THE PUBLISHING HOUSE
OF THE ROMANIAN ACADEMY

CHEMISTRY
Research article

ON THE FOURTH ATOM-BOND CONNECTIVITY INDEX OF ARMCHAIR POLYHEX NANOTUBES

Mohammad REZA FARAHANI[1]

[1] Department of Applied Mathematics, Iran University of Science and Technology (IUST) Narmak, Tehran, Iran
Corresponding author: Mohammad Reza FARAHANI, E-mail: mr_farahani@mathdep.iust.ac.ir

Received February 22, 2013

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 $ABC(G)=\sum_{e=uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_u d_v}}$, where d_v denotes the degree of vertex v of G. Recently, *M. Ghorbani et al.* introduced a new version of atom-bond connectivity (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 $N_G(u)=\{v\in V(G)|uvE(G)\}$. In this paper, formula for calculating the above topological descriptor in armchair polyhex nanotube $TUAC_6$ family is given.

Key words: nanotubes, fourth, atom-bond, connectivity, armchair polyhex.

INTRODUCTION

It is clear that any molecule is a collection of Atoms and Bonds that connect all its atoms.

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.

The chemical graph theory is an important branch of mathematical chemistry. In this branch, there are many molecular descriptors (or *Topological Index*), that have very useful properties to study of chemical molecules. A topological index is a real number associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry.

One of the oldest connectivity indices is the *Randić connectivity index*, introduced by *Milan Randić* in 1975, who has shown this index to reflect molecular branching and called the *branching index* [1] that later became the well-known *Randić connectivity index*. It is defined on the ground of vertex degrees

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

where d_u denotes G degree of vertex u.

In 2009, Furtula *et al.* [2, 3] introduced atom-bond connectivity (ABC) index, which it has been applied up until now to study the stability of alkanes and the strain energy of 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.* introduced a new version of atom-bond connectivity (ABC_4) index as

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

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 $N_G(u)=\{v\in V(G)|uv\in E(G)\}$.

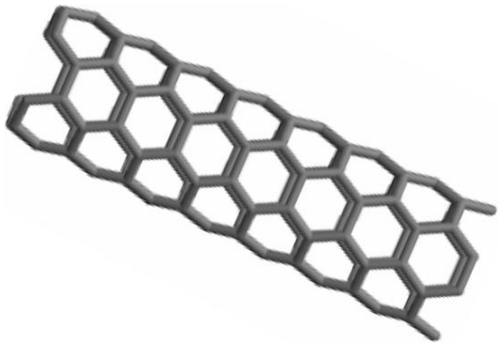

Fig. 1. The 3D Lattice of Armchair polyhex nanotubes $TUAC_6$ [8,7].

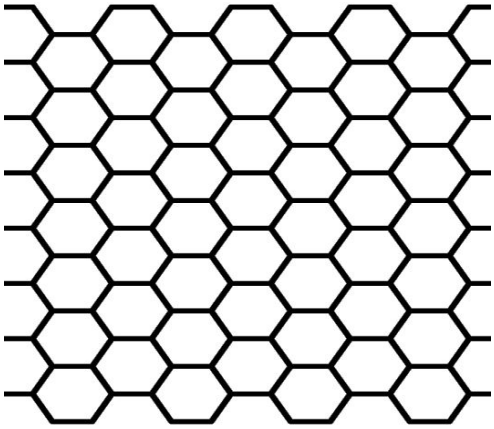

Fig. 2. The 2D Lattice of Armchair polyhex nanotubes $TUAC_6$ [8,7].

In References 4–12 some topological indices of armchair polyhex nanotube $TUAC_6$ (Figure 1) is computed. In this paper, we continue this work to compute the fourth atom-bond connectivity index of molecular graphs related to armchair polyhex nanotube $TUAC_6$. Our notation is standard and mainly taken from References [13, 14].

RESULTS

The aim of this section is to obtain a closed formula of ABC_4 of general representation of armchair polyhex nanotubes $TUAC_6$ (or VC_6) and we have following theorems, immediately.

Theorem. 1. Let G be the armchair nanotube $TUAC_6[m,n]$ $\forall m,n\in$. Then the fourth atom-bond connectivity index of G is equal to

$$ABC_4\left(VPHX\left[m,n\right]\right)=\left(4n+\frac{2\sqrt{2}}{5}+\sqrt{\frac{11}{10}}+\frac{\sqrt{14}}{8}+\frac{\sqrt{30}}{6}-\frac{16}{9}\right)m$$

Proof. Consider the armchair polyhex nanotubes $G=TUAC_6$ (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 $|V(TUAC_6[m,n])|=2m(n+1)$ $m,n\in$ and obviously the number of edges/bonds is $|E(TUAC_6[m,n])|=3mn+2m$.

There are two partitions $V_2=\{v\in V(G)\,|\,d_v=2\}$ and $V_3=\{v\in V(G)|\,d_v=3\}$ of $V(TUAC_6[m,n])$, since the degree of an arbitrary vertex/atom of a molecular graph armchair polyhex is equal to 2 or 3. Next, these partitions imply that $E(TUAC_6[m,n])$ can be divided in three partitions $E_6=\{u,v\in V(TUAC_6[m,n])|\,d_u=d_v=3\}$, $E_5=\{u,v\in V(TUAC_6[m,n])|\,d_u=3\&d_v=2\}$ and $E_4=\{u,v\in V(TUAC_6[m,n])|\,d_u=d_v=2\}$.

From Figure 2, it is easy to see that the size of edge/bond partitions E_4, E_5 and E_6 are equal to are equal to m, $2m$ and $3mn-m$, respectively. From Figure 3, one can see that for every atom/vertex $v\in V_2$, $S_v=2+3=5$, since for its adjacent vertices u, w; $d_u=2$ and $d_w=3$ ($u\in V_2$, $w\in V_3$) and obviously $S_u=5$. Whereas $S_w=2\times3+2$, 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 a (which belong to V_3), $S_a=3\times3=9$.

From Figure 2, the first and end (1^{th}, $2n+1^{th}$) rows consider all members of V_2 and $|V_2|=2m$, also all similar vertices to w belong to second and $2n^{th}$ rows. Therefore $\forall\, m,n\geq1$, we have following computations for the fourth atom-bond connectivity index of armchair polyhex $G=TUAC_6[m,n]$:

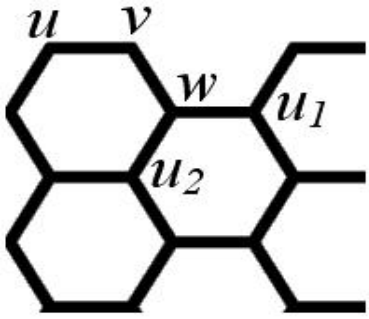

Fig. 3. A particular of 2D Lattice of Armchair polyhex $TUAC_6$.

Here, the new version

$$ABC_4(TUAC_6[m,n])=\sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_uS_v}}$$

$$=\sum_{u_2v_2\in E_4}\sqrt{\frac{S_{u_2}+S_{v_2}-2}{S_{u_2}S_{v_2}}}+\sum_{u_2v_3\in E_5}\sqrt{\frac{S_{u_2}+S_{v_3}-2}{S_{u_2}S_{v_3}}}+\sum_{u_3v_3\in E_6}\sqrt{\frac{S_{u_3}+S_{v_3}-2}{S_{u_3}S_{v_3}}}$$

$$=(m)\sqrt{\frac{5+5-2}{5\times5}}+(2m)\sqrt{\frac{5+8-2}{5\times8}}+(m)\sqrt{\frac{8+8-2}{8\times8}}+(2m)\sqrt{\frac{8+9-2}{8\times9}}$$

$$+(9mn-4m)\sqrt{\frac{9+9-2}{9\times9}}$$

$$=\frac{m2\sqrt{2}}{5}+m\sqrt{\frac{11}{10}}+\frac{m\sqrt{14}}{8}+\frac{m}{3}\sqrt{\frac{15}{2}}+\frac{4(9mn-4m)}{9}$$

$$=\left(4n+\frac{2\sqrt{2}}{5}+\sqrt{\frac{11}{10}}+\frac{\sqrt{14}}{8}+\frac{\sqrt{30}}{6}-\frac{16}{9}\right)m$$

Thus, $ABC_4(TUAC_6[m,n])\approx(4n+1.2172946)m$. Here the proof of theorem is completed. □

Example 1. Let $A=TUAC_6[8,7]$ be a nanotube armchair polyhex with 128 atoms and 184 chemical bonds. Then one can see that $ABC_4(A)=233.73836$.

Example 2. The fourth atom-bond connectivity index of $TUAC_6[m,n]$ for $m=2, 4, \ldots, 10$ and $n=1, 2, \ldots, 10$ are listed as follows

$ABC_4(TUAC_6[2,1])=10.4345891957273$
$ABC_4(TUAC_6[2,2])=18.4345891957273$
$ABC_4(TUAC_6[2,3])=26.4345891957273$
$ABC_4(TUAC_6[2,4])=34.4345891957273$
$ABC_4(TUAC_6[2,5])=42.4345891957273$
$ABC_4(TUAC_6[2,6])=50.4345891957273$
$ABC_4(TUAC_6[2,7])=58.4345891957273$
$ABC_4(TUAC_6[2,8])=66.4345891957273$
$ABC_4(TUAC_6[2,9])=74.4345891957273$
$ABC_4(TUAC_6[2,10])=82.4345891957273$

$ABC_4(TUAC_6[4,1])=20.8691783914545$
$ABC_4(TUAC_6[4,2])=36.8691783914545$
$ABC_4(TUAC_6[4,3])=52.8691783914545$
$ABC_4(TUAC_6[4,4])=68.8691783914545$
$ABC_4(TUAC_6[4,5])=84.8691783914545$
$ABC_4(TUAC_6[4,6])=100.869178391455$
$ABC_4(TUAC_6[4,7])=116.869178391455$
$ABC_4(TUAC_6[4,8])=132.869178391455$
$ABC_4(TUAC_6[4,9])=148.869178391455$
$ABC_4(TUAC_6[4,10])=164.869178391455$

$ABC_4(TUAC_6[6,1])=31.3037675871818$
$ABC_4(TUAC_6[6,2])=55.3037675871818$
$ABC_4(TUAC_6[6,3])=79.3037675871818$
$ABC_4(TUAC_6[6,4])=103.3037675871818$
$ABC_4(TUAC_6[6,5])=127.3037675871818$
$ABC_4(TUAC_6[6,6])=151.3037675871818$
$ABC_4(TUAC_6[6,7])=175.3037675871818$
$ABC_4(TUAC_6[6,8])=199.3037675871818$
$ABC_4(TUAC_6[6,9])=223.3037675871818$
$ABC_4(TUAC_6[6,10])=247.3037675871818$

$ABC_4(TUAC_6[8,1])=41.738356782909$
$ABC_4(TUAC_6[8,2])=73.738356782909$
$ABC_4(TUAC_6[8,3])=105.738356782909$
$ABC_4(TUAC_6[8,4])=137.738356782909$
$ABC_4(TUAC_6[8,5])=169.738356782909$
$ABC_4(TUAC_6[8,6])=201.738356782909$
$ABC_4(TUAC_6[8,7])=233.738356782909$
$ABC_4(TUAC_6[8,8])=265.738356782909$
$ABC_4(TUAC_6[8,9])=297.738356782909$
$ABC_4(TUAC_6[8,10])=329.738356782909$

$ABC_4(TUAC_6[10,1])=52.1729459786363$
$ABC_4(TUAC_6[10,2])=92.1729459786363$
$ABC_4(TUAC_6[10,3])=132.172945978636$
$ABC_4(TUAC_6[10,4])=172.172945978636$
$ABC_4(TUAC_6[10,5])=212.172945978636$
$ABC_4(TUAC_6[10,6])=252.172945978636$
$ABC_4(TUAC_6[10,7])=292.172945978636$
$ABC_4(TUAC_6[10,8])=332.172945978636$
$ABC_4(TUAC_6[10,9])=372.172945978636$
$ABC_4(TUAC_6[10,10])=412.172945978636$

Corollary 1. The fourth atom-bond connectivity index of $TUAC_6[m,n]$ for all positive integer number q and $n=1, 2, \ldots, 10$ are equal to: $ABC_4(TUAC_6[2q,n])=q\times ABC_4(TUAC_6[2,n])$.

CONCLUSIONS

In this paper, I was counting a new connectivity topological index for a family of carbon nanotubes. This topological index (fourth atom-bond connectivity index) is useful for surveying structure of some connected nanotubes and connected nanostructures, which is based on degrees of their vertices.

REFERENCES

1. M. Randić, On Characterization of Molecular Branching, J. Am. Chem. Soc., 97(23), pp. 6609 (1975).
2. B. Furtula, A. GRAOVAC, D. VUKIČEVIĆ, Disc. Appl. Math., 157, pp. 2828 (2009).
3. D. Vukičević and B. Furtula. Journal of Mathematics Chemical. 46, pp. 1369, (2009).
4. A.R. Ashrafi and A. Loghman, PI index of armchair polyhex nanotubes, ARS Combinatoria. 80, pp. 193–199, (2006).

5. A. Iranmanesh and A.R. Ashrafi. Balaban index of an armchair polyhex TUC4C8(R) and TUC4C8(S) nanotorus, Journal of Computational and Theoretical Nanoscience. 4(3), pp. 514–517, (2007).
6. H. Deng., The PI Index of TUAC6[2p,q], MATCH Communications in Mathematical and in Computer Chemistry. 55, pp. 461–476, (2006).
7. M.V. Diudea. M. Stefu, B. Pârv and P. E. John, Armchair Polyhex Nanotubes, Croatica Chemica Acta. 77111–115, (2004).
8. M.V. Diudea., Hosoya polynomial In Tori, MATCH Communications in Mathematical and in Computer Chemistry. 45, pp. 109-122, (2002).
9. M. Eliasi and B. Taeri. Distance in Armchair Polyhex Nanotubes, MATCH Communications in Mathematical and in Computer Chemistry. 62, pp. 295-310, (2009).
10. M.R. Farahani. Some Connectivity Indices and Zagreb Index of Polyhex Nanotubes, Acta Chimica Slovenica. 59(4), pp. 779–783, (2012).
11. X. Shoujun and Z. Heping. Hosoya polynomials of armchair open-ended nanotubes, International Journal of Quantum Chemistry. 107, (2007), 586–596.
12. S. Yousefi and A.R. Ashrafi, Distance Matrix and Wiener Index of Armchair Polyhex Nanotubes, Studia Univ. Babes-Bolyai. Chemia, 53(4), pp. 111–116, (2008).
13. R. Todeschini and V. Consonni, Handbook of Molecular Descriptors, Wiley-TUACH, Weinheim (2000).
14. N. Trinajstić, Chemical Graph Theory, 2nd. CRC Press, Boca Raton, FL, (1992), 20-75.