Computing *GA* index and *ABC* index of V – phenylenic nanotube

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Among topological descriptors topological indices are very important and they have a prominent role in chemistry. One of them is atom - bond connectivity (*ABC*) index defined as $ABC(G)=\sum_{uv\in E}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$, where $d_G(u)$ denotes degree of vertex u. In this paper we compute this new topological index for V – phenylenic nanotube.

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1. Introduction

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. If *e* is an edge of *G*, connecting the vertices *u* and *v*, then we write *e* = *uv* and say "*u* and *v* are adjacent". A connected graph is a graph such that there is a path between all pairs of vertices. A simple graph is an unweighted, undirected graph without loops or multiple edges. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted.

Molecular descriptors play a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [1]. One of the best known and widely used is the connectivity index, χ, introduced in 1975 by Milan Randić [2], who has shown this index to reflect molecular branching. Recently Estrada et al. [3,4] introduced atom-bond connectivity (*ABC*) index, which it has been applied up until now to study the stability of alkanes and the strain energy of cyclo - alkanes. This index is defined as follows:

$$ABC(G)=\sum_{e=uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}},$$

where $d_G(u)$ stands for the degree of vertex *u*. The geometric – arithmetic index is another topological index based on degrees of vertices defined by Vukičevič *et al.* [5] as:

$$GA(G)=\sum_{e=uv\in E(G)}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}.$$

The goal of this paper is to study the *ABC* index and then *GA* index of *V* – phenylenic nanotube. Our notation is standard and mainly taken from standard books of chemical graph theory [6]. All graphs considered in this paper are finite, undirected, simple and connected. One can see the references [7 -26], for more details about topological indices.

2. Main results and discussion

The goal of this section is computing the *ABC* index and *GA* of a lattice of $TUC_4C_6C_8[p, q]$, with *q* rows and *p* columns. Then we compute these topological indices for their nanotubes, see Figs. 1 and 2. At first consider the following examples:

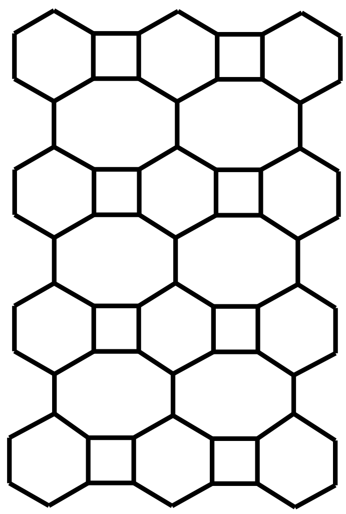

Fig. 1. 2 - D graph of lattice $C_4C_6C_8[3, 4]$.

Example 1. Let P_n be a path with n vertices. It is easy to see that P_n has exactly 2 edges with endpoints degrees 1 and 2. Other edges endpoints are of degree 2.

$$ABC(P_n) = (n-1)\frac{\sqrt{2}}{2}.$$

Example 2. Consider the graph C_n of a cycle with n vertices. Every vertex of a cycle is of degree 2. In other words,

$$ABC(C_n) = n\frac{\sqrt{2}}{2}.$$

Example 3. A star graph with $n + 1$ vertices is denoted by S_n. This graph has a central vertex of degree n and the others are of degree 1. Hence the *ABC* index is as follows:

$$ABC(C_n) = \sqrt{n(n-1)}.$$

Consider now 2 dimensional graph of lattice $G = TUC_4C_6C_8[p, q]$ depicted in Fig. 1. Degrees of edge endpoints of this graph are as follows:

Edge Endpoints	[2, 2]	[2, 3]	[3, 3]
Number of Edges of This Type	$2q + 4$	$4p + 4q - 8$	$9pq - 8q - 5p + 4$

On the other hand by summation these values one can see that:

$$ABC(G) = (9pq - 8q - 5p + 4)\frac{2}{3} + (4p + 6q - 4)\frac{\sqrt{2}}{2} + ()$$
$$= (6pq - \frac{16}{3}q - \frac{10}{3}p + \frac{8}{3}) + (3q + 2p - 2)\sqrt{2}.$$

Hence, we proved the following Theorem:

Theorem 2. Consider 2 - *D* graph of lattice $G = C_4C_6C_8[p, q]$. Then

$$ABC(G) = (6pq - \frac{16}{3}q - \frac{10}{3}p + \frac{8}{3}) + (3q + 2p - 2)\sqrt{2},$$

$$GA(G) = 9pq + (8\frac{\sqrt{6}}{5} - 6)q + (8\frac{\sqrt{6}}{5} - 5)p + 8 - 16\frac{\sqrt{6}}{5}.$$

In continuing consider the graph of nanotube $H = C_4C_6C_8[p, q]$, shown in Fig. 2. Similar to the last Theorem we have the following values for endpoint degrees of vertices of *H*:

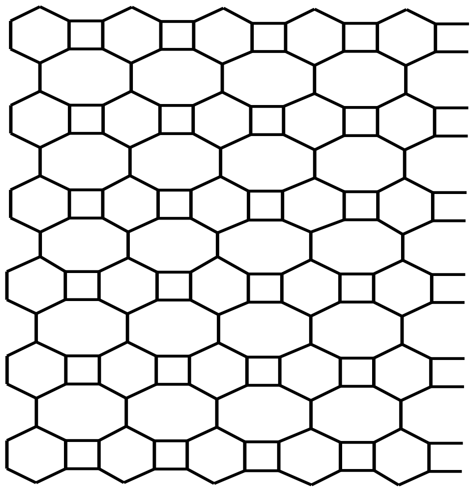

Fig. 2. 2 - D graph of $TUC_4C_6C_8[5,6]$ nanotube.

Edge Endpoints	[2, 3]	[3, 3]
Number of Edges of This Type	$4p$	$2pq+9p$

Thus, we can deduce the following formula for *ABC* index:

$$ABC(G) = (2pq + 9p)\frac{2}{3} + 4p\frac{\sqrt{2}}{2} = \frac{4}{3}pq + (6 + 2\sqrt{2})p.$$

So, the proof of the following Theorem is clear:

Theorem 3. Consider 2 - *D* graph of nanotube $H = TUC_4C_8[p, q]$. Then

$$ABC(H) = (2pq + 9p)\frac{2}{3} + 4p\frac{\sqrt{2}}{2} = \frac{4}{3}pq + (6 + 2\sqrt{2})p,$$

$$GA(H) = 2pq + (9 + 8\frac{\sqrt{6}}{5})p.$$

Theorem 4. Consider the graph of nanotori $K = C_4C_6C_8[p, q]$ in Fig. 3. Then the *ABC* index of *K* is as follows:

$$ABC(K) = 6pq,\ GA(K) = 9pq.$$

Proof. It is easy to see that this graph has 9*pq* edges. Since this graph is a cubic graph, the proof is completed.

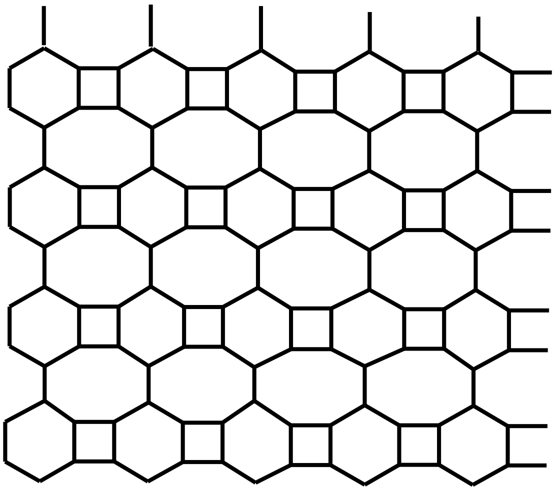

Fig. 3. 2 - D graph of $K = C_4C_6C_8[5,4]$ *nanotori.*

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