ON THE FIFTH ATOM-BOND CONNECTIVITY INDEX
OF ARMCHAIR POLYHEX NANOTUBE

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Abstract. Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry. One of them is atom-bond connectivity (ABC) index of a graph G and defined as $ABC(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{(Q_u + Q_v - 2)}{Q_u Q_v}}$, where Q_v is some quantity that in a unique manner can be associated with the vertex u of graph G . Recently, Calimi introduced a new version of atom-bond connectivity (ABC_5) index as $ABC_5(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{(M_u + M_v - 2)}{M_u M_v}}$, where M_u denotes the products of the degrees of adjacent vertices of u . In this paper, formula for calculating the above topological descriptor in armchair polyhex nanotube $TUAC_6[m,n]$ $m, n \geq 1$ family is given.

Keywords: nanotubes, fourth atom-bond connectivity index, armchair polyhex.

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1.   Introduction

All the graphs considered in this paper are simple and connected. Graph theory has successfully provided chemists with a variety of useful tools [3, 4, 5, 6], among which are the topological indices. In theoretical chemistry, assigning a numerical value to the molecular structure that will closely correlate with the physical quantities and activities. Molecular structure descriptors (also called topological indices) are used for modeling physicochemical, pharmacologic, toxicologic, biological and other properties of chemical compounds. Let $G = (V, E)$ be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge sets of it are represented by $V = V(G)$ and $E = E(G)$, respectively. In chemical graphs, the vertices correspond to the atoms of the molecule, and the edges represent to the chemical bonds. Also, 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. Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry. One of the best known and widely used is the connectivity index, introduced in 1975 by Milan Randi´c [7], who has shown this index to reflect molecular branching and defined as follows:

$\chi(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$, where d_u denotes the degree of vertex u of G . Another important classes of connectivity indices is *atom-bond connectivity (ABC) index*, introduced by Furtula et al.[8] , by setting Q_u and Q_v to be the degree of a vertex u and v , defined as $ABC_1(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{(d_u+d_v-2)}{d_u d_v}}$, which it has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. The second and third members of this class were introduced by A. Graovac and M. Ghorbani[10] and M. R. Farahani,[9] on distance version, separately. The fourth member of this class was considered by M. Ghorbani et al.[11], by setting Q_u to be the sum of degrees of all vertices adjacent to vertex u. In this extend, Calimli[12] proposed the new atom bond connectivity (ABC_5) index and obtained the exact value for infinite class of dendrimers, defined as follows $ABC_5(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{(M_u+M_v-2)}{M_u M_v}}$, where M_u denotes the products of the degrees of adjacent vertices of u . On the continuation of this work, we consider another infinte class molecular graphs armchair polyhex nanotube $TUAC_6[m,n]$. In Refs [13, 14, 15, 16, 17, 18, 19] some topological indices of armchair polyhex nanotube $TUAC_6[m,n]$ (Figure 1) is computed. In this paper, we continue this work to compute the fifth atom-bond connectivity index of molecular graphs related to armchair polyhex nanotube $TUAC_6[m,n]$

2. Result

The aim of this section is to obtain a closed formula of ABC_5 of general representation of armchair polyhex nanotubes $TUAC_6[m,n]$

Figure 1. The 3D Lattice of Armchair polyhex nanotubes $TUAC_6[8,7]$.

Theorem 2.1. Let G be the armchair nanotube $TUAC_6[m,n]$, for every $m, n \geq 1$. Then the fifth atom

bond connectivity index of G is equal to $(\frac{\sqrt{10}}{6} + \frac{2}{3}\sqrt{\frac{11}{6}} + \frac{1}{9}\sqrt{\frac{17}{2}} + \frac{2}{9}\sqrt{\frac{43}{6}} +$
$\frac{2n}{3}\sqrt{13} - \frac{8}{27}\sqrt{13})m$.

Proof. Consider the armchair polyhex nanotubes $G = TUAC_6[m, n]$ (Figure 1).
Suppose m and n denote the number of hexagons in the first row/column of the
$2D-$ lattice of $TUAC_6[m, n]$ (Figure 2), respectively. Thus the number of
vertices/atoms in this nanotube is equal to $|V(G)| = 2m(n + 1)$ $m, n \geq 1$ and
obviously the number of edges/bonds is $|E(G)| = 3mn + 2m$. For the convinence
let us partition the vertex set and edge set of G as follows. Since the degree of an
arbitrary vertex/atom of a molecular graph armchair polyhex is equal to 2. Thus
let $V(G) = V_1 \cup V_2$, where $V_1 = \{v \epsilon V(G)|d_v = 2\}$ and $V_2 = \{v \epsilon V(G)|d_v = 3\}$
and let $E(G) = E_1 \cup E_2 \cup E_3$, where $E_1 = \{uv \epsilon E(G)|d_u = d_v = 3\}$, $E_2 =$
$\{uv \epsilon E(G)|d_u = 3 \ d_v = 2\}$ and $E_3 = \{uv \epsilon E(G)|d_u = d_v = 2\}$. From Figure 2,
it is easy to see that the size of edge/bond partitions E_3, E_2 and E_1 are equal to
$m, 2m$ and $3mn - m$, respectively and one can observe that for every atom/vertex
$v \epsilon V_1$, $M_v = 2 \times 3 = 6$, since for its adjacent vertices u, w, observe that $d_u = 2$
and $d_w = 3$ ($u \epsilon V_1, w \epsilon V_2$) and obviously $M_u = 2 \times 3 = 6$, whereas $M_w =$
$3 \times 3 \times 2 = 18$, since for $N_w = \{u_1, u_2, v\}$, the degree of vertices/atoms
$u_1, u_2,$ is equal to three. Also, for all other vertices x (which belong to V_2),
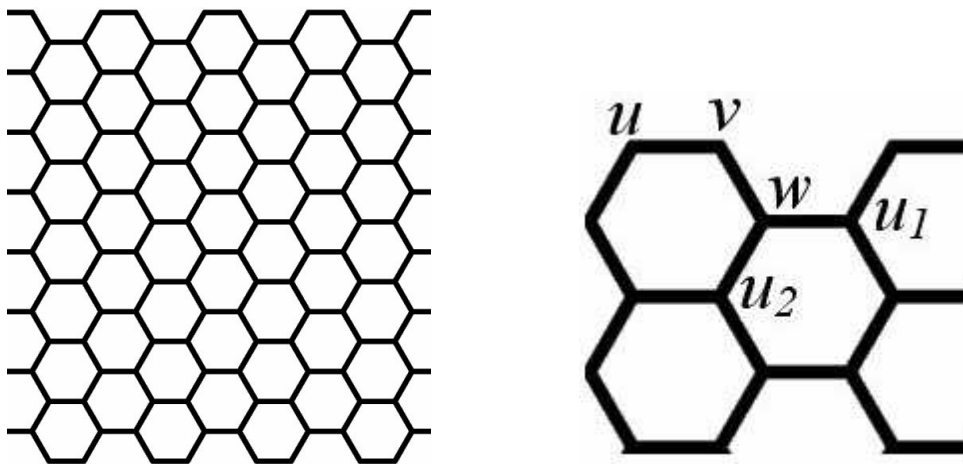$S_x = 3 \times 3 \times 3 = 27$.

Figure 2. The 2D Lattice of Armchair polyhex nanotubes $TUAC_6[8,7]$.

From Figure 2, the first and end (1th, $2n + 1^{th}$) rows consider all members of
V_1 and $|V_1| = 2m$, also all similar vertices to w belong to second and $2n^{th}$ rows.
Therefore $\forall$ $m, n \geq 1$, we have following computations for the fifth atom-bond
connectivity index of armchair polyhex $G = TUAC_6[m, n]$:

$$ABC_5(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{(M_u + M_v - 2)}{M_u M_v}}$$

$$= \sum_{e=uv \in E_1} \sqrt{\frac{(M_u+M_v-2)}{M_u M_v}} + \sum_{e=uv \in E_2} \sqrt{\frac{(M_u+M_v-2)}{M_u M_v}} +$$

$$\sum_{e=uv \in E_3} \sqrt{\frac{(M_u+M_v-2)}{M_u M_v}}$$

$$= m\sqrt{\frac{6+6-2}{6\times6}} + 2m\sqrt{\frac{6+18-2}{6\times18}} + m\sqrt{\frac{18+18-2}{18\times18}} + 2m\sqrt{\frac{18+27-2}{18\times27}} +$$

$$(9mn-4m)\sqrt{\frac{27+27-2}{27\times27}}$$

$$= \frac{m}{6}\sqrt{10} + \frac{2m}{3}\sqrt{\frac{11}{6}} + \frac{m}{9}\sqrt{\frac{17}{2}} + \frac{2m}{9}\sqrt{\frac{43}{6}} + \frac{2(9mn-4m)}{27}\sqrt{13}$$

$$= (\frac{\sqrt{10}}{6} + \frac{2}{3}\sqrt{\frac{11}{6}} + \frac{1}{9}\sqrt{\frac{17}{2}} + \frac{2}{9}\sqrt{\frac{43}{6}} + \frac{2n}{3}\sqrt{13} - \frac{8}{27}\sqrt{13})m$$

$$\approx (2.40730n + 1.28025)m$$

Example 2.2. For $TUAC_6[8,7]$ with 128 atoms and 184 chemical bonds. Then one can see that

$$ABC_5(TUAC_6[8,7]) = 144.8492.$$

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