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 $\text{ABC}(G) = \sum_{uv \in E} \sqrt{d_G(u) + d_G(v) - 2}/d_G(u)d_G(v)$, 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, $\chi$, 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:

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

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 \( \Delta \), and minimal non-pendent vertex degree \( \delta_1 \). 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 \( \overline{G} \). Then
\[
ABC(G) + ABC(\overline{G}) \geq \frac{2^{3/4}n(n-1)\sqrt{k-1}}{k^{3/4}(\sqrt{k} + \sqrt{2})}
\]
where \( k = \max\{\Delta, n - \delta - 1\} \), and where \( \Delta \) and \( \delta \) 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 \( \overline{G} \). Then
\[
ABC(G) + ABC(\overline{G}) \leq (p + \overline{p})\sqrt{\frac{n-3}{n-2} \left(1 - \sqrt{\frac{2}{n-2}}\right)} + \binom{n}{2}\sqrt{\frac{2}{k} - \frac{2}{k^2}}
\]
where \( p, \overline{p} \) and \( \delta_1, \overline{\delta}_1 \) are the number of pendent vertices and minimal non–pendent vertex degrees in \( G \) and \( \overline{G} \), respectively, and \( k = \min\{\delta_1, \overline{\delta}_1\} \). 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 $(n_u + n_v - 2)/n_un_v < 1$. So

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

$$< p \sqrt{\frac{n-2}{n-1} + m - p}.$$

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

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

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

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

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 $n_un_v \geq 2(n-2)$. This implies that $\sqrt{n_un_v} \geq \sqrt{2(n-2)}$ and so

$$\frac{1}{\sqrt{n_un_v}} \leq \frac{1}{\sqrt{2(n-2)}}.$$ 

Hence,

$$ABC_2(T) = \sqrt{n-2} \left( \sum_{uv \in T} \frac{1}{\sqrt{n_un_v}} + \sum_{uv \in T, d_u, d_v \neq 1} \frac{1}{\sqrt{n_un_v}} \right)$$

$$\leq \sqrt{n-2} \left( \frac{p}{\sqrt{n-1}} + \frac{n-p-1}{\sqrt{2(n-2)}} \right) = p \sqrt{\frac{n-2}{n-1} + \frac{\sqrt{2}}{2}(n-p-1)}.$$
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 \( C_4C_8[4, 4] \).](image)
**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:

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

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:

<table>
<thead>
<tr>
<th>Edge Endpoints</th>
<th>[2, 2]</th>
<th>[2, 3]</th>
<th>[3, 3]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Edges of This Type</td>
<td>$2p + 2q + 4$</td>
<td>$4p + 4q - 8$</td>
<td>$12pq - 8(p + q) + 4$</td>
</tr>
</tbody>
</table>

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 $H$. 

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

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

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.

REFERENCES