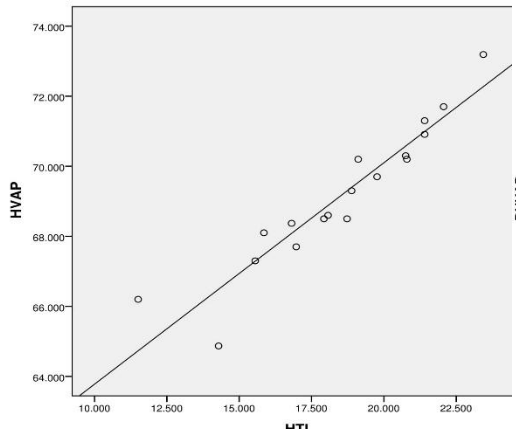


Fig 1.Fig 2.



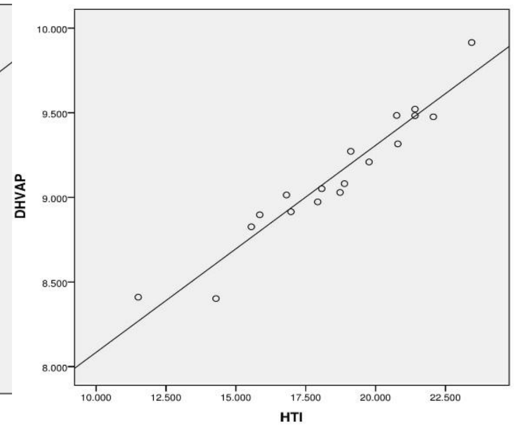


Fig 3.Fig 4.

Table II: Correlation Coefficient of HTI with Different Measurements

Harmonic Temperature index with	Correlation coefficient (R)
Entropy(S)	0.902
Acentric factor(AcentFac)	0.941
Enthalpy of vaporization(HVAP)	0.962
Standard enthalpy of vaporization(DHVAP)	0.902

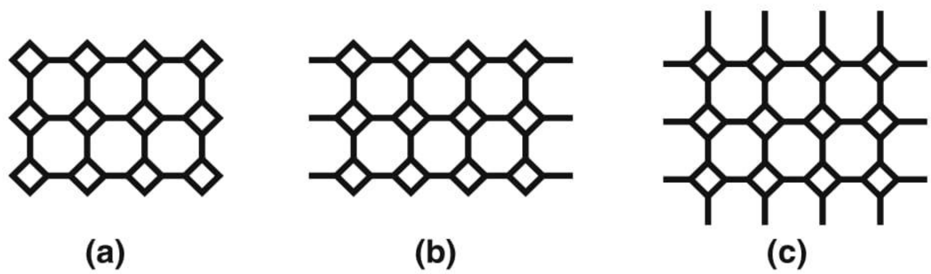


Figure 5:a) 2D-lattice of $TUC_4C_8[4,3]$. b) $TUC_4C_8[4,3]$nanotube. c) $TUC_4C_8[4,3]$nanotorus

Fig 1,2,3,4shows the Scatter plot between entropy(S), acentric factor (AcentFac), enthalpy of vaporization (HVAP), standard enthalpy of vaporization (DHVAP) of octane isomers and Harmonic temperature index respectively.The correlation coefficient (R) of the entropy, acentric factor, enthalpy of vaporization, standard enthalpy of vaporization with the Harmonic temperature index is shown in Table II.

III. Result for 2D-Lattice of $\mathbf{TUC_4C_8[p,q]}$

The line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$is shown in Figure 6(b).

Theorem 3.1. Let G be the line graph of the subdivision graph of 2D-Lattice of $TUC_4C_8[p,q]$.Then

$$HTI(G)=\frac{1}{3}(4-11p-11q+18pq)\big(-3+2(-p-q+6pq)\big)+(2+p+q)\big(-2+2(-p-q+6pq)\big)+\frac{-16+8p+8q}{\frac{3}{-3+2(-p-q+6pq)}+\frac{2}{-2+2(-p-q+6pq)}}$$

Proof. The subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$ and the graph G are shown in Fig. 6(a) and (b), respectively. In G there are total $2(6pq-p-q)$vertices among which $4(p+q)$vertices are of temperature $\frac{2}{2(6pq-p-q)-2}$ and allthe remaining vertices are of temperature$\frac{3}{2(6pq-p-q)-3}$. The total number of edges of G is $18pq-5p-5q$.Therefore we get the edge partition based on the temperature of thevertices as shown inTable III. Therefore

$$HTI(G) = \sum_{uv\in E(G)} \frac{2}{T_u + T_v}$$

$$HTI(G) = 2\left[\frac{(2p+2q+4)}{\frac{2}{2(6pq-p-q)-2}+\frac{2}{2(6pq-p-q)-2}} + \frac{(4p+4q-8)}{\frac{2}{2(6pq-p-q)-2}+\frac{3}{2(6pq-p-q)-3}} + \frac{18pq-11p-11q+4}{\frac{3}{2(6pq-p-q)-3}+\frac{3}{2(6pq-p-q)-3}}\right]$$

$$= \frac{1}{3}(4-11p-11q+18pq)\big(-3+2(-p-q+6pq)\big) + (2+p+q)\big(-2+2(-p-q+6pq)\big)\frac{-16+8p+8q}{\frac{3}{-3+2(-p-q+6pq)}+\frac{2}{-2+2(-p-q+6pq)}}.$$

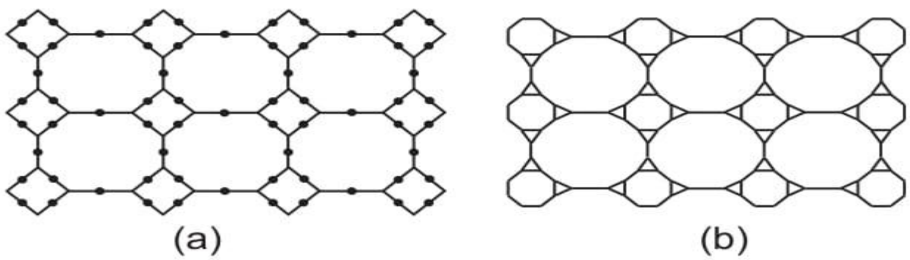


Figure 6: (a)subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$(b)line graph of sub-division graph of $TUC_4C_8[4,3]$.

Table III: The edge partition of the graphG.

(T_u, T_v), where$uv \in E(G)$	Number of edges
$\left(\frac{2}{2(6pq-p-q)-2}, \frac{2}{2(6pq-p-q)-2}\right)$	$2p+2q+4$
$\left(\frac{2}{2(6pq-p-q)-2}, \frac{3}{2(6pq-p-q)-3}\right)$	$4p+4q-8$
$\left(\frac{3}{2(6pq-p-q)-3}, \frac{3}{2(6pq-p-q)-3}\right)$	$18pq-11p-11q+4$

IV. Result for $TUC_4C_8[p,q]$Nanotube.

The line graph of the subdivision graph of $TUC_4C_8[p,q]$nanotube is shown inFigure 7(b).

Theorem 3.2. Let H be the line graph of the subdivision graph of ofTUC$_4$C$_8$[p, q] nanotube. Then

$$HTI(H) = \frac{1}{3}(-3-2p+12pq)(-11p+18pq) + p(-2-2p+12pq) + \frac{8p\big(-1+p(-1+6q)\big)\big(-3+2p(-1+6q)\big)}{-6+5p(-1+6q)}.$$

Proof. The subdivision graph of $TUC_4C_8[p,q]$ nanotube and the graph H are shown in Fig. 7(a) and (b),respectively. In H there are total $12pq-2p$vertices among which $4p$ vertices are of temperature $\frac{2}{(12pq-2p)-2}$ and all the remaining vertices are of temperature$\frac{3}{(12pq-2p)-3}$. The total number of edges of $H$is$18pq-5p$.Therefore we get the edge partition, based on the temperature of the vertices as shown inTable IV.Thus,

$$HTI(H) = 2\text{p}\left(\frac{2}{\left(\frac{2}{(12pq-2p)-2}\right)+\left(\frac{2}{(12pq-2p)-2}\right)}\right) + 4\text{p}\left(\frac{2}{\left(\frac{2}{(12pq-2p)-2}\right)+\left(\frac{3}{(12pq-2p)-3}\right)}\right) + \left(\frac{2(18pq-11p)}{\left(\frac{3}{(12pq-2p)-3}\right)+\left(\frac{3}{(12pq-2p)-3}\right)}\right)$$

$$= \frac{1}{3}(-3-2p+12pq)(-11p+18pq) + p(-2-2p+12pq) + \frac{8p\big(-1+p(-1+6q)\big)\big(-3+2p(-1+6q)\big)}{-6+5p(-1+6q)}.$$

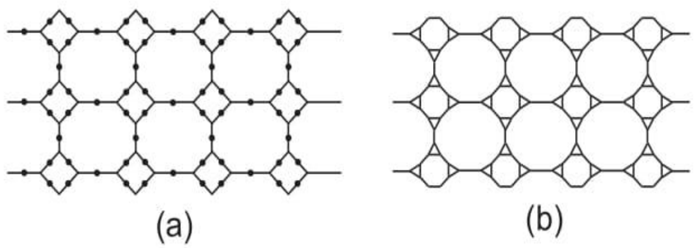


Figure 7: (a) subdivision graph of $TUC_4C_8[4,3]$ nanotube, (b) line graph of subdivision graph of $TUC_4C_8[4,3]$nanotube.

Table IV: The edge partition of the graphH.

(T_u, T_v), where $uv \in E(H)$	Number of edges
$\left(\frac{2}{(12pq-2p)-2}, \frac{2}{(12pq-2p)-2}\right)$	2p
$\left(\frac{2}{(12pq-2p)-2}, \frac{3}{(12pq-2p)-3}\right)$	4p
$\left(\frac{3}{(12pq-2p)-3}, \frac{3}{(12pq-2p)-3}\right)$	18pq − 11p

V. **Result for $\mathbf{TUC_4C_8[p,q]}$ Nanotorus**.

The line graph of the subdivision graph of $TUC_4C_8[p,q]$nanotorus is shown in Figure 8(b)

Theorem 3.3 Let K be the line graph of the subdivision graph of $TUC_4C_8[p,q]$nanotorus. Then

$$HTI(K) = 6pq(-3+12pq).$$

Proof. The subdivision graph of $TUC_4C_8[p,q]$ nanotorus and the graph K are shown in Fig. 8(a) and (b), respectively. In K there are total $12pq$ vertices all of them are of temperature $\frac{3}{(12pq)-3}$ The total number of edges of Kis $18pq$ .Therefore we get the edge partition, based on the temperature of the vertices as shown inTable V.Thus,

$$HTI(K) = (18\text{pq})\left(\frac{2}{\left(\frac{3}{12pq-3}\right)+\left(\frac{3}{12pq-3}\right)}\right)$$

$$= 6pq(-3+12pq)$$

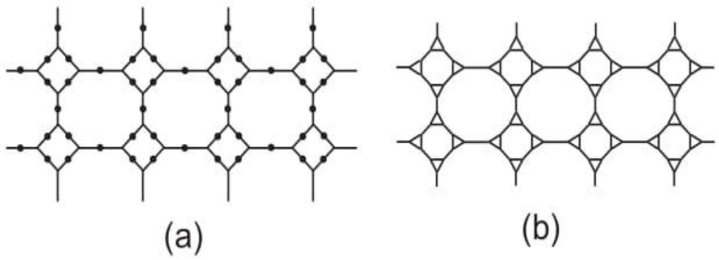


Figure 8: (a) Subdivision graph of $TUC_4C_8[4,2]$nanotorus, (b) line graph of subdivision graph of $TUC_4C_8[4,2]$ nanotorus.

Table V: The edge partition of the graph K.

(T_u, T_v), where $uv \in E(K)$	Number of edges
$\left(\frac{3}{(12pq)-3}, \frac{3}{(12pq)-3}\right)$	18pq

VI. Conclusion

In this paper, we have introduced a new topological index namely, Harmonic temperature index of molecular graph. It has been shown that this index can be used as predictive tool in QSPR/QSAR researches. We have obtained the expressions for the Harmonic Temperature index of the line graph of subdivision graph of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.

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