GA index and Zagreb indices of nanocones

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The GA index of a molecular graph G is a recently proposed topological index defined as $GA(G) = \sum_{uv \in E} \frac{2\sqrt{\deg(u)\deg(v)}}{\deg(u) + \deg(v)}$, where *deg(u)* denotes the degree of vertex *u* in *G*. In this paper the *GA* and Zagreb indices of some nanocones are computed.

1. Introduction

In the past years, nanostructures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications. One pentagonal carbon nanocones originally discovered by Ge and Sattler in 1994 [1]. For mathematical properties of nanocones we encourage the reader to consult papers [2-5] and references therein.

We now recall some algebraic notations that will be used in the paper. If *e* is an edge of *G*, connecting the vertices *u* and *v* then we write *e = uv*. The distance between a pair of vertices *u* and *w* of *G* is denoted by *d(u,w)*. The first non trivial topological index was introduced early by Wiener [6]. He defined his index as the sum of distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds. We encourage the reader to consult papers [3,4] and references therein, for further study on the topic.

Following Vukičević and Furtula [7], the *GA* index of a molecular graph *G* is defined as $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\deg(u)\deg(v)}}{\deg(u) + \deg(v)}$, where *deg(u)* denotes the degree of vertex *u* in *G* and sum is taken over all unordered pairs {*u,v*} of distinct vertices in *G*. Recently some researchers considered another variants of the new topological index into account [8-13].

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestic [14]. They are defined as:

$$M_1 = \sum_{v \in V(G)} \deg(v)^2 \text{ and } M_2 = \sum_{uv \in E(G)} \deg(u)\deg(v).$$

The historical background, computational techniques and mathematical properties of Zagreb indices are reported in the papers [15-17] and their references.

The problem of computing topological indices of nanostructures is introduced firstly by Diudea and his co-authors [18-23] and then continued by one the present authors (ARA) [24-36]. In the present article, we take the nanocones into consideration to compute their *GA* and Zagreb index. Our notation is standard and mainly taken from the famous books of Trinajestic [37] and other standard books on graph theory.

2. Main results

The nanocones are constructed from a graphene sheet by removing a wedge and joining the edges produces a cone with a single triangle, square or pentagonal defects at the apex. In some recent papers [2-5] the authors investigated the mathematical properties of this interesting class of nano-materials. The aim of this section is to derive exact formulas for the *GA* and Zagreb indices of nanocones depicted in Figs. 1-4.

Suppose $C_n(k)$ denotes an arbitrary nano-cone, where *n* denotes the number of edges in the single triangle, square, pentagon, etc. To compute these topological indices, we first obtain the number of vertices and edges of the nanocones depicted in Figs. 1-4. From these figures, one can see that the number of vertices and edges obeyed from the recurrence equations $x_k - x_{k-1} = n(2k + 1)$ and $y_k - y_{k-1} = n(3k + 1)$, respectively. By solving these equations, we can see that $|V(C_n(k))| = n(k+1)^2$ and $|E(C_n(k))| = \frac{1}{2}n(k + 1)(3k + 2)$. By these calculations one can see that the number of vertices in the last layer is $n(2k + 1)$ in which the number of vertices of degree two and three are nk and $n(k+1)$, respectively.
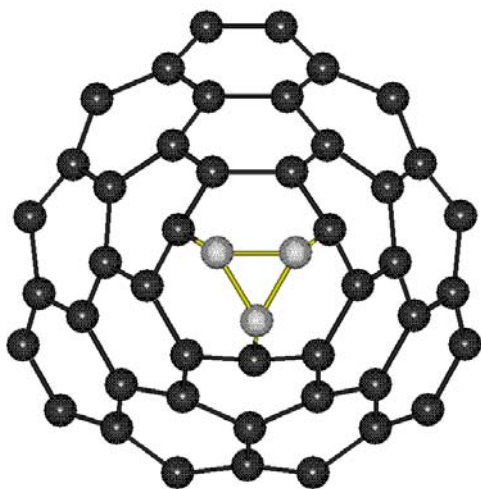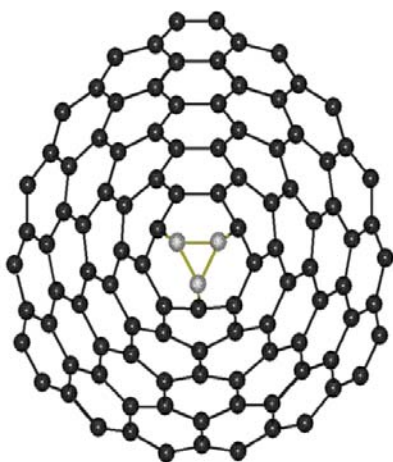
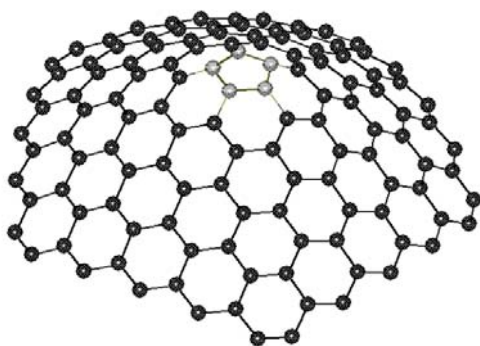*Fig 1. A NC₃(3) Nanocone.*

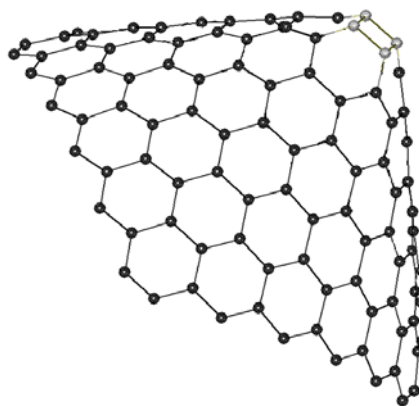*Fig. 2. A NC₃(5) Nanocone.*

Fig. 3. A NC₅(4) Nanocone.

Fig. 4. A NC₄(5) Nanocone.

Therefore by substitution, $GA_1(C_n(k)) = n[\frac{1}{2}k(3k + 1) + (4k/5)6^{\frac{1}{2}} + 1]$, $M_1(C_n(k)) = n(k + 1)(9k + 4)$ and $M_2(C_n(k)) = n[\frac{1}{2}k(27k + 9) + 12k + 4]$.

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