On the fourth atom-bond connectivity index of nanocones

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Atom bond connectivity index is a topological index was defined as $ABC(G) = \sum_{UV\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$ where $d(v)$ denotes the degree of vertex v of G. Recently, *M. Ghorbani et al*. introduced a new version of atom-bond connectivity (ABC4) index as $ABC_4(G) = \sum_{UV\in E(G)} \sqrt{\frac{S(u)+S(v)-2}{S(u)S(v)}}$ where $S_u = \sum_{v\in N_G(u)} d_v$ and $N_G(u) = \{v \in V(G) | uv \in E(G)\}$. In this paper we compute the fourth atom-bond connectivity index for nanocones.

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1. Introduction

The graph theory has successfully provided chemists with a variety of very useful tools, namely, the topological index. A topological index is a numeric quantity of the structural graph of a molecule. This graph has atoms as vertices and two atoms are adjacent if there is a bond between them. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$.

Molecular descriptors have found a wide application in QSPR/QSAR studies [2]. Among them, topological indices have a prominent place. One of the best known and widely used is the connectivity index, χ, introduced in 1975 by *Milan Randic* [1], who has shown this index to reflect molecular branching. Some novel results about branching can be found in [3, 4, 5] and in the references cited therein. However, many physico-chemical properties are dependent on factors rather different than branching.

In order to take this into account but at the same time to keep the spirit of the Randic index, *Ernesto Estrada et al*. proposed a new index, nowadays known as the atom bond connectivity (ABC) index [6]. This index is defined as follows:

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

where $d(v)$ denotes the degree of vertex v of G. Recently, *M. Ghorbani et al*. [7] introduced a new version of atom-bond connectivity (ABC_4) index as

$$ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{S(u)+S(v)-2}{S(u)S(v)}}$$

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

Farahani [8] presented a fourth atom-bond connectivity index of V-Phenylenic Nanotubes and Nanotori and *Farahani* [9] presented fourth atom-bond connectivity index of armchair polyhex nanotubes. We encourage the reader to consult papers for some applications.

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 [10]. These are constructed from a graphene sheet by removing a 60° wedge and joining the edges to produce a cone with a single pentagonal defect at the apex [11].

In this paper, we continue this work to compute the fourth atom-bond connectivity index of carbon nanocones. Our notation is standard and mainly taken from References 12 and 13.

2. Main results

The goal of this section is to computing the fourth atom-bond connectivity index of carbon nanocones (Fig. 1). Let $CNC_n[k]=C_n[k]$. Obviously, $|V(C_n[k])| = n(k+1)^2$ and $|E(C_n[k])| = \frac{n}{2}(k+1)(3k+2)$.

Before computing a extended formula for fourth atom-bond connectivity indices, we compute these values for the following examples:

Example 1. Consider the graph of carbon nanocones $C_3[1]$ depicted in Fig. 1. This graph has 15 edges. If u and v be endpoints of edge e, then there are 3 edges with $S(u) = S(v) = 5$, 6 edges with $S(u) = 7$, $S(v) = 5$, 3 edges with $S(u) = 7$, $S(v) = 9$, and 3 edges of type with $S(u) = S(v) = 9$. In other words,

$$ABC_4(C_3\ [1]) = 3.\sqrt{\frac{5+5-2}{5.5}} + 6.\sqrt{\frac{5+7-2}{5.7}} + 3.\sqrt{\frac{7+9-2}{7.9}} + 3.\sqrt{\frac{9+9-2}{9.9}}$$

$$ABC_4(C_3\ [1]) = 3.\frac{\sqrt{8}}{5} + 6\,.\frac{\sqrt{14}}{7} + 3.\frac{\sqrt{2}}{3} + 3.\frac{4}{9} = \frac{11\sqrt{2}}{5} + \frac{6\sqrt{14}}{7} + \frac{4}{3}.$$

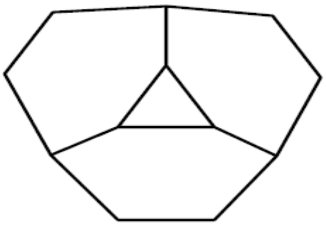

Fig. 1. 2–D graph of carbon nanocones $C_3[1]$ with n=3, k=1.

Example 2. Consider the graph of carbon nanocones $C_4[2]$ depicted in Fig. 1. This graph has 15 edges, 4 edges with $S(u) = S(v) = 5$, 8 edges with $S(u) = 5$, $S(v) = 7$, 8 edges with $S(u) = 7$, $S(v) = 9$, 8 edges with $S(u) = 6$, $S(v) = 7$ and 20 edges of type with $S(u) = S(v) = 9$. So,

$$ABC_4(C_4\ [2]) = 4.\sqrt{\frac{5+5-2}{5.5}} + 8.\sqrt{\frac{5+7-2}{5.7}} + 8.\sqrt{\frac{6+7-2}{6.7}} + 8.\sqrt{\frac{7+9-2}{7.9}} + 20.\sqrt{\frac{9+9-2}{9.9}}$$

$$ABC_4(C_4\ [2]) = 4.\frac{\sqrt{8}}{5} + 8\,.\frac{\sqrt{14}}{7} + 8\,.\sqrt{\frac{11}{42}} + 8.\frac{\sqrt{2}}{3} + 20.\frac{4}{9} = \frac{64\sqrt{2}}{15} + \frac{8\sqrt{14}}{7} + 8\,.\sqrt{\frac{11}{42}} + \frac{80}{9}.$$

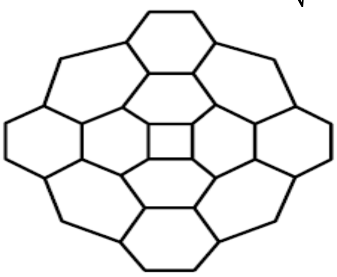

Fig. 2. 2–D graph of carbon nanocones $C_4[2]$ with n=4, k=2.

The main result of this paper is as follows:

Theorem 3. Let $n \geq 2$ and $k \geq 1$ be a positive integers. Then,

$$ABC_4(C_n\ [k]) = \frac{n(5k+6)\sqrt{2}}{15} + 2n\,.\frac{\sqrt{14}}{7} + 2(k-1)n\,.\sqrt{\frac{11}{42}} + \frac{nk}{2}.(3k-1).\frac{4}{9}$$

Proof. It can be easily seen that

$$ABC_4(C_n\ [k]) = n.\frac{\sqrt{8}}{5} + 2n\,.\frac{\sqrt{14}}{7} + 2(k-1)n\,.\sqrt{\frac{11}{42}} + nk.\frac{\sqrt{2}}{3} + \frac{nk}{2}.(3k-1).\frac{4}{9}$$
$$= \frac{n(5k+6)\sqrt{2}}{15} + 2n\,.\frac{\sqrt{14}}{7} + 2(k-1)n\,.\sqrt{\frac{11}{42}} + \frac{nk}{2}.(3k-1).\frac{4}{9}$$

3. Conclusions

In this paper the fourth atom-bond connectivity index of carbon nanocone is computed for the first time. To the best of our knowledge it is the first paper considering the fourth atom-bond connectivity index of carbon nanocone into account. We present a powerful method for calculating such indices.

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