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Atom bond connectivity temperature index

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Abstract. In the study of QSPR/QSAR, topological indices such as Zagreb index, Randic index and 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 atom bond connectivity temperature index $ABCT(G)$ 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 atom bond connectivity temperature index $ABCT(G)$ of line graphs of subdivision graphs of $2D-$lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.

Keywords. temperature of a vertex, atom bond connectivity temperature index, nanostructures.

1 Introduction

Molecular descriptors are playing significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [13]. There are numerous of topological descriptors that have found some applications in theoretical chemistry, especially in $QSPR/QSAR$research [2,6,7]. 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) [11].

Topological indices are numerical parameters of a graph which are invariant undergraph isomorphism. For a collection of recent results on topological indices, we refer the interested reader to the articles [1,3,5].

Let G be a connected graph of order n and size m. Let $V(G)$ and $E(G)$ be vertex and edge sets of G, respectively. An edge joining the vertices u and v is denoted by uv. The degree of a vertex u in a

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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 Fajtlowiczas [12].

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

where d_u is the degree of a vertex u and n is the size of a graph G. Ernesto Estrada et al. proposed a new index, nowadays known as the atom-bond connectivity (ABC) index [4]. This index is defined as follows:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u} + \frac{1}{d_v} - \frac{2}{d_u d_v}}.$$

Recently Kishori P N, et al. have introduced temperature index, Harmonic TI and geometric arithmetic TI of a graph in [9], [8] and [10], respectively and we extend this study for atom bond connectivity temperature index. Inspired by the work on degree based topological indices and atom bond connectivity index, we now define the atom bond connectivity temperature index $ABCT(G)$ of a molecular graph G as follows:

$$ABCT(G) = \sum_{uv \in E(G)} \sqrt{\left| \frac{T_u + T_v - 2}{T_u T_v} \right|},$$

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

2 On chemical applicability of the atom bond connectivity 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 Atom Bond Connectivity temperature index of the corresponding molecular graph. The productivity of $ABCT$ is tested using a dataset of octane isomers (Table I), found at

$$http://www.moleculardescriptors.eu/dataset.htm.$$

It is shown in Table II, that the $ABCT$-index has a good correlation with the entropy (R = 0. 856), acentric factor (R = 0.879), standard enthalpy of vaporization (R = 0.912) and enthalpy of vaporization (R =0.887) of octane isomers.

Table I. Experimental values of the entropy, acentric factor, enthalpy of vaporization, standard enthalpy of vaporization and the corresponding values of atom bond connectivity temperature index of octane isomers.

Alkane	S	$AcentFac$	$HVAP$	$DHVAP$	$ABCT$
n-octane	111.67	0.397898	73.19	9.915	28.985
2-methyl-heptane	109.84	0.377916	70.3	9.484	26.242
3-methyl-heptane	111.26	0.371002	71.3	9.521	23.672
4-methyl-heptane	109.32	0.371504	70.91	9.483	23.672
3-ethyl-hexane	109.43	0.362472	71.7	9.476	27.6115
2,2-dimethyl-hexane	103.42	0.339426	67.7	8.951	21.523
2,3-dimethyl-hexane	108.02	0.348247	70.2	9.272	24.5604
2,4-dimethyl-hexane	106.98	0.344223	68.5	9.029	24.211
2,5-dimethyl-hexane	105.72	0.35683	68.6	9.051	23.5269
3,3-dimethyl-hexane	104.74	0.322596	68.5	8.973	21.524
3,4-dimethyl-hexane	106.59	0.340345	70.2	9.316	24.4023
2-methyl-3-ethyl-pentane	106.06	0.332433	69.7	9.20	9 22.770
3-methyl-3-ethyl-pentane	101.48	0.306899	69.3	9.081	23.862
2,2,3-trimethyl-pentane	101.31	0.300816	67.3	8.826	20.067
2,2,4-trimethyl-pentane	104.09	0.30537	64.87	8.402	18.008
2,3,3-trimethyl-pentane	102.06	0.293177	68.1	8.897	20.552
2,3,4-trimethyl-pentane	102.39	0.317422	68.37	9.014	20.194
2,2,3,3-tetramethylbutane	93.06	0.255294	66.2	8.410	14.748

Figure 1 $(a-d)$ shows the Scatter plot between entropy S, acentric factor $AcentFac$, enthalpy of vaporization $HVAP$, standard enthalpy of vaporization $DHVAP$ of octane isomers and atom bond connectivity temperature index respectively. The correlation coefficient R of the entropy, acentric factor, enthalpy of vaporization, standard enthalpy of vaporization with the atom bond connectivity temperature index is as reported in Table II.

Table II. Correlation coefficient of atom bond connectivity temperature index.

Atom bond connectivity temperature index with	correlation coefficient (R)
Entropy (S)	0.856
Acentric factor $(AcentFac)$	0.879
Enthalpy of vaporization $(HVAP)$	0.887
Standard enthalpy of vaporization $(DHVAP)$	0.912

3 Result for $2D-$Lattice of $TUC_4C_8[p,q]$

Figure 2 $(a),(b)$ and (c) show $2D-$lattice of $TUC_4C_8[4,3]$, $TUC_4C_8[4,3]$ nanotube and $TUC_4C_8[4,3]$ nanotorus, respectively. The line graph of the subdivision graph of $2D-$lattice of $TUC_4C_8[p,q]$ is shown in Figure $VI(b)$.

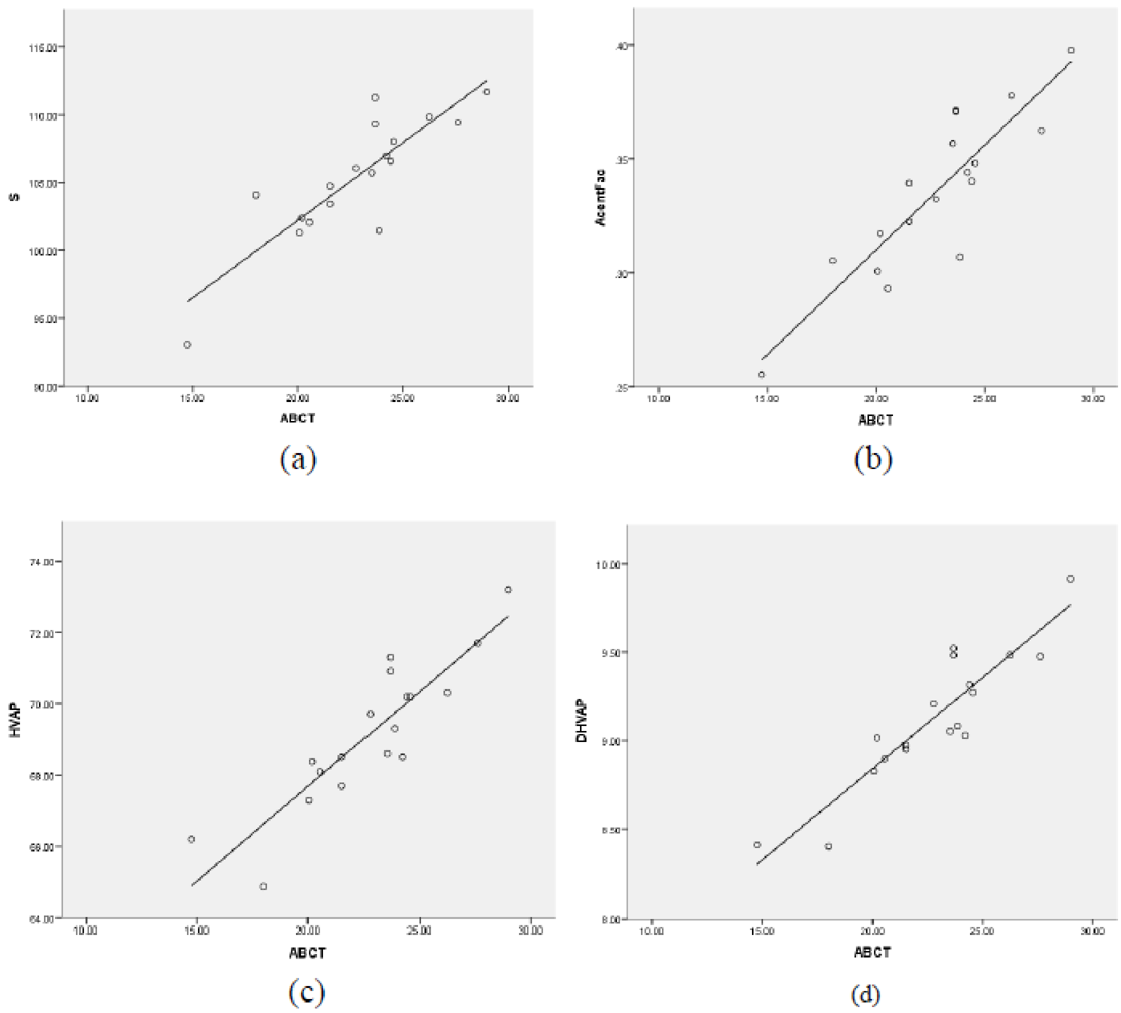

Figure 1. Scatter plot of $ABCT$ of octane isomers with (a) S, (b) $AcentFac$, (c) $HVAP$ and (d) $DHVAP$ respectively.

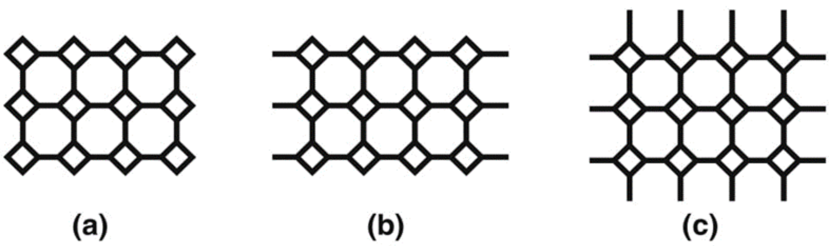

Figure 2. a) $2D-$lattice of $TUC_4C_8[4,3]$. b) $TUC_4C_8[4,3]$ nanotube. c) $TUC_4C_8[4,3]$ nanotorus.

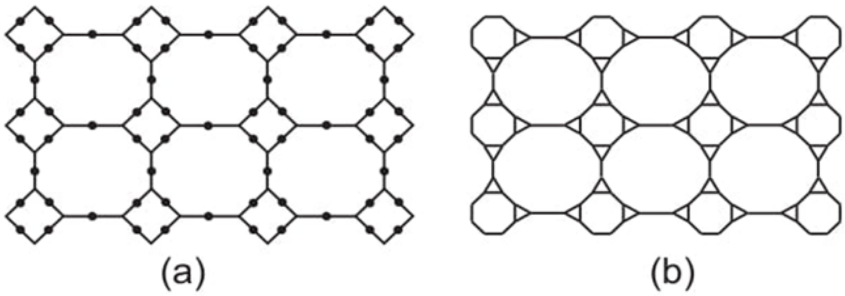

Figure 3. (a) subdivision graph of $2D-$lattice of $TUC_4C_8[4,3]$, (b) line graph of sub-division graph of $TUC_4C_8[4,3]$.

Table III. The edge partition of the graph G.

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

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

$$\begin{aligned} ABCT(G) &= 2\sqrt{2}\,(2+p+q)\sqrt{-\left(1+q-p\,[-1+6q]\right)\left(2+q-p\,[-1+6q]\right)} \\ &+ \frac{2}{3}\,(4-11q-11p+18pq)\sqrt{-\left(3+2q-2p\,[-1+6q]\right)\left(3+q-p\,[-1+6q]\right)} \\ &+ 4(-2+p+q)\sqrt{-4-\frac{4}{3}p^2(1-6q)^2-5q-\frac{4q^2}{3}+p[-5+\frac{82q}{3}+16q^2]}. \end{aligned}$$

Proof. The subdivision graph of $2D-$lattice of $TUC_4C_8\,[p,q]$ and the graph G are shown in Figure 3 (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 all the 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

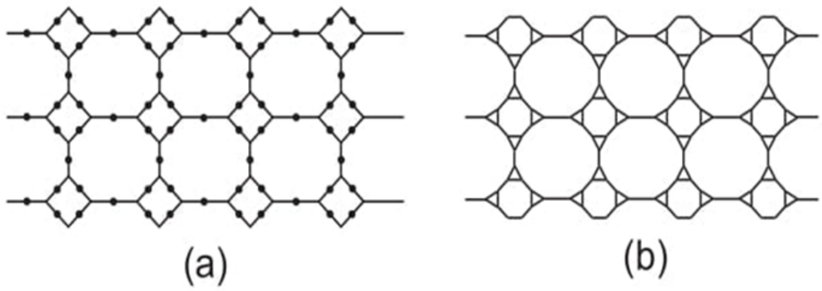

Figure 4. (a) subdivision graph of $TUC_4C_8[4,3]$ nanotube, (b) line graph of subdivision graph of $TUC_4C_8[4,3]$ nanotube.

of the vertices as shown in Table III. Therefore

$$
\begin{aligned}
ABCT(G) &= \sum_{uv\in E(G)} \sqrt{\left|\frac{T_u+T_v-2}{T_uT_v}\right|}\\
&= (2p+2q+4)\sqrt{\left|\frac{\left(\frac{2}{2(6pq-p-q)-2}\right)+\left(\frac{2}{2(6pq-p-q)-2}\right)-2}{\left(\frac{2}{2(6pq-p-q)-2}\right)\left(\frac{2}{2(6pq-p-q)-2}\right)}\right|}\\
&+ (4p+4q-8)\sqrt{\left|\frac{\left(\frac{2}{2(6pq-p-q)-2}\right)+\left(\frac{3}{2(6pq-p-q)-3}\right)-2}{\left(\frac{2}{2(6pq-p-q)-2}\right)\left(\frac{3}{2(6pq-p-q)-3}\right)}\right|}\\
&+ (18pq-11p-11q+4)\sqrt{\left|\frac{\left(\frac{3}{2(6pq-p-q)-3}\right)+\frac{3}{2(6pq-p-q)-3}-2}{\left(\frac{3}{2(6pq-p-q)-3}\right)\left(\frac{3}{2(6pq-p-q)-3}\right)}\right|}\\
&= 2\sqrt{2}(2+p+q)\sqrt{-(1+q-p[-1+6q])(2+q-p[-1+6q])}\\
&+ \frac{2}{3}(4-11q-11p+18pq)\sqrt{-(3+2q-2p[-1+6q])(3+q-p[-1+6q])}\\
&+ 4(-2+p+q)\sqrt{-4-\frac{4}{3}p^2(1-6q)^2-5q-\frac{4q^2}{3}+p\left[-5+\frac{82q}{3}+16q^2\right]}.
\end{aligned}
$$

□

4 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 4 (b).

Table IV. The edge partition of the graph H.

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

Theorem 4.1. *Let H be the line graph of the subdivision graph of of $TUC_4C_8\,[p,q]$ nanotube. Then*

$$ABCT\,(H) = \frac{1}{3}\,(-11p+18pq)\,|-3-2p+12pq|\,\sqrt{\left|-2+\frac{6}{-3-2p+12pq}\right|}$$
$$+2p\sqrt{\frac{2}{3}\left|(-3-2p+12pq)\,(-2-2p+12pq)\left(-2+\frac{3}{-3-2p+12pq}+\frac{2}{-2-2p+12pq}\right)\right|}$$
$$+p\,|-2-2p+12pq|\,\sqrt{\left|-2+\frac{4}{-2-2p+12pq}\right|}.$$

Proof. The subdivision graph of $TUC_4C_8\,[p,q]$ nanotube and the graph H are shown in Figure VII (a) and (b) respectively. In H there are $12pq-2p$ 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 in Table IV. Thus,

$$ABCT\,(H) = 2p\sqrt{\left|\frac{\left(\frac{2}{(12pq-2p)-2}+\frac{2}{(12pq-2p)-2}-2\right)}{\frac{2}{(12pq-2p)-2}\times\frac{2}{(12pq-2p)-2}}\right|}$$
$$+4p\sqrt{\left|\frac{\left(\frac{2}{(12pq-2p)-2}+\frac{3}{(12pq-2p)-3}-2\right)}{\frac{2}{(12pq-2p)-2}\times\frac{3}{(12pq-2p)-3}}\right|}$$
$$+(18pq-11p)\sqrt{\left|\frac{\left(\frac{3}{(12pq-2p)-3}+\frac{3}{(12pq-2p)-3}-2\right)}{\frac{3}{(12pq-2p)-3}\times\frac{3}{(12pq-2p)-3}}\right|}$$
$$=\frac{1}{3}\,(-11p+18\text{pq})\,|-3-2p+12pq|\,\sqrt{\left|-2+\frac{6}{-3-2p+12\text{pq}}\right|}$$
$$+2p\sqrt{\frac{2}{3}\left|(-3-2p+12pq)\,(-2-2p+12pq)\left(-2+\frac{3}{-3-2p+12pq}+\frac{2}{-2-2p+12pq}\right)\right|}$$
$$+\;p|-2-2p+12pq|\sqrt{\left|-2+\frac{4}{-2-2p+12pq}\right|}.$$

□

5 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).

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

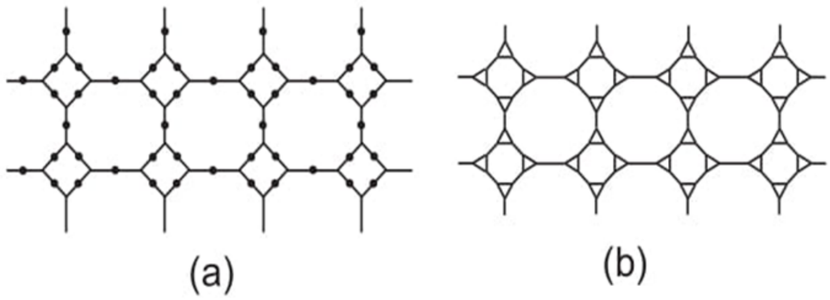

Figure 5. (a) Subdivision graph of $TUC_4C_8[4,2]$ nanotorus, (b) line graph of subdivision graph of $TUC_4C_8[4,2]$ nanotorus.

Theorem 5.1. *Let K be the line graph of the subdivision graph of $TUC_4C_8\,[p,q]$ nanotorus. Then*

$$ABCT\,(K) = 6pq(-3+12pq)\sqrt{\left|-2+\frac{6}{-3+12pq}\right|}.$$

Proof. The subdivision graph of $TUC_4C_8\,[p,q]$ nanotorus and the graph K are shown in Figure VIII (a) and (b), respectively. In K there are $12pq$ 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 V. Therefore,

$$\begin{aligned} ABCT\,(K) =& 18pq\sqrt{\left|\frac{\left(\frac{3}{12pq-3}+\frac{3}{12pq-3}-2\right)}{\frac{3}{12pq-3}\times\frac{3}{12pq-3}}\right|} \\ =& 6pq(-3+12pq)\sqrt{\left|-2+\frac{6}{-3+12pq}\right|}. \end{aligned}$$

□

6 Conclusion

In this paper, we have introduced a new topological index namely, atom bond connectivity 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 atom bond connectivity 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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