Computing some connectivity indices of Nanotubes

Mohammad R. Farahani a*

a Department of Applied Mathematics, Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran

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ABSTRACT

Let G be a simple connected graph in chemical graph theory and e=uv be an edge of G. Atom-Bond Connectivity index, Randic connectivity index, geometric-arithmetic index and sum-connectivity index of G are defined as

\[ ABC(G) = \sum_{e=uv \in E(G)} \left( \frac{d_u + d_v - 2}{d_u d_v} \right) \]

\[ \chi(G) = \sum_{u,v \in V(G)} \frac{1}{\sqrt{d_u d_v}} \]

\[ G(A(G) = \sum_{e=uv \in E(G)} \left( \frac{2d_u d_v}{d_u + d_v} \right) \]

\[ X(G) = \sum_{u,v \in V(G)} \frac{1}{\sqrt{d_u + d_v}} \]

respectively. In this paper we compute ABC(G), \( \chi(G) \), G(A(G) and X(G) indices of \( G_1=\text{TUC}_4 \) and \( G_2=\text{TUC}_4 \text{C}_8 \) Nanotubes.

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1. Introduction

Let G be a simple connected graph in chemical graph theory. The vertex set and edge set of G denoted by V(G) and E(G) respectively and its vertices correspond to the atoms and the edges correspond to the bonds.

There exists many topological indices in mathematical chemistry. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry. A topological index is a numeric quantity from the structural graph of a molecule and is invariant on the automorphism of the graph. Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, Wiener index [4-7]. Wiener index is defined as the sum of distances between any two atoms in the molecules, in terms of bonds (or edges) and denoted by W(G).

\[ W(G) = \frac{1}{2} \sum_{u \neq v \in V(G)} d(u,v) \]

where the distance \( d(u,v) \) between two vertices u and v is the number of edges in a shortest path connecting them.

Three simplest topological indices are the number of vertices, the number of edges and degree of a vertex v of the graph G and we denoted by \( \eta, e \) and \( d_v \), respectively. The degree of a vertex v is the number of vertices joining to v.

Let \( e=uv \) be an edge of the graph G, Randic Connectivity Index of G was introduced by Milan Randic in 1975 [8] as

\[ \chi(G) = \sum_{u,v \in V(G)} \frac{1}{\sqrt{d_u d_v}} \]

where \( d_u \) and \( d_v \) are the degrees of the vertices u and v, respectively.

Of course, a new version of Randic connectivity index (First-connectivity index) called Sum-connectivity index was introduced by Zhou and Trinajstić [3, 9] in 2008. For a connected graph G, its sum-connectivity index \( X(G) \) is defined as

\[ X(G) = \sum_{u,v \in V(G)} \frac{1}{\sqrt{d_u + d_v}} \]

Randic connectivity index is an oldest connectivity topological indices, for an arbitrary graph with connected structure in chemical graph theory. Recently in 2009, Vukicevic and Furtula [5, 6] introduced Atom-Bond Connectivity index \( ABC(G) \) and Geometric-Arithmetic index \( G(A(G) \) as

\[ ABC(G) = \sum_{e=uv \in E(G)} \left( \frac{d_u + d_v - 2}{d_u d_v} \right) \]

And

\[ G(A(G) = \sum_{e=uv \in E(G)} \left( \frac{2d_u d_v}{d_u + d_v} \right) \]

respectively. In this paper, we compute these connectivity topological indices of \( G_1=\text{TUC}_4 \) and \( G_2=\text{TUC}_4 \text{C}_8 \) nanotubes.

* Corresponding author. Tel.: +98-9192478265; e-mail: mr_farahani@mathdep.iust.ac.ir

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2. Main results and discussion

In this section, Randic index, geometric-arithmetic index, atom-bond connectivity index and sum-connectivity index of $TUC_4[m,n]$ and $TUC_4C_8[m,n]$ nanotubes are computed. Let us recall some definitions and notations.

**Definition 1.** [10] Consider an arbitrary vertex $v$ with degree $d_v$ of simple connected graph $G=(V(G),E(G))$ and we denoted the minimum degree with $\delta = \min \{d_v \mid v \in V(G)\}$ and the maximum degree with $\Delta = \max \{d_v \mid v \in V(G)\}$. By according to the vertices degree, we have several partitions of vertex set $V(G)$ and edge set $E(G)$ of graph $G$, as follow:

- $\forall i, 1 \leq i \leq \Delta, E_i = \{e = uv \in E(G) \mid d_v + d_u = i\}$,
- $\forall j, \delta \leq j \leq \Delta^*, E_j^* = \{e = uv \in E(G) \mid d_v \times d_u = j\}$

and $\forall k, \delta \leq k \leq \Delta, V_k = \{v \in V(G) \mid d_v = k\}$.

Before going to calculate favorite connectivity indices, we divide the vertex set $V(G)$ of an arbitrary molecular graph in four partitions as follow

- $V_1 = \{v \in V(G) \mid d_v = 3\}$,
- $V_2 = \{v \in V(G) \mid d_v = 2\}$,
- $V_3 = \{v \in V(G) \mid d_v = 1\}$,
- $E_4 = E_4^* = \{u,v \in V(G) \mid d_u = d_v = 2\}$,
- $E_5 = E_5^* = \{u,v \in V(G) \mid d_u = 3 \& d_v = 2\}$,
- $E_6 = E_6^* = \{u,v \in V(G) \mid d_u = d_v = 3\}$.

Note that, all atoms in chemical graph theory have at most three adjacent atoms (vertices) and for Carbon atoms at most four adjacent atoms. Thus the degree of an arbitrary vertex $v$ (or atom) is equal to 1 or 2 or 3 or 4.

Molecular graphs $TUHRC_4(S)$ and $TUSC_4C_8(S)$ are tow family of nanotubes. Now we compute Randic index, geometric-arithmetic index, atom-bond connectivity index and sum-connectivity index of $G_1=TUC_4[m,n]$ and $G_2=TUC_4C_8[m,n]$ nanotubes.

**Theorem 1** Consider nanotube $G_i=TUHRC_4(S)$ for every $m,n>1$. Then

- Atom-Bond connectivity index of $G_i$ is equal to
  $$ABC(TUC_4[m,n]) = m \left( \frac{(2n-1)\sqrt{6}}{2} + 2\sqrt{2} \right).$$
- Geometric-Arithmetic index of $G_i$ is equal to
  $$GA(TUC_4[m,n]) = \left( 4n + \frac{8\sqrt{2}}{3} - 2 \right) m.$$
\[ \chi(TUC_4[m,n]) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \]
\[ = \sum_{e=uv \in E^*_G} \frac{1}{\sqrt{d_u + d_v}} + \sum_{e=uv \in E_G^*} \frac{1}{\sqrt{d_u + d_v}} \]
\[ = \sqrt{16} \left[ \frac{1}{\sqrt{16}} + \frac{1}{\sqrt{8}} \right] \]
\[ = \frac{4mn - 2m}{4} + \frac{4m}{2\sqrt{2}} \]
\[ = m \left( \frac{2n - 1}{2} + \sqrt{2} \right). \]
\[ X(TUC_4[m,n]) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \]
\[ = \sum_{e=uv \in E^*_G} \frac{1}{\sqrt{d_u + d_v}} + \sum_{e=uv \in E_G^*} \frac{1}{\sqrt{d_u + d_v}} \]
\[ = \sqrt{16} \left[ \frac{1}{\sqrt{16}} + \frac{1}{\sqrt{8}} \right] \]
\[ = \frac{4mn - 2m}{4} + \frac{4m}{2\sqrt{2}} \]
\[ = m \left( \frac{2n - 1}{2} + \sqrt{2} \right). \]
\[ ABC(TUC_4[m,n]) = \sum_{e=uv \in E(G)} \frac{d_u + d_v - 2}{d_u d_v} \]
\[ = |E_8| \sqrt{\frac{8 - 2}{16} + |E_6| \sqrt{\frac{6 - 2}{8}}} \]
\[ = (4mn - 2m) \left( \frac{\sqrt{6}}{4} \right) + 4m \left( \frac{\sqrt{2}}{2} \right) \]
\[ = m \left( \frac{2n - 1}{2} \sqrt{6} + 2\sqrt{2} \right). \]
\[ GA(TUC_4[m,n]) = \sum_{e=uv \in E(G)} \frac{2d_u}{d_u + d_v} \]
\[ = |E_8^*| \frac{2\sqrt{6}}{8} + |E_6^*| \frac{2\sqrt{8}}{6} \]
\[ = (4mn - 2m) + 4m \left( \frac{\sqrt{6}}{3} \right) \]
\[ = 4n + \frac{8\sqrt{2}}{3} - 2 \]

Now, by computing Randic connectivity index \( \chi(TUC_4[m,n]), \) sum-connectivity index \( X(TUC_4[m,n]), \) atom-bond connectivity index \( ABC(TUC_4[m,n]), \) and geometric-arithmetic index \( GA(TUC_4[m,n]) \) for every \( m \& n \in \mathbb{N} - \{1\} \) the proof of Theorem 1 is completed. □

**Corollary 1** By according to Randic connectivity index \( \chi(G_1=\text{TUC}_4[m,n]) \) sum-connectivity index \( X(G_1) \) atom-bond connectivity index \( ABC(G_1), \) and geometric-arithmetic index \( GA(G_1) \) in Theorem 1, we see that m is addition parameter. In other word, we can write four new indices with one variable n that independent of m as follow

\[ ABC_m(G_1) = \frac{ABC(G_1)}{m} = \frac{(2n - 1)\sqrt{6} + 2\sqrt{2}}{2}, \]
\[ GA_m(G_1) = \frac{GA(G_1)}{m} = \left( 4n + \frac{8\sqrt{2}}{3} - 2 \right) \]
\[ X_m(G_1) = \frac{X(G_1)}{m} = \frac{2n - 1}{2} + \sqrt{2} \]

and
\[ X_m(G_1) = X(G_1) = \frac{(2n - 1)\sqrt{2}}{2} + \frac{\sqrt{6}}{3}. \]

**Corollary 2** By use of above corollary and look at the planar figure of nanotube \( G_1=\text{TUC}_4[m,n] \) We see that, it's may be increased the graph \( G_1 \) as horizontal by increase m with any problem.

**Theorem 2** For all integer numbers \( m \& n \in \mathbb{N} - \{1\} : \)

I. Randic connectivity index \( \chi(G_2=\text{TUC}_4C_8[m,n]) \) nanotube is equal to
\[ \chi(TUC_4C_8[m,n]) = \left( 4n + \frac{2\sqrt{6}}{2} + \frac{1}{3} \right) \]

II. Sum-connectivity index \( X(TUC_4C_8[m,n]) \) nanotube is equal to
\[ X(TUC_4C_8[m,n]) = \left( 2\sqrt{6}n + 4\sqrt{5} - \sqrt{6} + \frac{1}{3} \right) \]

III. Atom-Bond connectivity index \( ABC(TUC_4C_8[m,n]) \) nanotube is equal to
\[ ABC(TUC_4C_8[m,n]) = \left( 8n + \frac{9\sqrt{2} - 4}{3} \right) \]

IV. Geometric-Arithmetic index of \( G_2=\text{TUC}_4C_8[m,n] \) nanotube is equal to
Proof. The proof is analogous to the proof of above theorem. Let $G_2$ be nanotubes $TUC_4C_8[m,n]$ \((m,n \in \mathbb{N} - \{1\})\). If we enumerate all octagons (any cycle $C_8$) in the first row by number 1, 2, ..., $m$ and enumerate all octagons in the first column by 1, 2, ..., $n$, then there exists $mn$ numbers of these octagons. Also, the number of quadrangles in the first row and end row is $m + m$ and implies that in general case of Nanotubes $TUC_4C_8[m,n]$ have $8mn + 4m$ vertices.

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By according to Definition 1, one can see the size of two partitions of vertex set $V(G_2)$ are equal to $2m + 2m$ and $8mn$. Therefore, the size of edge set $E(TUC_4C_8[m,n])$ will be 

$$V(G_2) = \frac{2(4m) + 3(8mn)}{2} = 12mn + 4m.$$ 

Now, by refer to Figure 3, readers can see that the yellow color edges are members of edge set $E_4$ and $E_4^*$ and the number of them is $m + m$. Other edges of quadrangles in the first row and end row, such that exit from vertices as degree 2 are members of edge set $E_5$ or $E_5^*$. So, all remaining edges are in $E_6$ and $E_6^*$.

ABC$TUC_4C_8[m,n]$ for nanotube $G_2=TUC_4C_8\{m,n\}$ similar nanotube $G_1=TUHRC_4\{m,n\}$. Thus we have following corollary:

Corollary 3 For nanotube $G_2=TUC_4C_8\{m,n\}$:

$$\chi_6(G_2) = \left(4n + \frac{24\sqrt{6}}{2} + \frac{1}{3}\right),$$

$$X_6(G_2) = \left(2\sqrt{6n} + 4\sqrt{\frac{6\sqrt{6}}{3}} + 1\right),$$

$$ABC_6(G_2) = \left(8n + \frac{9\sqrt{2} - 4}{3}\right).$$

Here, we complete the proof of Theorem 2. $\Box$

It is easy to see that Corollary 1 and Corollary 2 are true for nanotube $G_2=TUC_4C_8\{m,n\}$ similar nanotube $G_1=TUHRC_4\{m,n\}$. Thus we have following corollary:

Corollary 3 For nanotube $G_2=TUC_4C_8\{m,n\}$:

$$\chi_6(G_2) = \left(4n + \frac{24\sqrt{6}}{2} + \frac{1}{3}\right),$$

$$X_6(G_2) = \left(2\sqrt{6n} + 4\sqrt{\frac{6\sqrt{6}}{3}} + 1\right),$$

$$ABC_6(G_2) = \left(8n + \frac{9\sqrt{2} - 4}{3}\right).$$

Here, we complete the proof of Theorem 2. $\Box$
and 

\[ GA_n(G_2) = \left(12n + \frac{8\sqrt{6}}{5}\right) \].

3. Conclusion:

In this paper, we focus on the connected structure of two families nanotubes. The structure of \( TUHRC_4(S) \) and \( TUSC_4C_8(S) \) are similar and they are near families. Also, we count some connectivity indices of them. These connectivity indices are atom-bond connectivity index, geometric-arithmetic index, Randic connectivity index and sum-connectivity index.

References