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A Note on atom bond connectivity index

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ABSTRACT

The atom bond connectivity index of a graph is a new topological index was defined by E. Estrada as $ABC(G) = \sum_{uv\in E}\sqrt{(d_G(u)+d_G(v)-2)/d_G(u)d_G(v)}$, where $d_G(u)$ denotes degree of vertex *u*. In this paper we present some bounds of this new topological index.

Keywords: Topological index, ABC Index, nanotube, nanotori.

1. INTRODUCTION

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. 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. A simple graph is an unweighted, undirected graph without loops or multiple edges. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted.

Molecular descriptors play a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [1]. One of the best known and widely used is the connectivity index, χ, introduced in 1975 by Milan Randić [2], who has

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shown this index to reflect molecular branching. Recently Estrada et al. [3, 4, 5] 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 cyclo - alkanes. This index is defined as follows:

$$ABC(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}\ ,$$

where $d_G(u)$ stands for the degree of vertex *u*.

Recently, Graovac and Ghorbani defined a new version of the atom-bond connectivity index namely the second atom-bond connectivity index:

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

Some upper and lower bounds for the ABC_2 index of general graphs have been given in [6]. The goal of this paper is to study the properties of *ABC* and ABC_2 indices. Our notation is standard and mainly taken from standard books of chemical graph theory [7]. All graphs considered in this paper are finite, undirected, simple and connected. One can see the references [8 – 17], for more details about topological indices.

2. MAIN RESULTS AND DISCUSSION

In this section, we present some properties of atom bond connectivity indices. We refer the readers to references [18, 19].

The first Zagreb index is defined as $M_1(G) = \sum_{uv\in E} d_G(u) + d_G(v)$, where $d_G(u)$ denotes the degree of vertex *u*. The modified second Zagreb index $M_2^*(G)$ is equal to the sum of the products of the reciprocal of the degrees of pairs of adjacent vertices of the underlying molecular graph *G*, that is,

$$M_2^*(G) = \sum_{uv\in E} \frac{1}{d_G(u)d_G(v)}.$$

Theorem 1 ([18]). Let G be a connected graph with n vertices, p pendent vertices, m edges, maximal degree Δ, and minimal non-pendent vertex degree δ_1. Let M_1 and M_2^* be the first and modified second Zagreb indices of G. Then

$$ABC(G) \leq p\sqrt{1-\frac{1}{\Delta}} + \sqrt{[M_1 - 2m - p(\delta 1 - 1)](M_2^* - \frac{p}{\Delta}}).$$

Corollary 1 ([18]).With the same notation as in Theorem 1, $ABC(G) \leq \sqrt{(M_1 - 2m)M_2^*}$, with equality if and only if G is regular or bipartite semi–regular.

Theorem 2 ([19, Nordhaus–Gaddum–Type]). Let G be a simple connected graph of order n with connected complement $\bar{G}$. Then

$$ABC(G) + ABC(\bar{G}) \geq \frac{2^{3/4} n(n-1)\sqrt{k-1}}{k^{3/4}(\sqrt{k}+\sqrt{2})} \tag{1}$$

where $k = \max\{\Delta,\ n - \delta - 1\}$, and where Δ and δ are the maximal and minimal vertex degrees of G. Moreover, equality in (1) holds if and only if $G \approx P_4$.

Theorem 3 ([17]). Let G be a simple connected graph of order n with connected complement $\bar{G}$. Then

$$ABC(G) + ABC(\bar{G}) \leq (p + \bar{p})\sqrt{\frac{n-3}{n-2}}\left(1 - \sqrt{\frac{2}{n-2}}\right) + \binom{n}{2}\sqrt{\frac{2}{k} - \frac{2}{k^2}} \tag{2}$$

where p, $\bar{p}$ and δ_1, $\bar{\delta}_1$ are the number of pendent vertices and minimal non–pendent vertex degrees in G and $\bar{G}$, respectively, and $k = \min\{\delta_1,\ \bar{\delta}_1\}$. Equality holds in (2) if and only if $G \approx P_4$ or G is an r-regular graph of order $2r + 1$.

Theorem 4. Let G be a connected graph of order n with m edges and p pendent vertices, then

$$ABC_2(G) < p\sqrt{\frac{n-2}{n-1}} + (m - p).$$

Proof. Clearly, we can assume that $n \geq 3$. For each pendent edge uv of graph G we have $n_u = 1$ and $n_v = n - 1$. For each non-pendent edge uv of graph G we have $(n_u + n_v - 2)/n_u n_v < 1$. So

$$ABC_2(G) = \sum_{uv \in E} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} = \sum_{uv \in E, d_u = 1} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} + \sum_{uv \in E, d_u, d_v \neq 1} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}}$$
$$< p\sqrt{\frac{n-2}{n-1}} + m - p.$$

A simple calculation shows that the Diophantine equation $x + y - 2 = xy$ does not have any integer solution. Then the upper bound does not happen.

Theorem 5. Let T a tree of order $n > 2$ with p pendent vertices. Then

$$ABC_2(T) \leq p\sqrt{\frac{n-2}{n-1}} + \frac{\sqrt{2}}{2}(n - p - 1) \qquad (2)$$

with equality if and only if $T \cong K_{1,n-1}$ or $T \cong S(2r, s)$ where $n = 2r + s + 1$.

Proof. For any edge uv of trees we have $n_u + n_v = n$. If T be an arbitrary tree with $n \geq 3$ vertex, then ABC_2 is simplified as

$$ABC_2(T) = \sqrt{n-2} \sum_{uv \in E(T)} \frac{1}{\sqrt{n_u n_v}}.$$

Now we assume, the tree T have p pendent vertex, then there are exist p edge that $n_u = 1$ and $n_v = n - 1$. For each non-pendent edge uv of tree T, $2 \leq n_u, n_v \leq n - 2$ and then $n_u n_v \geq 2(n-2)$. This implies that $\sqrt{n_u n_v} \geq \sqrt{2(n-2)}$ and so $\frac{1}{\sqrt{n_u n_v}} \leq \frac{1}{\sqrt{2(n-2)}}$.

Hence,

$$ABC_2(T) = \sqrt{n-2}\left(\sum_{\substack{uv \in E(T), \\ d_u = 1}} \frac{1}{\sqrt{n_u n_v}} + \sum_{\substack{uv \in E(T), \\ d_u, d_v \neq 1}} \frac{1}{\sqrt{n_u n_v}} \right)$$
$$\leq \sqrt{n-2}\left(\frac{p}{\sqrt{n-1}} + \frac{n-p-1}{\sqrt{2(n-2)}} \right) = p\sqrt{\frac{n-2}{n-1}} + \frac{\sqrt{2}}{2}(n-p-1). \qquad (7)$$

Suppose now that equality holds in (6), we can consider the following cases:

Case (a): $p = n - 1$. From equality in (7), we must have $n_u = n-1$ and $n_v = 1$ for each edge $uv \in E(T)$ and $n_u \geq n_v$, that is, each edge uv must be pendent. Since T is a tree, $T \cong K_{1,n-1}$.

Case (*b*): $p < n - 1$. In this case the diameter of T is strictly greater than 2. So there is a neighbor of a pendent vertex, say u, adjacent to some non-pendent vertex k. Since $n_u = n - 2$ and $n_v = 2$ for each non−pendent edge $uv \in E(T)$, $n_u \geq n_v$ we conclude that the degree of each neighbor of a pendent vertex is two and each such vertex is adjacent to vertex k. In addition, also the remaining pendent vertices are adjacent to vertex k. Hence T is isomorphic to $T \cong S(2r, s)$ where $n=2r+s+1$. Conversely, one can see easily that the equality in (1) holds for star $K_{1,n-1}$ or $S(2r,s)$ where $n = 2r + s + 1$.

3. ATOM BOND CONNECTIVITY INDEX OF NANOSTRUCTURES

The goal of this section is computing the *ABC* index of a lattice of $TUC_4C_8[p, q]$, with q rows and p columns. Then we compute this topological index for its nanotubes. Finally, we calculate *ABC* index of $TUC_4C_8[p, q]$, see Figure 1.

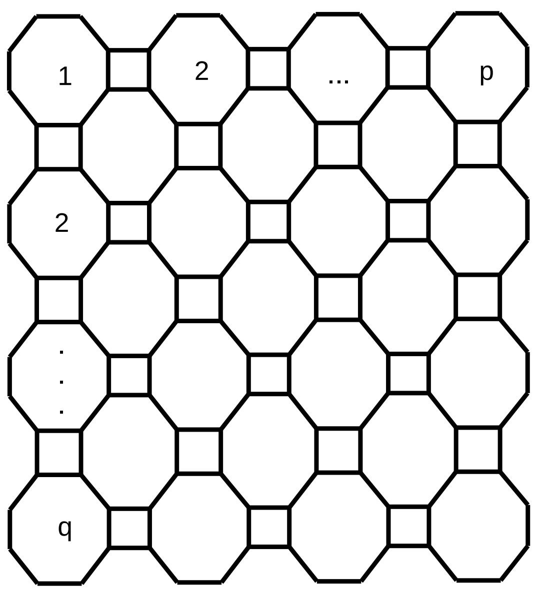

Figure 1. $2 - D$ graph of Lattice $C_4C_8[4, 4]$.

Example 1. Let P_n be a path with n vertices. It is easy to see that P_n has exactly 2 edges with endpoints degrees 1 and 2. Other edges endpoints are of degree 2.

$$ABC(P_n) = (n-1)\frac{\sqrt{2}}{2}.$$

Example 2. Consider the graph C_n of a cycle with n vertices. Every vertex of a cycle is of degree 2. In other words,

$$ABC(C_n) = n\frac{\sqrt{2}}{2}.$$

Example 3. A star graph with n + 1 vertices is denoted by S_n. This graph has a central vertex of degree n and the others are of degree 1. Hence the *ABC* index is as follows:

$$ABC(C_n) = \sqrt{n(n-1)}.$$

Consider now 2 dimensional graph of lattice $G = TUC_4C_8[p, q]$ depicted in Figure 1. Degrees of edge endpoints of this graph are as follows:

Edge Endpoints	**[2, 2]**	**[2, 3]**	**[3, 3]**
Number of Edges of This Type	$2p + 2q + 4$	$4p + 4q$-8	$12pq$-$8(p + q) + 4$

On the other hand by summation these values one can see that:

$$ABC(G) = (12pq - 8p - 8q + 4)\frac{2}{3} + (2p + 2q + 4)\frac{\sqrt{2}}{2} + (4p + 4q - 8)\frac{\sqrt{2}}{2}$$

$$= 8pq + \frac{2}{3}(4 - 8p - 8q) + (3p + 3q - 2)\sqrt{2}.$$

Hence, we proved the following theorem:

Theorem 6. Consider 2 - D graph of lattice $G = C_4C_8[p, q]$. Then

$$ABC(G) = 8pq + \frac{2}{3}(4 - 8p - 8q) + (3p + 3q - 2)\sqrt{2}.$$

In continuing consider the graph of nanotube $H = C_4C_8[p, q]$, shown in Figure 2. Similar to Theorem 6, we have the following values for endpoint degrees of vertices of H.

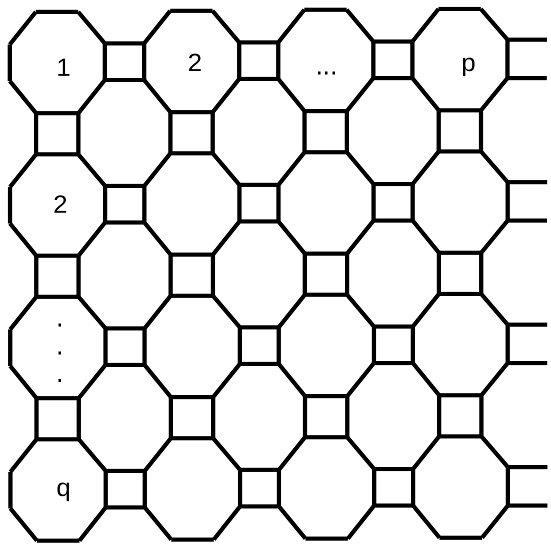

Figure 2. $2 - D$ Graph of $C_4C_8[4,4]$ Nanotube.

Edge Endpoints	**[2, 2]**	**[2, 3]**	**[3, 3]**
Number of Edges of This Type	$2p$	$4p$	$12pq$-$8p$

Thus, we can deduce the following formula for *ABC* index:

$$ABC(H)=\frac{2}{3}(12pq-8p)+2p\frac{\sqrt{2}}{2}+4p\frac{\sqrt{2}}{2}=8pq-\frac{16}{3}p+3p\sqrt{2}.$$

So, the proof of the following theorem is clear.

Theorem 8. Consider 2 - D graph of nanotube $H = TUC_4C_8[p, q]$. Then

$$ABC(H)=8pq-\frac{16}{3}p+3p\sqrt{2}.$$

Theorem 9. Consider the graph of nanotori $K = C_4C_8[p, q]$ in Figure 3. The *ABC* index of K is $ABC(K)=8pq$.

Proof. It is easy to see that this graph has $12pq$ edges. On the other hand, K is 3 regular graph and this complete the proof.

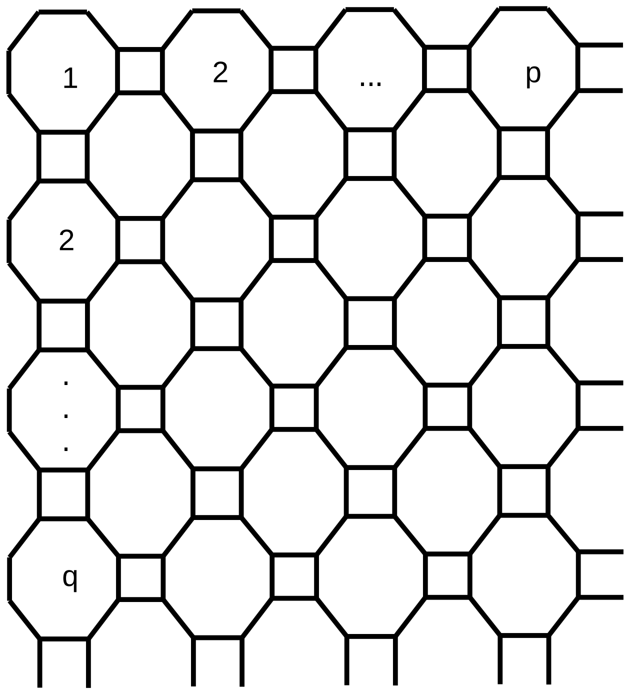

Figure 3. $2 - D$ graph of $K = C_4C_8[4,4]$ Nanotorus.

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