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FORTH ATOM-BOND CONNECTIVITY INDEX OF SOME FAMOUS NANOTUBES

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ABSTRACT. Let $G = (V, E)$ be a simple connected graph. The sets of vertices and edges of G are denoted by $V = V(G)$ and $E = E(G)$, respectively. In such a simple molecular graph, vertices represent atoms and edges represent bonds. The goal of this paper is to compute the ABC_4 index for some nanotubes designed by Diudea.

Keywords: *Molecular graph, Atom-bond connectivity index,* ABC_4 *index.*

INTRODUCTION

Chemical graph theory is a branch of graph theory whose focus of interest is to find topological indices of chemical graphs (i.e. graphs that represent chemical molecules) which correlate well with chemical properties of the corresponding molecules. A molecular graph is a collection of points representing the atoms in the molecule and a set of lines representing the covalent bonds. These points are named vertices and the lines are named edges in the graph theory language.

Many topological indices are closely correlated with some physico-chemical characteristics of the underlying compounds. All graphs considered in this study are finite, simple and connected graphs (without loops and multiple edges). For a connected graph G, $V(G)$ and $E(G)$denote the set of vertices and edges, and $|V(G)|$ and $|E(G)|$ the number of vertices and edges, respectively. The degree d_u of a vertex $u \in V(G)$ is the number of vertices of G adjacent to u.

A connected graph is a graph such that there is a path between all pairs of vertices. Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry. First connectivity index has been introduced in 1975 by Milan Randić [1]; it reflects the molecular

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branching and by this reason was called the branching index, later becaming the well-known Randić connectivity index. It is defined as:

$$\chi(G) = \sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

In 2009, Furtula et al. [2] introduced the Atom-Bond Connectivity (ABC) index, which found applications in the study of stability of alkanes and cycloalkanes. This index is defined as follows:

$$ABC_1(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

Recently, M. Ghorbani et al. [3] introduced a new version of atom-bond connectivity index, named *ABC*4:

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

where S_v is the sum of degrees of all vertices adjacent to vertex v. In other words, $S_u = \sum_{v\in N_G(u)} d_v$ and $N_G(u) = \{v \in V(G) | uv \in E(G)\}$.

The goal of this paper is to compute a close formula of ABC_4 index of a famous family of nanotubes such as HC_5C_7, VC_5C_7 and VAC_5C_7 designed by Diudea [4]. Our notation is standard and for more information and background biography, refers to paper series [5-12].

RESULTS AND DISCUSSION

The structure of HC_5C_7, VC_5C_7 and VAC_5C_7 nanotubes consists of cycles with the length five and seven (or C_5C_7 net). A C_5C_7 net is a trivalent decoration made by alternating C5 and C7. It can cover either a cylinder or a torus. For a review, historical details and further bibliography see refs. [4] and the 3-dimensional lattice of HC_5C_7, VC_5C_7 and VAC_5C_7 nanotubes in Figures 1, 4 and 7.

Theorem 1. *Let* G *be the nanotube* $VC_5C_7[p,q]$. *Then the fourth atom bond connectivity index of* G *is*

$$ABC_4(VC_5C_7[p,q]) = 10pq\sqrt{\frac{11}{42}} + 11pq\left(\frac{3\sqrt{2}+4}{9}\right).$$

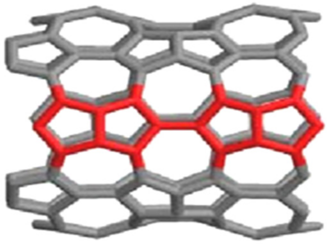

Figure 1. The 3D lattice of VC_5C_7 nanotube

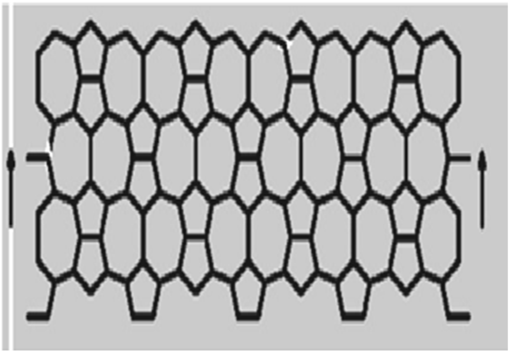

Figure 2. The 2D lattice of $VC_5C_7[16,8] = VC_5C_7[4p,4q]$ nanotube

Proof. We denoted the number of paired pentagons in the first row by p. In this nanotube the two first rows of vertices and edges are repeated alternatively and we denoted the number of this repetition by q. Consider the nanotube $G = VC_5C_7[p,q]$. The number of vertices in this nanotube is equal to $|V(VC_5C_7[p,q])| = 16pq$ and obviously the number of edges is equal to $|E(VC_5C_7[p,q])| = 24pq - 3p$. There are two partitions $V_2 = \{v \in V(G) | d_v = 2\}$ and $V_3 = \{v \in V(G) | d_v = 3\}$ of $(VC_5C_7[p,q])$, and $E(VC_5C_7[p,q])$ can be divided in three partitions,

$$E_4 = \{u,v \in V(VC_5C_7[p,q]) \mid d_u = d_v = 2\},\ E_5 = \{u,v \in V(VC_5C_7[p,q]) | d_u = 3\ \&d_v = 2\}$$
$$\text{and } E_6 = \{u,v \in V(VC_5C_7[p,q]) | d_u = d_v = 3\}.$$

From Figure 2, it is easy to see that the size of edge partitions E_4, E_5 and E_6 are equal to $p, 10p$ and $24pq - 14p$, respectively. We assume u, v, u_1, u_2, u_3 and b are some of the vertices of this graph. From Figure 3, one can see that for every atoms

$$u \in V_2, S_u = 3 + 3 = 6, S_v = 2 + 2 + 3 = 7, S_{u_2} = S_{u_3} = 2 + 3 = 5 \text{ and}$$
$$S_{u_1} = 3 + 3 + 3 = 9.$$

Also for all other vertices b (which belong to V_a), $S_b = 3 \times 3 = 9$.

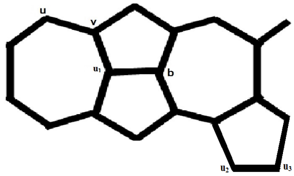

Figure 3. A particular of 2D lattice of $VC_5C_7[p,q]$ nanotube

$$\begin{aligned}
&ABC_4\,(VC_5C_7[p,q]) \\
&= \sum_{uv\in E_5}\sqrt{\frac{S_u+S_v-2}{S_u\times S_v}}+\sum_{vu_1\in E_6}\sqrt{\frac{S_v+S_{u_1}-2}{S_v\times S_{u_1}}}+\sum_{bu_1\in E_6}\sqrt{\frac{S_{u_1}+S_b-2}{S_{u_1}\times S_b}} \\
&+\sum_{u_2u_3\in E_4}\sqrt{\frac{S_{u_2}+S_{u_3}-2}{S_{u_2}\times S_{u_3}}} \\
&= 10p\sqrt{\frac{6+7-2}{6\times 7}}+(24pq-14p)\sqrt{\frac{7+9-2}{7\times 9}}+(24pq-14p)\sqrt{\frac{9+9-2}{9\times 9}} \\
&+\ p\sqrt{\frac{5+5-2}{5\times 5}}=\ 10p\sqrt{\frac{11}{42}}+(24pq-14p)\sqrt{\frac{14}{63}}+(24pq-14p)\sqrt{\frac{16}{81}}+p\sqrt{\frac{8}{25}} \\
&= \frac{\left(4+3\sqrt{2}\right)(24pq-14p)}{9}+2p\left(5\frac{\sqrt{11}}{42}+\frac{\sqrt{2}}{5}\right).
\end{aligned}$$

Theorem 2. *Let G be the nanotube $HC_5C_7[p,q]$. Then the fourth atom bond connectivity index of G is*

$$ABC_4(HC_5C_7[p,q]) = 4p + (12pq-5p)\left(\frac{9\sqrt{14}+6\sqrt{30}+32}{36}\right).$$

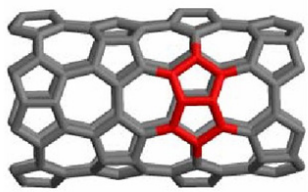

Figure 4. The 3D lattice of HC_5C_7 nanotube

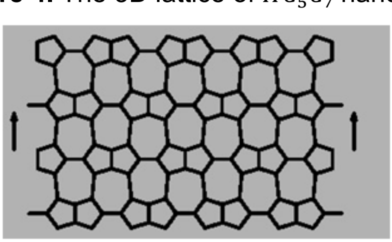

Figure 5. The 2D lattice of $HC_5C_7[16,8]$ nanotube

Proof. In this nanotube we denoted the number of heptagons in one row by p, and the three first rows of vertices and edges are repeated alternatively, we denoted the number of this repetition by q. Consider the nanotube $G = HC_5C_7[p,q]$. The number of vertices in this nanotube is equal to $|V(HC_5C_7[p,q])| = 16\,pq$ and the number of edges is equal to $|E(HC_5C_7[p,q])| = 24pq - 2p$. There are two partitions V_2 and V_3 of $V(HC_5C_7[p,q])$ and $E(HC_5C_7[p,q])$ can be divided in two partitions E_5 and E_6. From Figure 5, it is easy to see that, the size of edge partitions E_5 and E_6 are equal to $8p$ and $24pq - 10p$, respectively. From Figure 6, one can see that for every atom $u \in V_2$, S_u=3+3=6, S_v=2+3×2=8, S_w=2+3×2=8, S_{u_1}=3+3+3=9, and $\forall b \in V_3, S_b$=3×3=9.

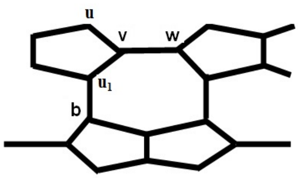

Figure 6. A particular of 2D lattice of $HC_5C_7[p,q]$ nanotube

$$ABC_4\,(HC_5C_7[p,q]) = \sum_{uv\in E_5}\sqrt{\frac{S_u+S_v-2}{S_u\times S_v}} + \sum_{vw\in E_6}\sqrt{\frac{S_v+S_w-2}{S_v\times S_w}} + \sum_{vu_1\in E_6}\sqrt{\frac{S_v+S_{u_1}-2}{S_v\times S_{u_1}}} + \sum_{bu_1\in E_6}\sqrt{\frac{S_{u_1}+S_b-2}{S_{u_1}\times S_b}}$$

$$= 8p\sqrt{\frac{6+8-2}{6\times 8}} + (24pq-10p)\sqrt{\frac{8+8-2}{8\times 8}} + (24pq-10p)\sqrt{\frac{8+9-2}{8\times 9}} + (24pq-10p)\sqrt{\frac{9+9-2}{9\times 9}}$$

$$= 8p\sqrt{\frac{12}{48}} + (24pq-10p)\sqrt{\frac{14}{64}} + (24pq-10p)\sqrt{\frac{15}{72}} + (24pq-10p)\sqrt{\frac{16}{81}}$$

$$= \; 4p + (12pq - 5p)\left(\frac{9\sqrt{14}+6\sqrt{30}+32}{36}\right).$$

Theorem 3. *Let G be the nanotube $VAC_5C_7[p,q]$. Then the fourth atom bond connectivity index of G is:*

$$ABC_4(VAC_5C_7[p,q]) = p\left(\frac{4\sqrt{2}+2\sqrt{110}+20}{5}\right)+$$
$$(24pq-13p+3)\left(\frac{9\sqrt{14}+6\sqrt{30}+32}{72}\right)$$

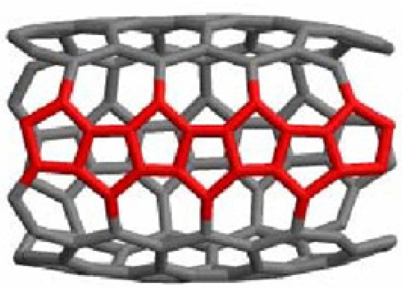

Figure 7. The 3D lattice of VAC_5C_7 nanotube

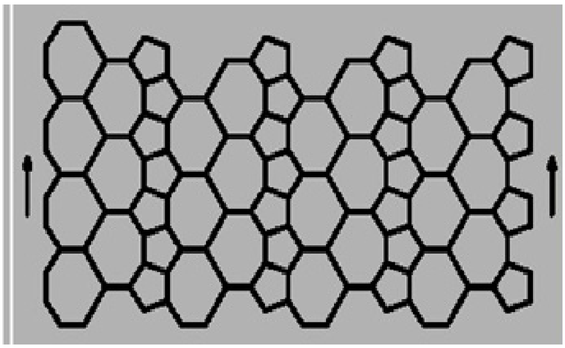

Figure 8. The 2D lattice of $VAC_5C_7[16,8]$ nanotube

Proof. Consider the nanotube $= VAC_5C_7[p,q]$. The number of vertices in this nanotube is equal to $|V(VAC_5C_7[p,q])| = 16pq+2$ and the number of edges is equal to $|E(VAC_5C_7[p,q])| = 24pq-3p+3$. There are two partitions V_2 and V_3 of $V(VAC_5C_7[p,q])$, and $E(VAC_5C_7[p,q])$ can be divided in three partitions E_4, E_5 and E_6. From Figure 8, it is easy to see that the size of edge partitions E_4, E_5 and E_6 are equal to $2p$, $8p$ and $24pq-13p+3$, respectively. From Figure 9, one can see that for every atoms u and

$$v \in V_2, S_u = S_v = 2+3 = 5,\ S_w = 2+3\times 2 = 8,\ S_{u_1} = 2+3\times 2 = 8,$$

$$S_{u_2} = 3+3 = 6,\ S_{u_3} = 3+3+3 = 9$$

and for all other vertices b (which belong to V_a), $S_b = 3\times 3 = 9$.

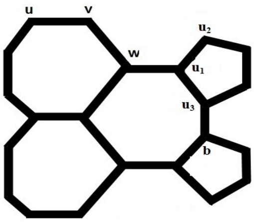

Figure 9. A particular of 2D lattice of $VAC_5C_7[p,q]$ nanotubes

It follows that:

$$ABC_4(G) = \sum_{uv\in E_4}\sqrt{\frac{S_u+S_v-2}{S_u\times S_v}}+\sum_{vw\in E_5}\sqrt{\frac{S_v+S_w-2}{S_v\times S_w}}+\sum_{u_1w\in E_6}\sqrt{\frac{S_w+S_{u_1}-2}{S_w\times S_{u_1}}}+\sum_{u_1u_2\in E_5}\sqrt{\frac{S_{u_1}+S_{u_2}-2}{S_{u_1}\times S_{u_2}}}+\sum_{u_1u_3\in E_6}\sqrt{\frac{S_{u_1}+S_{u_3}-2}{S_{u_1}\times S_{u_3}}}+\sum_{bu_3\in E_6}\sqrt{\frac{S_{u_3}+S_b-2}{S_{u_3}\times S_b}}$$

$$= 2p\sqrt{\frac{8}{25}}+8p\sqrt{\frac{11}{40}}+(24pq-13p+3)\sqrt{\frac{14}{64}}+8p\sqrt{\frac{12}{48}}+(24pq-13p+3)\sqrt{\frac{15}{72}}+(24pq-13p+3)\sqrt{\frac{16}{81}}$$

$$= p\left(\frac{4\sqrt{2}+2\sqrt{110}+20}{5}\right)+(24pq-13p+3)\left(\frac{9\sqrt{14}+6\sqrt{30}+32}{72}\right).$$

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