Short communication

Computing Fourth Atom-bond Connectivity Index of V-Phenylenic Nanotubes and Nanotori

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Abstract

Among topological descriptors connectivity topological indices are very important and they have a prominent role in chemistry. One of them is atom-bond connectivity (*ABC*) index defined as $ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$, in which degree of vertex v denoted by d_v. Recently, a new version of atom-bond connectivity (ABC_4) index was introduced by *M. Ghorbani et.al* in 2010 and is defined as $ABC_4(G)=\sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_uS_v}}$, 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 this new topological index for *V-Phenylenic Nanotube and Nanotori*.

Keywords: V-phenylenic, nanotube, nanotori, topological index, Atom bond connectivity index.

1. Introduction

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«.

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 which applies graph theory to mathematical modeling of chemical phenomena.[1–3] This theory had an important effect on the development of the chemical sciences.

In mathematical chemistry, numbers encoding certain structural features of organic molecules and derived from the corresponding molecular graph, are called *graph invariants* or more commonly *topological indices*.

Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry. In other words, if G be the connected graph, then we can introduce many connectivity topological indices for it, by distinct and different definition. A connected graph is a graph such that there is a path between all pairs of vertices. One of the best known and widely used is the connectivity index, introduced in 1975 by *Milan Randić*[1], who has shown this index to reflect molecular branching and defined as follows:

$$\chi(G)=\sum_{e=uv\in E(G)}\frac{1}{\sqrt{d_ud_v}}, \tag{1}$$

where d_u denotes G degree of vertex u.

One of the important classes of connectivity indices is atom-bond connectivity (ABC) index defined as

$$ABC_{\text{general}}(G)=\sum_{uv\in E(G)}\sqrt{\frac{Q_u+Q_v-2}{Q_uQ_v}}, \tag{2}$$

where Q_v is some quantity that in a unique manner can be associated with the vertex v of the graph G. The first member of this class was considered by *E. Estrada et. al.,*[5] by setting Q_v and Q_u to be the degree of a vertex v and u:

$$ABC_1(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}. \tag{3}$$

The second and third members of this class were introduced by *A. Graovac* and *M. Ghorbani*[6] and *M. R. Farahani,*[7–9] separately as follow:

$$ABC_2(G)=\sum_{uv\in E(G)}\sqrt{\frac{n_u+n_v-2}{n_u n_v}}, \quad (4)$$

$$ABC_3(G)=\sum_{uv\in E(G)}\sqrt{\frac{m_u+m_v-2}{m_u m_v}}, \quad (5)$$

where n_u denotes the number of vertices of G whose distances to vertex u are smaller than those to other vertex v of the edge $e = uv$ ($n_u = \{x|x\in V(G), d(u,x)<d(x,v)\}$) and n_v is defined analogously. And m_u denotes the number of vertices of G whose distances to vertex u are smaller than those to other vertex v of the edge $e = uv$ ($m_u = \{f|f \in E(G), d(u,f)<d(f,v)\}$) and m_v is defined analogously.

Suppose S_v as the summation of degrees of all neighbors of vertex v in G. In other words, $S_u = \sum_{v\in N_G(u)} d_v$ and $N_G(u) = \{v\in V(G)|uv \text{ in } E(G)\}$. The fourth member of this class was considered by *M. Ghorbani et al.*[10], by setting Q_v to be the number S_v of vertex v:

$$ABC_4(G)=\sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_u S_v}} \quad (6)$$

In Refs[11–22] some topological indices of V-phenylenic nanotube and V-phenylenic nanotori are computed. In this paper, we continue this work to compute the fourth atom-bond connectivity index of molecular graphs related to V-phenylenic nanotube and nanotori. Our notation is standard and mainly taken from Refs.[1,2,23,24]

2. Main Results and Discussion

The goal of this section is to computing the ABC_4 index of V-phenylenic nanotube and nanotori. The novel phenylenic and naphthylenic lattices proposed can be constructed from a square net embedded on the toroidal surface. Phenylenes are polycyclic conjugated molecules, composed of four membered ring (= square) and six-membered rings (= hexagons) such that every four membered ring (4-membered cycle) is adjacent to two 6-membered cycles, and no two six-membered rings are mutually adjacent. Each four-membered ring lies between two six-membered rings, and each hexagon is adjacent only two four-membered rings. Because of such structural features phenylenes are very interesting conjugated species.[25–30] The rapid development of the experimental study of phenylenes motivated a number of recent theoretical studies of thee conjugated π-electron systems.[29]

Following *M. V. Diudea*[24] we denote a V-Phenylenic nanotube and V-Phenylenic nanotorus by *G=VPHX[m,n]* and *H = VPHY[m,n]*, respectively. The general representation of these nano structures are shown in Figure 1 and Figure 2. For more information and background materials, refer to paper series[11–30] again.

Now we have following theorems, immediately.

Theorem 1. $\forall m,n\in N$, the fourth atom-bond connectivity index of *V-Phenylenic Nanotube VPHX[m,n]* is equal to

$$ABC_4\big(VPHX\,[m,n]\big) = (4n+\sqrt{\frac{5}{6}}+\sqrt{\frac{7}{6}}-2)m \quad (7)$$

Proof. Consider the *V-phenylenic nanotube G = VPHX[m,n]* with *6mn* vertices and *9mn-m* edges (Figure 1). In V-phenylenic molecule, there are two partitions $V_2 = \{v \in V(G)|d_v = 2\}$ and $V_3 = \{v \in V(G)|d_v = 3\}$ of $V(VPHX[m,n])$, since the degree of an arbitrary vertex/atom of a molecular graph is equal to 2 or 3. Next, the two partitions of $E(G)$ are $E_5 = \{u,v \in V(G)|d_u = 3\&d_v = 2\}$ and $E_6 = \{u,v \in V(G)|d_u = d_v = 3\}$.

Also, two adjacent vertices v_1,v_2 of a vertex $v\in V_2$ have degree three, then $S_v = 2 \times 3 = 6$ and two edges vv_1 and vv_2 belong to E_5 (and $|E_5| = 2|V_2| = 4m$). Also, for all vertices u in first and end row of V-phenylenic nanotube with degree three, $N(u) = \{v_1,v_2,v_3\}$ such that $v_1\in V_2$ and $v_2,v_3\in V_3$ ($uv_1\in E_5$ and $uv_3,uv_2\in E_6$), thus $S_u = 2 \times 3 + 2 = 8$. Finally, for other vertices $S_w = 9$, because all other vertices and their edges belong to V_3 and E_6, respectively. So, the fourth atom-bond connectivity index of *VPHX[m,n] (m,n ≥ 1)* will be

$$\begin{aligned}ABC_4(VPHX[m,n]) &= \sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_u S_v}}\\ &=(4m)\sqrt{\frac{6+8-2}{6\times 8}}+(2m)\sqrt{\frac{8+8-2}{8\times 8}}+\\ &(2m)\sqrt{\frac{8+9-2}{8\times 9}}+(9mn-9m)\sqrt{\frac{9+9-2}{9\times 9}}\\ &=\frac{4m}{\sqrt{4}}+\frac{2m\sqrt{14}}{8}+\frac{2m}{2}\sqrt{\frac{5}{6}}+(9mn-9m)\frac{4}{9}\\ &=\left(4n+\sqrt{\frac{5}{6}}+\sqrt{\frac{7}{6}}-2\right)m\end{aligned} \quad (8)$$

Thus, the proof is completed.

Theorem 2. $\forall n,k \in N$ the fourth atom-bond connectivity index of all *k-regular* graph K with n vertices is equal to $\frac{n\sqrt{2(k^2-1)}}{2k}$.

Proof. Let K be a *k-regular* graph with n vertices. Then clearly, all vertices and edges of K belong to V_k and E_{2k}, respectively. For every vertex v of K, $S_v = k^2$, thus $ABC_4(K)=|E(K)|\sqrt{\frac{k^2+k^2-2}{k^2\times k^2}}=\frac{|E(K)|}{k^2}\sqrt{2(k^2-1)}=\frac{n\sqrt{2(k^2-1)}}{2k}$.

Example 1. Let K_n be the complete graph on n vertices. Then $|E(K_n)| = \frac{1}{2}n(n-1)$ *and* implies that $ABC_4(K_n)$

$ABC_4(K_n) = \frac{n\sqrt{2n(n-2)}}{2(n-1)}$

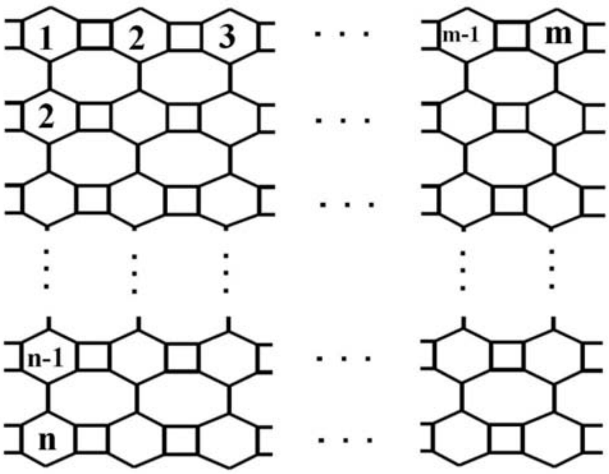

Figure 1. The Molecular Graph of V-Phenylenic Nanotube *VPHX[m,n].*

Example 2. Let C_n be the cycle of length n. Then for every $v\in V(C_n))$ $d_v = 2$ $S_v = 4$, So $ABC_4(C_n) = n\sqrt{6}/4$

Lemma 1. Let Q_n be a *Cubic* graph such that all n vertices of Q_n have degree 3. Then its fourth atom-bond connectivity index is equal to $2n/3$.

Proof. The proof is clear, by using proof of Theorem 2.

Theorem 2. $\forall m,n \geq 1$, *the fourth atom-bond connectivity index of V-Phenylenic Nanotori H = VPHY[m,n] is equal to* $ABC_4(H) = 4\,mn$.

Proof. The proof is easily, since by considering the *V-phenylenic nanotori H = VPHY[m,n]* with *6 mn* vertices and *9mn* edges (Figure 1). We see that this nanotori is a *Cubic* graph and all vertices belong to V_3 and $\forall v \in V(VPHY[m,n])$ $S_v = 9$. This implies that all edges belong

$$ABC_4(VPHX[m,n]) = (9mn)\sqrt{\frac{9+9-2}{9\times 9}} = (9mn)\frac{4}{9} = 4mn.$$

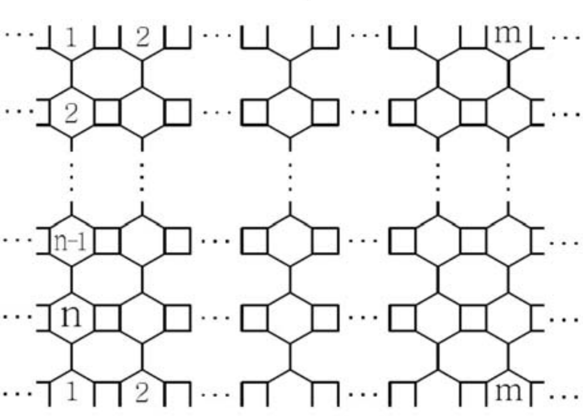

Figure 2. The Molecular Graph of V-Phenylenic Nanotorus *VPHY[m,n].*

to E_6, immediately. Thus $\forall m,n \geq 1 m,n \geq 1$, we have the following computations.

3. Conclusions

In this report, we study some properties of a new connectivity index of (molecular) graphs that called fourth atom-bond connectivity index. This connectivity index (ABC_4) index was proposed by *M. Ghorbani et.al* recently and was defined as

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

such that $\sum_{v\in N_G(u)} d_v$ is the

summation of degrees of all neighbors of vertex (atom) v in G ($N_G(u) = \{v\in V(G) | uv\in E(G)\}$.). In continue, closed analytical formulas for ABC_4 of a physico chemical structure of Phenylenic nanotubes and Nanotorus are given. These nano structures are V-Phenylenic Nanotube *VPHX[m,n]* and V-Phenylenic Nanotorus *VPHY[m,n].* The structures of V-Phenylenic Nanotube and V-Phenylenic Nanotorus consist of several $C_4C_6C_8$ net. A $C_4C_6C_8$ net is a trivalent decoration made by alternating C_4, C_6 and C_8. Phenylenes are polycyclic conjugated molecules, composed of four-and six-membered rings such that every four membered ring (= square) is adjacent to two six-membered rings (= hexagons). In other words, a composition of four-, six-and eight-membered rings in the structures of *VPHX[m,n]* and *VPHY[m,n]* is a $C_4C_6C_8$ net.

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Povzetek

Med topološkimi deskriptorji so zaradi pomena v kemiji zelo pomembni topološki indeksi. Mednje sodi indeks atomske povezanosti (*ABC*), definiran kot $ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$, kjer vozel grafa označuje d_V. Leta 2010 je uvedel Ghorbani s sodelavci konektivnost atom-vez kot indeks (ABC_4) in ga definiral kot $ABC_4(G)=\sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_uS_v}}$, kjer je $S_u=\sum_{v\in N_G(u)}d_v$ in $N_G(u)=\{v\in V(G)|uv\in E(G)\}$. V tem članku smo izračunali novi topološki indeks za *V* fenilensko nanocevko in nanozvitek.