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Geometric Arithmetic Temperature Index of Paraline Graphs Of V-Phenylenic Nanostructures

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ABSTRACT

Geometric Arithmetic Temperature Index of Paraline Graph of 2D lattice TUC4C6C8[m, n] and Geometric Arithmetic Temperature Index of Paraline Graph of TUC4C6C8[m, n] nanotube are calculatedis computed in this paper.

KEYWORDS:Temperature of a vertex, Geometric Arithmetic Temperature Index, nanotubes.

1. INTRODUCTION

Molecular descriptors are playing significant role in chemistry, pharmacology etc. Among them, topological indices have a prominent role. Topological indices are numerical parameters of a graph which are invariant under isomorphism. As numerical descriptors of the molecular structure yielded from the corresponding nanostructures, topological indices have been proofed over several applications in nanoengineering, for example, Quantitative Structure-Activity Relationship ($QSAR$), Quantitative Structure-Property Relationship ($QSPR$) study. Generally topological indices can be categorised in three classes: degree-based, distance-based andspectrum-based indices. Among them degree-based indices have great applicationsin chemical graph theory.

Let Gbe 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 graph $G$is the number of edges incidence to $u$and is denoted by duor d(u). The temperature of a vertex $u$of a connected graph $G$is defined by Siemion Fajtlowiczas in [10].

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

where $d(u)$ is the degree of a vertex$u$, and $n$is Harmonic index is one of the most important indices in chemical and mathematical fields. It is a variant of the Randic index which is the most successful molecular descriptor in structure property and structure activity relationships studies. The Harmonic index gives somewhat better correlations with physical and chemical properties compared with the well-known Randic index. It is defined for the first time by S. Fajtlowicz in [11]. The harmonic index of a graph $G$is defined as,

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

It has been found that the harmonic index correlates well with the Randi´c index [16] and [17] and the -electronic energy of benzenoid hydrocarbons [18] and [19]. Favaron et al. [20] considered the relation between harmonic index and the eigenvalues of graphs. Recently Kishori P. Narayankar and Dickson S. introduced Harmonic temperatureindex HTI in [7] and is defined as.

$$HTI(G) = \sum_{uv\epsilon E(G)} \frac{2}{T(u)+T(v)}$$

where $T(u)$ and $T(v)$ are the temperatures of the vertices u and v, respectively. Other topological index with respect to temperature is defined in [8].The Phenylenes belong to the family of polycylic non-benzenoid alternate conjugated

hydrocarbons in which the carbon atoms form hexagon and squares. Each square is adjacent to two detached hexagons. From this, some larger compounds can be formed such as V-phenylenic $2D$ lattice, V-Phenylenic nanotube and nanotorus. The structures of V-Phenylenic nanotubes and nanotorus consist of several

$C4C6C8$nets. A $C4C6C8$net is a trivalent decoration made by alternate $C4$, $C6$and $C8$. V-phenylenic nanotubes and nanotori are most comprehensively studied nanostructures due to widespread applications in the production of catalytic, gas-sensing and corrosion resistant materials. Let $TUC4C6C8[m,n]$ represents the V -phenylenic nanostructures where m denotes the number of hexagons in a row and $n$denotes

the number of rows of hexagons in V-Phenylenic $2D$-lattice, V-Phenylenic nanotube and nanotorus. With this brief introduction, in the forth coming sections Geometric Arithmetic

Temperature Index of Paraline Graph of 2D lattice $TUC4C6C8[m,n]$ and Geometric Arithmetic Temperature Index of Paraline Graph Of $TUC4C6C8[m,n]$ nanotube are calculated.

2. Geometric Arithmetic Temperature Index of ParalineGraph of $2D$ lattice $TUC4C6C8[m,n]$

In this section, we compute the Geometric Arithmetic Temperature Index of the paraline graph of $2D$ lattice $TUC4C6C8[m,n]$.

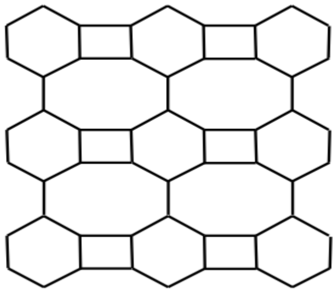

Figure 1: The $2D$ lattice $TUC4C6C8[3,3]$

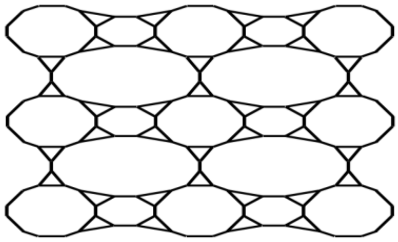

Figure 2: The $2D$ lattice $TUC4C6C8[3,3]$

The total number of vertices in the paraline graph of $2D$ lattice $TUC4C6C8[m,n]$ is $2(9mn - m - 2n)$ and the total number of edges is $27mn - 5m - 10n$, where m denotes the number of hexagons in a row and $n$denotes the number of rows of hexagons which is given in [15]. Figure 2.1 depicts the $2D$ lattice $TUC4C6C8[m,n]$ and Figure 2.2 depicts the paraline graph of $2D$ lattice of $TUC4C6C8[m,n]$.

Theorem 2.1. The Geometric Arithmetic Temperature Index of paraline graph of

$2D$ lattice $TUC4C6C8[m,n]$is

$$GATI(G^*) = (2m + 6n + 4) + \frac{2(4m+4n-8)\sqrt{6[2(9mn - m - 2n) - 2][2(9mn - m - 2n) - 3]}}{10(9mn - m - 2n) - 12} + (27mn - 11m - 20n + 4)$$

Proof . Let G^* be the paraline graph of $2D$ lattice $TUC4C6C8[m,n]$. Then the cardinality of vertex set of $G^*$is $|V(G^*)| = 2(9mn - m - 2n)$ and the cardinality of edge set of G^* is $|E(G^*)| = 27mn - 5m - 10n$, where $m$denotes the number of hexagons in a row and $n$denotes the number of rows of hexagons. The following table represents the edge partition of paraline graph of $2D$ lattice $TUC4C6C8[m,n]$ based on degrees of end vertices of each edge.

Edge partition of paraline graph of $2D$ lattice $TUC4C6C8[m,n]$	
(du, dv) where $uv \in E(G)$	Number of edges
(2, 2)	2m + 6n + 4
(2, 3)	4m + 4n – 8
(3, 3)	27mn – 11m – 20n + 4

Now the temperature of vertices of paraline graph of $2D$ lattice $TUC4C6C8[m,n]$ based on degrees of end vertices of each edge is given by the following table.

(Tu, Tv) where $uv \in E(G)$	Number of edges
$\left(\frac{2}{2(9mn-m-2n)-2}, \frac{2}{2(9mn-m-2n)-2}\right)$	2m + 6n + 4
$\left(\frac{2}{2(9mn-m-2n)-2}, \frac{3}{2(9mn-m-2n)-3}\right)$	4m + 4n – 8
$\left(\frac{3}{2(9mn-m-2n)-3}, \frac{3}{2(9mn-m-2n)-3}\right)$	27mn – 11m – 20n + 4

We know that,

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

Hence,

$$GATI(G^*) = (2m+6n+4)\times \frac{2\sqrt{\frac{2}{2(9mn-m-2n)-2}\times\frac{2}{2(9mn-m-2n)-2}}}{\frac{2}{2(9mn-m-2n)-2}+\frac{2}{2(9mn-m-2n)-2}}$$

$$+(4m+4n-8)\times \frac{2\sqrt{\frac{2}{2(9mn-m-2n)-2}\times\frac{3}{2(9mn-m-2n)-3}}}{\frac{2}{2(9mn-m-2n)-2}\times\frac{3}{2(9mn-m-2n)-3}}$$

$$+(27mn-11m-20n+4)\times \frac{2\sqrt{\frac{3}{2(9mn-m-2n)-3}\times\frac{3}{2(9mn-m-2n)-3}}}{\frac{3}{2(9mn-m-2n)-3}+\frac{3}{2(9mn-m-2n)-3}}$$

$$= \frac{2(2m+6n+4)[2(9mn-m-2n)-2]}{4} \times \frac{2}{[2(9mn-m-2n)-2]}$$

$$+ 2(4m+4n-8) \times \frac{[2(9mn-m-2n)-2][2(9mn-m-2n)-3}{4(9mn-m-2n)-6+6(9mn-m-2n)-6}$$

$$\times \sqrt{\frac{6}{[2(9mn-m-2n)-2][2(9mn-m-2n)-3]}} + 2(27mn-11m-20n+4)$$

$$\times \frac{[2(9mn-m-2n)-3]}{6} \times \frac{3}{[2(9mn-m-2n)-3]}$$

$$= (2m+6n+4) + \frac{2(4m+4n-8)\sqrt{6[2(9mn-m-2n)-2].[2(9mn-m-2n)-3]}}{10(9mn-m-2n)-12}$$

$$+ (27mn-11m-20n+4).$$

3. Geometric ArithmeticTemperature Index of Paraline Graph of $TUC4C6C8[m,n]$nanotube

In this section, we compute the Geometric Arithmetic Temperature Index of the paraline graph of $TUC4C6C8[m,n]$ nanotube. The total number of vertices in the paraline graph of $TUC4C6C8[m,n]$ nanotube is $2(9mn-m)$ and the total number of edges is $27mn-5m$, where $m$denotes the number of hexagons in a row and $n$denotes the number of rows of hexagons which is given in [15]. *Figure* 2.3 depicts the $TUC4C6C8[m,n]$ nanotube and *Figure* 2.4 depicts the paraline graph of $TUC4C6C8[m,n]$ nanotube.

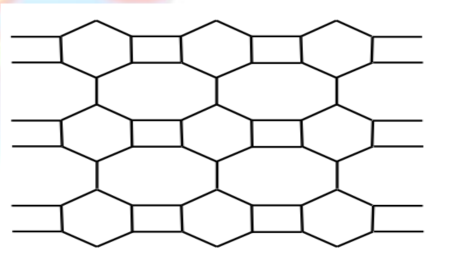

Figure 3: The $TUC4C6C8[3,3]$ nanotube

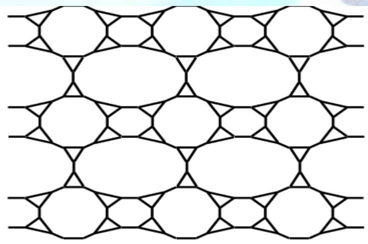

Figure 4: The paraline graph of $TUC4C6C8[3,3]$ nanotube

Theorem 3.1. The Geometric Arithmetic Temperature Index of paraline graph of $TUC4C6C8[m,n]$nanotube is

$$GATI(G^*) = 2m + \frac{8m\sqrt{6[2(9mn-m)-2][2(9mn-m)-3]}}{10(9mn-m)-12}$$

$+ (27mn - 11m)$

Proof. Let G^* be the paraline graph of $TUC4C6C8[m,n]$ nanotube. Then the cardinality of vertex set of G^* is $|V(G*)| = 2(9mn - m)$ and the cardinality of edge set of G^* is $|E(G^*)| = 27mn - 5m$, where m denotes the number of hexagons in a row and n denotes the number of rows of hexagons. The following table represents the edge partition of paraline graph of TUC4C6C8[m, n] nanotube based on degrees of end vertices of each edge.

Edge partition of paraline graph of $TUC4C6C8[m,n]$ nanotube	
(du, dv) where $uv \in E(G)$	Number of edges
$(2,2)$	2m
$(2,3)$	$4m$
$(3,3)$	$27mn - 11m$

Now the temperature of vertices of paraline graph of $TUC4C6C8[m,n]$ nanotube based on degrees of end vertices of each edge is given by the following table.

(Tu, Tv) where uv $\in$ E(G)	Number of edges
$\left(\frac{2}{2(9mn - m) - 2}, \frac{2}{2(9mn - m) - 2}\right)$	2m
$\left(\frac{2}{2(9mn - m) - 2}, \frac{3}{2(9mn - m) - 3}\right)$	4m
$\left(\frac{3}{2(9mn - m) - 3}, \frac{3}{2(9mn - m) - 3}\right)$	$27mn - 11m$

We know that,

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

Hence,

$$\mathrm{GATI}(G^*) = 2m \times \frac{2\sqrt{\frac{2}{2(9mn - m) - 2} \times \frac{2}{2(9mn - m) - 2}}}{\frac{2}{2(9mn - m) - 2} + \frac{2}{2(9mn - m) - 2}} + 4m \times \frac{2\sqrt{\frac{2}{2(9mn - m) - 2} \times \frac{3}{2(9mn - m) - 3}}}{\frac{2}{2(9mn - m) - 2} + \frac{3}{2(9mn - m) - 3}} + (27mn - 11m) \times \frac{2\sqrt{\frac{3}{2(9mn - m) - 3} \times \frac{3}{2(9mn - m) - 3}}}{\frac{3}{2(9mn - m) - 3} + \frac{3}{2(9mn - m) - 3}}$$

$$= \frac{4m[2(9mn - m) - 2]}{4} \times \frac{2}{[2(9mn - m) - 2]} + \frac{8m[2(9mn - m) - 2][2(9mn - m) - 3]}{2[2(9mn - m) - 3] + 3[2(9mn - m) - 2]} \times \sqrt{\frac{6}{[2(9mn - m) - 2][2(9mn - m) - 3]}} + \frac{2(27mn - 11m)[2(9mn - m) - 3]}{6} \times \frac{3}{[2(9mn - m) - 3]}$$

$$= 2m + \frac{8m\sqrt{6[2(9mn - m) - 2][2(9mn - m) - 3]}}{10(9mn - m) - 12} + (27mn - 11m).$$

Conflict of interest statement

Authors declare that they do not have any conflict of interest.

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