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On atom bond connectivity and GA indices of nanocones

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The *GA* index is a topological index was defined as $GA(G)=\sum_{uv\in E}\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$, in which degree of a vertex *u* denoted by *d*(*u*). Atom bond connectivity index is another topological index defined as $ABC(G)=\sum_{uv\in E}\sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$. In this paper we compute these topological indices for two types of nanocones.

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1. Introduction

Throughout this paper graph means simple connected graph. Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. Suppose Λ denotes the class of all graphs. A map $\mathrm{Top}:\sum\to\mathbb{R}^+$ is called a topological index, if $G\cong H$ implies that $Top(G) = Top(H)$. Obviously, the maps Top_1 and Top_2 defined as the number of edges and vertices, respectively, are topological indices. The Wiener [1] index is the first reported distance based topological index and is defined as half sum of the distances between all the pairs of vertices in a molecular graph. If $x, y\in V(G)$ then the distance $d_G(x, y)$ between x and y is defined as the length of any shortest path in G connecting x and y.

Nowadays thousands and thousands topological indices are defined for different goals, such as stability of alkanes, the strain energy of cycloalkanes, prediction of boiling point and etc. One of the important topological index is the geometric – arithmetic index (GA) considered by Vukičević and Furtula [2] as

$$GA(G)=\sum_{uv\in E}\frac{2\sqrt{\mathrm{d}(u)\,\mathrm{d}(v)}}{\mathrm{d}(u)+\mathrm{d}(v)},$$

in which degree of vertex u denoted by $d(u)$. Recently Furtula et al. [3] introduced atom bond connectivity (*ABC*) index, which it has been applied up until now to study the stability of alkanes, the strain energy of cycloalkanes. This index is defined as follows:

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

In this paper we compute these topological indices for two infinite families of carbon nanocones. Throughout this paper our notation is standard and mainly taken from standard book of graph theory such as [4, 5] as well as [6 - 31].

2. Main Results and discussions

Before computing a extended formula for atom bond connectivity and geometric – arithmetic indices, we compute these values for the following examples:

Example 1. Consider the graph of carbon nanocones $C_4[1]$ depicted in Fig. 1. This graph has 20 edges. If u and v be endpoints of edge e, then there are 8 edges with $d(u) = d(v) = 3$, 4 edges with $d(u) = d(v) = 2$ and 8 edges of type $d(u) = 2$, $d(v) = 3$. In other words,

$$GA(C_4[1]) = 12+16\frac{\sqrt{6}}{5} \text{ and}$$

$$ABC(C_4[1]) = \frac{16}{3}+6\sqrt{2}.$$

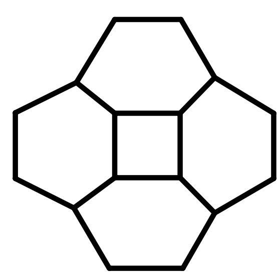

Fig. 1. 2 – D graph of carbon nanocones $C_4[1]$.

Example 2. Consider the graph of carbon nanocones $C_4[2]$ depicted in Fig. 2. This graph has 48 edges. Also, there are 24 edges with $d(u) = d(v) = 3$, 4 edges with $d(u) = d(v) = 2$ and 16 edges of type $d(u) = 2$, $d(v) = 3$. In other words,

$$GA(C_4[2]) = 28 + 32\frac{\sqrt{6}}{5} \text{ and}$$
$$ABC(C_4[2]) = \frac{48}{3} + 10\sqrt{2}\,.$$

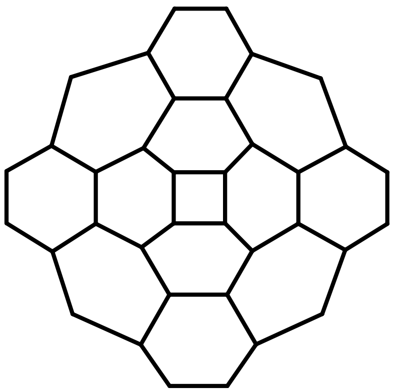

Fig. 2. 2 – D graph of carbon nanocones $C_4[2]$.

By continuing this method, one can see that in generally, this graph has $6n^2 + 10n + 4$ edges and $4(n + 1)^2$ vertices, $n = 1, 2, 3, \ldots$ · On the other hand the are $6n^2 + 6n$ edges with $d(u) = d(v) = 3$, 4 edges with $d(u) = d(v) = 2$ and $4n$ edges of type $d(u) = 2$, $d(v) = 3$. Hence we can deduce the following Theorem:

Theorem 3. Consider the graph of carbon nanocones $C_4[n]$. Then we have:

$$GA(C_4[n]) = 6n^2 + (6 + \frac{8\sqrt{6}}{5})n + 4 \text{ and}$$
$$ABC(C_4[n]) = (n+1)(4n + 2\sqrt{2})\,.$$

Example 4. Consider the graph of carbon nanocones $C_3[1]$ depicted in Fig. 3. This graph has 15 edges, 6 edges with $d(u) = d(v) = 3$, 3 edges with $d(u) = d(v) = 2$ and 6 edges of type $d(u) = 2$, $d(v) = 3$. In other words,

$$GA(C_3[1]) = 9 + 12\frac{\sqrt{6}}{5} \text{ and}$$
$$ABC(C_3[1]) = 4 + 9\sqrt{2}/2\,.$$

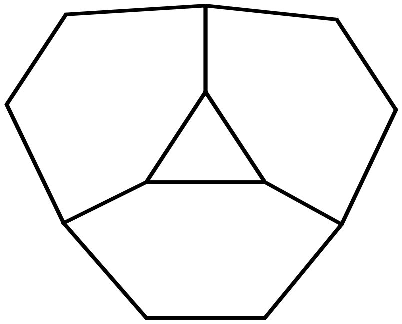

Fig. 3. 2 – D graph of carbon nanocones $C_3[1]$.

Example 5. Consider the graph of carbon nanocones $C_3[2]$ depicted in Fig. 4. This graph has 30 edges, 21 edges with $d(u) = d(v) = 3$, 3 edges with $d(u) = d(v) = 2$ and 12 edges of type $d(u) = 2$, $d(v) = 3$. In other words,

$$GA(C_3[2]) = 24 + 24\frac{\sqrt{6}}{5} \text{ and}$$
$$ABC(C_3[2]) = 14 + 15\sqrt{2}/2\,.$$

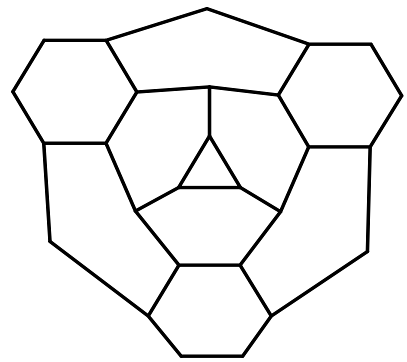

Fig. 4. 2 – D graph of carbon nanocones $C_3[2]$.

Similarly to Theorem 3, by continuing above method in generally, this graph has $15(n^2 - n + 2)/2$ edges and $3(n + 1)^2$ vertices, $n = 1, 2, 3, \ldots$ · On the other hand, there are $(15n^2 - 27n + 24)/2$ edges with $d(u) = d(v) = 3$, 3 edges with $d(u) = d(v) = 2$ and $6n$ edges of type $d(u) = 2$, $d(v) = 3$. This implies the following Theorem is proved:

Theorem 4. Consider the graph of carbon nanocones $C_3[n]$. Then we have:

$$GA(C_3[n]) = \frac{15n^2 - 27n + 24}{2} + 12n\frac{\sqrt{6}}{5} + 3 \text{ and}$$
$$ABC(C_3[n]) = 5n^2 - 9n + 8 + \frac{(6n+3)\sqrt{2}}{2}\,.$$

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