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GEOMETRIC ARITHMETIC TEMPERATURE INDEX OF CERTAIN NANOSTRUCTURES

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Abstract: In the study of $\mathbf{QSPR/QSAR}$, topological indices such as Zagreb index, geometric arithmetic 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 geometric arithmetic temperature index $\mathbf{GATI(G)}$ of a molecular graph $\mathbf{G}$, 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 geometric arithmetic temperature index $\mathbf{GATI(G)}$ of line graphs of subdivision graphs of $\mathbf{2D}$-lattice, nanotube and nanotorus of $\mathbf{TUC_4C_8[p,q]}$.

Keywords: Temperature of a vertex, geometric arithmetic temperature 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 numerous of topological descriptors that have found some applications in theoretical chemistry, especially in QSPR/QSAR research [2,3,4]. Within all topological indices one 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 under graph isomorphisms. For a collection of recent results on topological indices, we refer the interested reader to the articles [5,6,7].

Let G be a connected graph with n vertices and m edges. 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 Siemion Fajtlowicz as [8].

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

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

In [9], Vukiĉeviĉ et al. defined a new topological index “geometric arithmetic index” of a graph G denoted by $GA(G)$ and is defined by,

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u\, d_v}}{d_u + d_v}$$

Recently, Kishori P N and Dickson S has introduced temperature index of a graph in [10] and is defined as $\sum_{uv\in E(G)}[d_u + d_v]$ and we extend this study for geometric arithmetic temperature index.

Inspired by the work on degree based topological indices and geometric arithmetic index, we now define the geometric arithmetic temperature index $GATI(G)$ of a molecular graph G as follows.

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

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

II. ON CHEMICAL APPLICABILITY OF THE GEOMETRIC ARITHMETIC 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 geometric arithmetic temperature index of the corresponding molecular graph. The productivity of GATI was tested using a dataset of octane isomers, found at http://www.moleculardescriptors.eu/dataset.htm. It is shown that the geometric arithmetic T-index has a good correlation with the acentric factor $(R = 0.813)$, entropy $(R = 0.784)$, standard enthalpy of vaporization $(R = 0.855)$ and enthalpy of vaporization $(R = 0.816)$ of octane isomers.

Table 1: Experimental values of the entropy, acentric factor, enthalpy of vaporization, standard enthalpy of vaporization and the corresponding values of geometric arithmetic temperature index of octane isomers.

Alkane	**S**	**AcentFac**	**HVAP**	**DHVAP**	**GATI**
n-octane	111.67	0.397898	73.19	9.915	6.831
2-methyl-heptane	109.84	0.377916	70.3	9.484	6.446
3-methyl-heptane	111.26	0.371002	71.3	9.521	6.533
4-methyl-heptane	109.32	0.371504	70.91	9.483	6.533
3-ethyl-hexane	109.43	0.362472	71.7	9.476	6.620
2,2-dimethyl-hexane	103.42	0.339426	67.7	8.951	5.759
2,3-dimethyl-hexane	108.02	0.348247	70.2	9.272	5.233
2,4-dimethyl-hexane	106.98	0.344223	68.5	9.029	6.149
2,5-dimethyl-hexane	105.72	0.35683	68.6	9.051	6.063
3,3-dimethyl-hexane	104.74	0.322596	68.5	8.973	5.881
3,4-dimethyl-hexane	106.59	0.340345	70.2	9.316	6.320
2-methyl-3-ethyl-pentane	106.06	0.332433	69.7	9.209	6.320
3-methyl-3-ethyl-pentane	101.48	0.306899	69.3	9.081	6.000
2,2,3-trimethyl-pentane	101.31	0.300816	67.3	8.826	5.604
2,2,4-trimethyl-pentane	104.09	0.30537	64.87	8.402	5.372
2,3,3-trimethyl-pentane	102.06	0.293177	68.1	8.897	5.640
2,3,4-trimethyl-pentane	102.39	0.317422	68.37	9.014	5.933
2,2,3,3-tetramethylbutane	93.06	0.255294	66.2	8.410	4.959

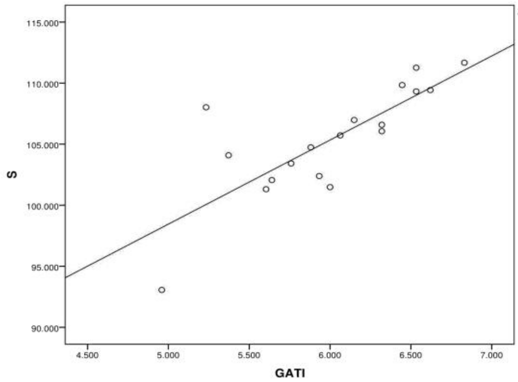

Fig.1

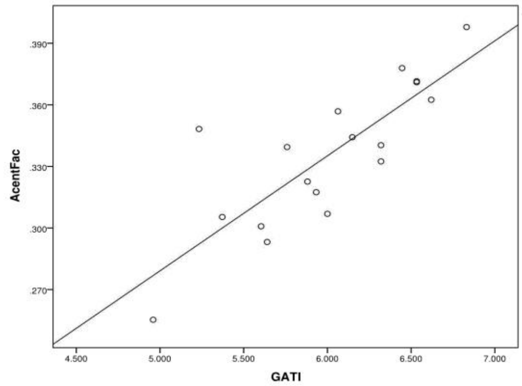

Fig.2

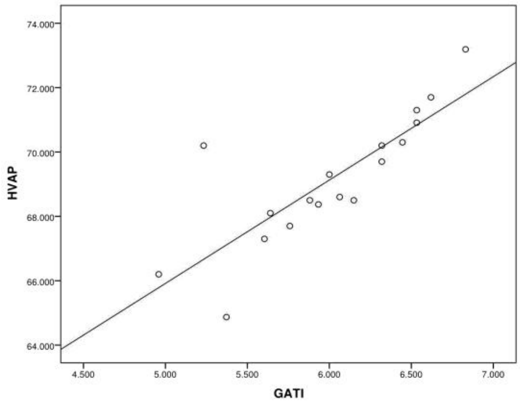

Fig.3

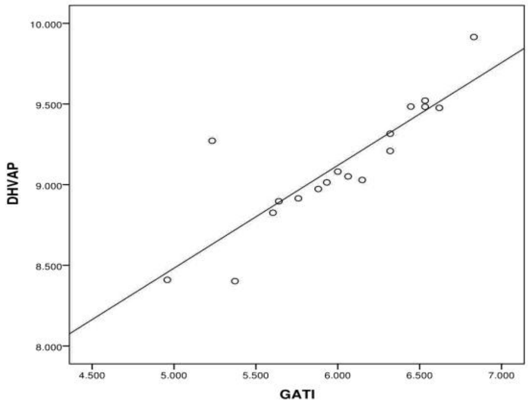

Fig.4

Fig 1,2,3,4 shows the Scatter plot between entropy (S), acentric factor (AcentFac), enthalpy of vaporization (HVAP), standard enthalpy of vaporization (DHVAP) of octane isomers and geometric arithmetic temperature index respectively.

Table 2. The correlation coefficient (R) of the entropy, acentric factor, enthalpy of vaporization, standard enthalpy of vaporization with the geometric arithmetic temperature index is as follows.

Geometric arithmetic temperature index with	**Correlation coefficient (R)**
Entropy(S)	0.784
Acentric factor(AcentFac)	0. 813
Enthalpy of vaporization(HVAP)	0. 816
Standard enthalpy of vaporization(DHVAP)	0. 855

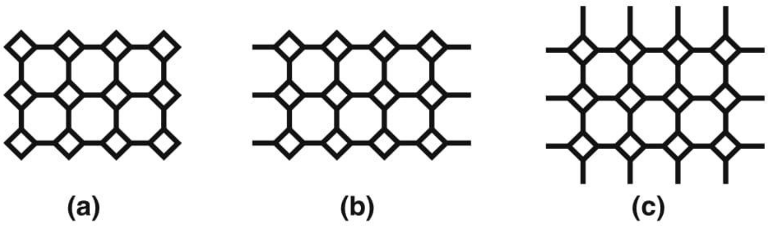

Figure 5: a) 2D-lattice of $TUC_4C_8[4,3]$. b) $TUC_4C_8[4,3]$ nanotube. c) $TUC_4C_8[4,3]$ nanotorus.

III. RESULT FOR 2D-LATTICE OF $TUC_4C_8[p,q]$

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

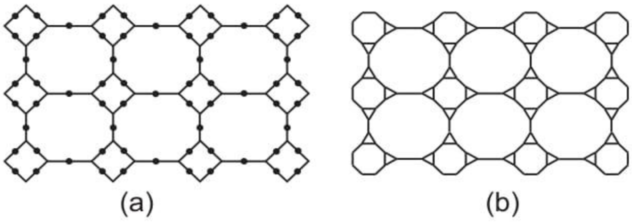

Figure 6: (a) subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$ (b) line graph of subdivision graph of $TUC_4C_8[4,3]$.

Table 3: The edge partition of the graph G.

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

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

$$GATI(G)=(2p+2q+4)+\frac{2(6pq-p-q-1)(12pq-2p-2q-3)\sqrt{\frac{3}{(6pq-p-q-1)(12pq-2p-2q-3)}}}{3pq-5p-5q-6}+(18pq-11p-11q+4).$$

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 remaining all the 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 the vertices as shown in Table 3. Therefore

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

$$GATI(G)=(2p+2q+4)+\frac{2(6pq-p-q-1)(12pq-2p-2q-3)\sqrt{\frac{3}{(6pq-p-q-1)(12pq-2p-2q-3)}}}{3pq-5p-5q-6}+(18pq-11p-11q+4).$$

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 in Figure 7(b).

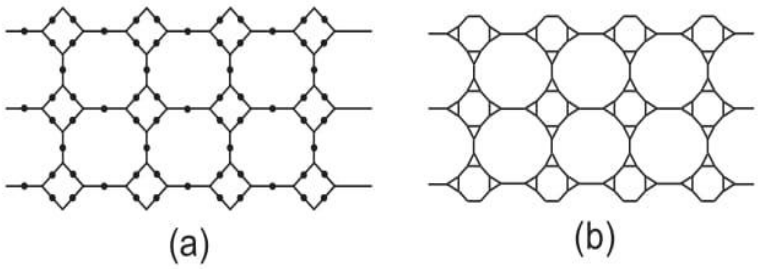

Figure 7: (a) subdivision graph of $TUC_4C_8[4,3]$ nanotube, (b) line graph of subdivision graph of $TUC_4C_8[4,3]$ nanotube.

Table 4: The edge partition of the graph H.

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

Theorem 3.2. Let H be the line graph of the subdivision graph of of $TUC_4C_8[p,q]$ nanotube. Then

$$GATI(H) = 2p + \frac{8p(12pq-2p-3)(12pq-2p-2)\sqrt{\frac{3}{(6pq-p-1)(12pq-2p-3)}}}{2(12pq-2p-3)+3(12pq-2p-2)} + 18pq - 11p\,.$$

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 remaining all the 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 in Table 4.

Therefore

$$GATI(H) = 2p + \frac{8p(12pq-2p-3)(12pq-2p-2)\sqrt{\frac{3}{(6pq-p-1)(12pq-2p-3)}}}{2(12pq-2p-3)+3(12pq-2p-2)} + 18pq - 11p.$$

V. RESULT FOR $TUC_4C_8[p,q]$ NANOTORUS.

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

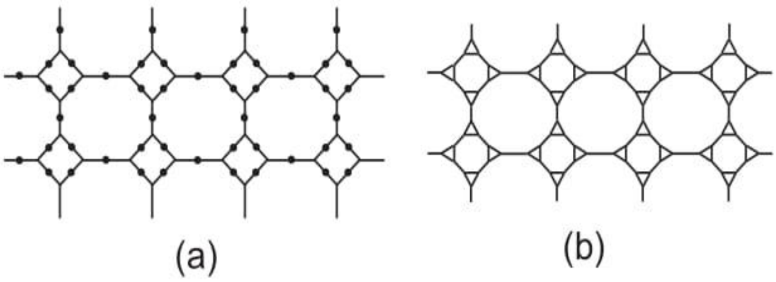

Figure 8: (a) subdivision graph of $\mathrm{TUC_4C_8}[4,2]$ nanotorus, (b) line graph of subdivision graph of $\mathrm{TUC_4C_8}[4,2]$ nanotorus.

Table 5: The edge partition of the graph K.

(T_uT_v) where uv ∈ E(K)	Number of edges
$\frac{3}{(12pq)-3}, \frac{3}{(12pq)-3}$	18pq

Theorem 3.3 Let K be the line graph of the subdivision graph of $\mathrm{TUC_4C_8}[\mathrm{p},\mathrm{q}]$ nanotorus. Then $GATI(K) = 18pq$.

Proof. The subdivision graph of $\mathrm{TUC_4C_8}[\mathrm{p},\mathrm{q}]$ 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 K is 18pq.Therefore we get the edge partition, based on the temperature of the vertices as shown in Table 5.

Therefore

$$GATI(K) = 18pq.2.\frac{\sqrt{\frac{3}{(12pq)-3}\cdot\frac{3}{(12pq)-3}}}{\frac{3}{(12pq)-3}+\frac{3}{(12pq)-3}}$$

$$GATI(K) = 18pq.$$

VI. CONCLUSION

In this paper, we have introduced a new topological index namely, geometric arithmetic 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 geometric arithmetic temperature index of the line graph of subdivision graph of 2D-lattice, nanotube and nanotorus of $\mathrm{TUC_4C_8}[\mathrm{p},\mathrm{q}]$.

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