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Short Communication

STUDY OF THE TOPOLOGICAL INDICES OF THE LINE GRAPHS OF H-PANTACENIC NANOTUBES

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ABSTRACT

In this paper, we computed the edge version of atom-bond connectivity and geometric arithmetic indices of H-Pantacenic nanotube. We also computed ABC4 and GA5 indices of the line graph of H-Pantacenic nanotube.

Keywords: Atom-bond connectivity index, geometric-arithmetic index, line graph, phenylenes, H-Pantacenic nanotube.

1. INTRODUCTION

Let *G* be a simple graph, with vertex set V(G) and edge set E(G). The line graph L(G) of graph *G* is the graph whose vertices are the edges of *G* and two vertices e and f are incident if and only if they have a common end vertex in G. The degree d_u of a vertex u is the number of vertices adjacent to u. Also, the degree d_e of an edge e of E(G) is the number of its joining vertices in V(L(G)). For a natural number l, we define $V_l(G)=\{u\in V(G)|d_u=l\}$.

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A molecular graph is a collection of points symbolize the atoms in the molecule and set of lines denotes the covalent bonds. These points and lines are known as vertices and edges in graph theory. A topological index is a map from the collection of chemical compounds described by molecular graphs to the set of real numbers. The clear contenders for topological indices are number of vertices and the number of edges. Topological indices are invariant under the graph isomorphisms. The benefit of topological indices are that they may be used directly as a straightforward arithmetical descriptors in a comparison with physical, chemical or biological parameters of molecules in Quantitative Structure Property Relationships (QSPR) and in Quantitative Structure Activity Relationships (QSAR).

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The edge adjacency matrix of a molecular graph is identical as vertex adjacency matrix of the line graph of this molecular graph. That's why the edge connectivity index of molecular graph is identical as Randić vertex connectivity index of the corresponding line graph**.** This remark opens new trends in the subject of topological indices: (i) an approach based on creating topological indices depends on the line graph of molecular graph; (ii) computation of the topological indices of the line graph of molecular graph.

The use of the line graphs in chemistry was initiated from the very beginning of structural chemistry. The first topological index based on line graph is introduced by Bertz in 1981, [1] in the advancement of the theory of molecular branching and complexity. There are various topological indices based on the line graph of molecular graph (see [2-4]). For more details about the applications of line graphs in chemistry, we refer the articles (see [5-7]).

Estrada et al. proposed a topological index based on the degrees of vertices of graphs in [8], which is named as the atom-bond connectivity index (*ABC*). The *ABC* index of a graph *G* is defined as

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

In beginning, the close connection among the heats of formation of alkanes and the *ABC* index is experienced. After that the *ABC* index turned out to be a resourceful tool to model the thermodynamic properties of organic chemical compounds (see [9]).

The fourth member of the class of *ABC* index was launched by M. Ghorbani et al. in [10]:

$$ABC_4(G)=\sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_u\times S_v}}$$

where $S_u=\sum_{v\in N_u}d_v$ and $N_u=\{v\in V(G)|uv\in E(G)\}$.

In [11], the edge version of *ABC* index was introduced:

$$ABC_e(G)=\sum_{ef\in E(L(G))}\sqrt{\frac{d_e+d_f-2}{d_e\times d_f}}.$$

Note that $ABC_e(G)=ABC(L(G))$.

In [12], D. Vukicevic and B. Furtula introduced the geometric arithmetic (GA) index. The *GA* index for graph *G* is defined by

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

The 5th *GA* index was introduced by Graovac et al. in [13]:

$$GA_5(G)=\sum_{uv\in E(G)}\frac{2\sqrt{S_u\times S_v}}{S_u+S_v}.$$

The edge version of *GA* index was introduced in [14]:

$$GA_e(G)=\sum_{ef\in E(L(G))}\frac{2\sqrt{d_e\times d_f}}{d_e+d_f}.$$

It is easily seen that $GAe(G)=GA(L(G))$. For more information on degree-based topological indices, we pass on to the articles [15-45].

The following lemma is helpful for computing the degree of a vertex of line graph.

Lemma 1. Let *G* be a graph with $u,v\in V(G)$ and $e=uv\in E(G)$. Then:

$$d_e=d_u+d_v-2.$$

In order to calculate the number of edges of an arbitrary graph, the following lemma is significant for us.

Lemma 2. Let *G* be a graph. Then

$$\sum_{u\in V(G)}d_u=2|E(G)|.$$

This is also known as handshaking Lemma.

In this paper, we computed two versions of degree-based indices *ABC* and *GA*, for the case of line graph of H-Pantacenic nanotube.

2. RESULTS AND DISCUSSION

The H-Pantacenic nanotube *K[p,q]* and its line graph are shown in Figures 1 and 2, respectively.

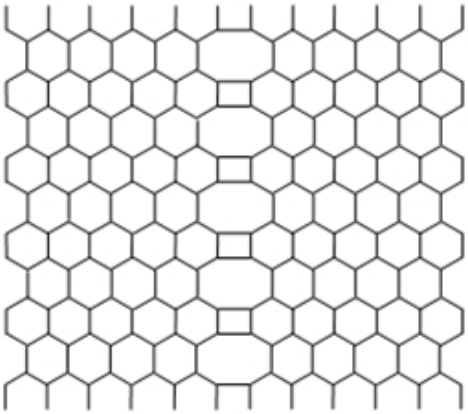
Theorem 1. Let *G=K[p,q]* be a graph of H-Pantacenic nanotube with 22pq vertices and *33pq-2q* edges. Then

$$(1)\, ABC_e(G) = \frac{33}{2}\sqrt{6}pq + q\left(2\sqrt{2} + \frac{4}{3}\sqrt{15} - 5\sqrt{6}\right).$$

$$(2)\, GA_e(G) = 66pq + q\left(\frac{8}{5}\sqrt{6} + \frac{32}{7}\sqrt{3} - 20\right).$$

Proof. In L(G),there are 33pq-2qvertices. It is easily seen from Fig. 2 and Lemma 1 that $|V_2(L(G))| = 2q$, $|V_3(L(G))| = 4q$ and $|V_4(L(G))| = 33pq-8q$. By using Lemma 2, we get $|E(L(G))| = 66pq-8q$.

Fig. 1. The H-Pantacenic nanotube *K[p,q]*.



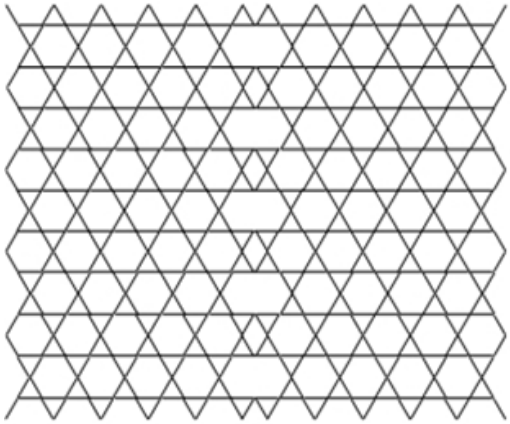
The edge set E(L(G)) divides into three edge partitions based on degrees of the end vertices, i.e. $E(L(G))=E1\,(L(G)) \cup E2\,(L(G)) \cup E3\,(L(G))$. The edge partition E1(L(G)) contains 4q edges uv, where du=2 and dv=3, the edge partition E2 (L(G)) contains 8q edges uv, where d_u=3 and d_v=4 and the edge partition E_3 (L(G)) contains 66pq-20q edges uv, where $d_u=d_v=4$.

$$\mathrm{ABC_e(G)} = \sum_{ef \in E(L(G))} \sqrt{\frac{d_e + d_f - 2}{d_e \times d_f}},$$

then

$$\mathrm{ABC_e(G)} = 4q\sqrt{\frac{2+3-2}{2\times 3}} + 8q\sqrt{\frac{3+4-2}{3\times 4}} + (66pq-20q)\sqrt{\frac{4+4-2}{4\times 4}}.$$

Fig. 2. The line graph of H-Pantacenic nanotube *K[p,q]*.



After simplification we get,

$$\mathrm{ABC_e(G)} = \frac{33}{2}\sqrt{6}pq + q\left(2\sqrt{2} + \frac{4}{3}\sqrt{15} - 5\sqrt{6}\right).$$

Similarly one can find the expression of $GA_e(G)$.

$$GA_e(G) = 66pq + q\left(\frac{8}{5}\sqrt{6} + \frac{32}{7}\sqrt{3} - 20\right). \blacksquare$$

Theorem 2. Let G_L=*L(K[p,q])* be a line graph of H-Pantacenic nanotube. Then:

$$(1)\ \mathrm{ABC_4}(G_L) = \frac{33}{8}\sqrt{30}pq + q\left(\frac{6}{35}\sqrt{70} + \frac{2}{15}\sqrt{210} + \frac{2}{35}\sqrt{770} + \frac{2}{15}\sqrt{138} + \frac{2}{15}\sqrt{435} - 2\sqrt{30}\right)$$

$$(2)\ \mathrm{GA_5}(G_L) = 66pq + q\left(\frac{95}{31}\sqrt{15} + \frac{2}{3}\sqrt{35} + \frac{8}{5}\sqrt{6} + \frac{8}{29}\sqrt{210} - 32\right).$$

Proof. The edge partition of G_L based on the degree sum of vertices lying at the unit distance from end vertices of each edge is given in Table 1.

Since

$$ABC_4(G_L) = \sum_{uv\in E(G_L)} \sqrt{\frac{S_u + S_v - 2}{S_u \times S_v}},$$

then after doing some calculations by using Table1, we get

$$ABC_4(G_L)=\frac{33}{8}\sqrt{30}pq+q\left(\frac{6}{35}\sqrt{70}+\frac{2}{15}\sqrt{210}+\frac{2}{35}\sqrt{770}+\frac{2}{15}\sqrt{138}+\frac{2}{15}\sqrt{435}-2\sqrt{30}\right)$$

Table 1.

$(S_u,S_v);uv\in E(G_L)$	*Number of Edges*
(6,10)	*4q*
(10,14)	*4q*
(10,15)	*4q*
(14,15)	*4q*
(15,16)	*8q*
(16,16)	*66pq-32q*

Similarly we can find the expression of $GA_5(G_L)$ by using Table 1.

$$GA_5(G_L)=66pq+q\left(\frac{95}{31}\sqrt{15}+\frac{2}{3}\sqrt{35}+\frac{8}{5}\sqrt{6}+\frac{8}{29}\sqrt{210}-32\right).\blacksquare$$

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