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Comparison between Atom–Bond Connectivity Indices of Graphs

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Abstract

The atom–bond connectivity index ABC is a much studied degree–based graph invariant with noteworthy applications in chemistry. Few years ago, a new distance–based variant of this index, ABC_{GG} , was introduced. We establish relations between the two ABC-indices. In particular, we determine classes of graph for which ABC is greater than (resp. equal to or less than) ABC_{GG}.

1 Introduction

In this paper we are concerned with finite, simple, undirected, and connected graphs, bearing in mind that all molecular graphs are of this type [21]. Let $G = (V(G), E(G))$

such a graph, with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n \geq 2$ and $|E(G)| = m \geq 1$. The edge whose end-vertices are v_i and v_j will be denoted by $v_i v_j$.

The degree of the vertex $v_i \in V(G)$ is denoted by d_i , $i = 1, 2, \ldots, n$. A vertex is said to be pendent if its neighborhood contains exactly one vertex. An edge of a graph is said to be pendent if one of its end-vertices is pendent.

The original atom–bond connectivity index (ABC) was introduced in the 1990s and is defined as [11]:

$$ABC = ABC(G) = \sum_{v_i\, v_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i\, d_j}}\,. \tag{1}$$

This molecular structure descriptor proved to have outstanding predictive power, especially with regard to thermodynamic properties of saturated hydrocarbons [10, 11, 13, 22, 23]. Its mathematical properties were also extensively investigated, see the recent articles [1, 3–5, 7, 8, 12, 14, 20, 25, 26, 29] and the references cited therein.

Let G be a connected graph and $e = v_i v_j \in E(G)$. The number of vertices of G whose distance to the vertex v_i is smaller than the distance to the vertex v_j is denoted by $n_i = n_i(e|G)$. Analogously, $n_j = n_j(e|G)$ is the number of vertices of G whose distance to the vertex v_j is smaller than to v_i.

Motivated by the success of the original ABC-index, Eq. (1), Graovac and Ghorbani [15] put forward its new variant, defined as

$$ABC_{GG} = ABC_{GG}(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{n_i + n_j - 2}{n_i\, n_j}}\,. \tag{2}$$

This distance–based variant of the atom–bond connectivity index was until now studied only to a limited extent [6, 15, 27, 28].

Throughout this paper, by K_n, $K_{p,q}$ $(p + q = n)$, $K_{1,n-1}$, P_n, and C_n, we denote, respectively, the complete graph, complete bipartite graph, star, path, and cycle on n vertices [2].

If $V(G)$ is the disjoint union of two nonempty sets $V_1(G)$ and $V_2(G)$, such that every vertex in $V_1(G)$ has degree r and every vertex in $V_2(G)$ has degree s, then G is said to be (r, s)-semiregular.

The double star $DS_{p,q}$ $(p+q=n)$, is the tree of order n, constructed by joining the central vertices of two stars $K_{1,p-1}$ and $K_{1,q-1}$.

For other undefined notations and terminology from graph theory, the readers are referred to [2].

In this paper, we are concerned with the comparison of the two ABC-indices. In particular, we determine classes of graph for which one of the relations $ABC > ABC_{GG}$, $ABC = ABC_{GG}$, or $ABC < ABC_{GG}$ holds. Directly from the definitions of the two ABC-indices, Eqs. (1) and (2) we obtain the following elementary results:

Example 1.

$$ABC(K_n) = \frac{n}{2}\sqrt{2n-4} \qquad \textit{and} \qquad ABC_{GG}(K_n) = 0$$

and therefore,

$$\begin{aligned} ABC(K_n) &= ABC_{GG}(K_n) && \textit{for } n=2, \\ ABC(K_n) &> ABC_{GG}(K_n) && \textit{for } n \geq 3. \end{aligned}$$

Example 2.

$$ABC(K_{p,q}) = ABC_{GG}(K_{p,q}) = pq\sqrt{\frac{p+q-2}{p\,q}}\,.$$

Example 3. *Let $n \geq 3$. Then,*

$$ABC(P_n) = \frac{n-1}{\sqrt{2}} \qquad \textit{and} \qquad ABC_{GG}(P_n) = \sum_{i=1}^{n-1}\sqrt{\frac{n-2}{i\,(n-i)}}$$

and therefore

$$\begin{aligned} ABC(P_n) &= ABC_{GG}(P_n) && \textit{for } n=2,3, \\ ABC(P_n) &< ABC_{GG}(P_n) && \textit{for } 4 \leq n \leq 9, \\ ABC(P_n) &> ABC_{GG}(P_n) && \textit{for } n \geq 10\,. \end{aligned}$$

Example 4.

$$ABC(C_n) = \frac{n}{\sqrt{2}} \qquad \textit{and} \qquad ABC_{GG}(C_n) = \begin{cases} 2\sqrt{n-2} & \textit{if } n \textit{ is even} \\ \dfrac{2n}{n-1}\sqrt{n-3} & \textit{if } n \textit{ is odd,} \end{cases}$$

and therefore

$$\begin{aligned} ABC(C_n) &= ABC_{GG}(C_n) && \textit{for } n=4,5, \\ ABC(C_n) &> ABC_{GG}(C_n) && \textit{for } n=3 \textit{ and } n \geq 6. \end{aligned}$$

Example 5. *For $p \geq 2$, the double star $DS_{p,p}$ has $2p$ vertices,*

$$ABC(DS_{p,p}) = 2(p-1)\sqrt{\frac{p-1}{p}} + \frac{\sqrt{2\,(p-1)}}{p}$$

$$ABC_{GG}(DS_{p,p}) = 2(p-1)\sqrt{\frac{2\,(p-1)}{2\,p-1}} + \frac{\sqrt{2\,(p-1)}}{p}$$

and therefore

$$ABC(DS_{p,p}) < ABC_{GG}(DS_{p,p})\,.$$

From the above examples we see that all the three cases $ABC < ABC_{GG}$, $ABC = ABC_{GG}$, and $ABC > ABC_{GG}$ may occur. In what follows we show how ABC and ABC_{GG} can be compared in the case of several special classes of graphs.

2 Comparing *ABC* indices of graphs

Theorem 6. *Let G be a connected bipartite (r,s)-semiregular graph. Then*

$$ABC(G) \geq ABC_{GG}(G) \tag{3}$$

with equality holding if and only if $G \cong K_{r,s}$ for $r,s \geq 1$.

Proof. If $G \cong K_{r,s}$, then in Example 2 we have seen that the equality holds in (3). Consider therefore the case $G \ncong K_{r,s}$. Then we have

$$ABC(G) = m\sqrt{\frac{r+s-2}{rs}} \qquad \text{and} \qquad ABC_{GG}(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{r+s+a_i+b_j-2}{(r+a_i)\,(s+b_j)}}$$

where $n_i = r + a_i$ and $n_j = s + b_j$. Since G is a connected bipartite (r,s)-semiregular graph and $G \ncong K_{r,s}$, we have $a_i, b_j \geq 1$. Moreover, $r \geq s \geq 2$.

First we have to show that

$$\sqrt{\frac{r+s-2}{rs}} > \sqrt{\frac{r+s+a_i+b_j-2}{(r+a_i)\,(s+b_j)}} \tag{4}$$

that is,

$$\left(\frac{1}{r} - \frac{1}{r+a_i}\right) + \left(\frac{1}{s} - \frac{1}{s+b_j}\right) > \frac{2}{r\,s} - \frac{2}{(r+a_i)\,(s+b_j)}$$

that is,

$$s\,a_i\,(s+b_j-2)+r\,b_j\,(r+a_i-2)>2\,a_i\,b_j$$

which is true, because $a_i, b_j \geq 1$ and $r \geq s \geq 2$.

By (4), we have

$$ABC(G)-ABC_{GG}(G)=\sum_{v_iv_j\in E(G)}\left[\sqrt{\frac{r+s-2}{rs}}-\sqrt{\frac{r+s+a_i+b_j-2}{(r+a_i)\,(s+b_j)}}\,\right]>0\,.$$

This completes the proof of the theorem. □

A tree is said to be starlike if exactly one of its vertices has degree greater than two. By $S(n_1, n_2, \ldots, n_k)$ we denote the starlike tree which has a vertex v_1 of degree $k \geq 3$ and which has the property $S(n_1, n_2, \ldots, n_k) \setminus \{v_1\} = P_{n_1} \cup P_{n_2} \cup \cdots \cup P_{n_k}$.

This tree has $n_1 + n_2 + \ldots + n_k + 1 = n$ vertices and it will be assumed that $n_1 \geq n_2 \geq \cdots \geq n_k \geq 1$.

Lemma 7. *For positive integer $n \geq 13$,*

$$\sqrt{n-2}\,\left[\frac{1}{\sqrt{n-1}}+\frac{1}{\sqrt{3(n-3)}}+\frac{1}{\sqrt{4(n-4)}}\right]<\frac{3}{\sqrt{2}}\,.$$

Proof. Consider the function

$$f(n)=\sqrt{n-2}\,\left[\frac{1}{\sqrt{n-1}}+\frac{1}{\sqrt{3(n-3)}}+\frac{1}{\sqrt{4(n-4)}}\right]\,.$$

Then we have

$$f(n+1)-f(n)=\sqrt{n-1}\,\left[\frac{1}{\sqrt{n}}+\frac{1}{\sqrt{3(n-2)}}+\frac{1}{\sqrt{4(n-3)}}\right]$$

$$-\ \sqrt{n-2}\,\left[\frac{1}{\sqrt{n-1}}+\frac{1}{\sqrt{3(n-3)}}+\frac{1}{\sqrt{4(n-4)}}\right]$$

$$=\ \left(\sqrt{\frac{n-1}{n}}-\sqrt{\frac{n-2}{n-1}}\right)+\left(\sqrt{\frac{n-1}{3(n-2)}}-\sqrt{\frac{n-2}{3(n-3)}}\right)+\left(\sqrt{\frac{n-1}{4(n-3)}}-\sqrt{\frac{n-2}{4(n-4)}}\right)$$

$$= \frac{1}{\sqrt{n(n-1)}\left(n-1+\sqrt{n^2-2n}\right)} - \frac{1}{\sqrt{3(n-2)(n-3)}\left(n-2+\sqrt{(n-2)^2-1}\right)}$$

$$- \frac{1}{\sqrt{(n-3)(n-4)}\left(\sqrt{n^2-5n+4}+\sqrt{n^2-5n+6}\right)} < 0$$

as

$$\sqrt{(n-3)(n-4)}\left(\sqrt{n^2-5n+4}+\sqrt{n^2-5n+6}\right) < \sqrt{n(n-1)}\left(n-1+\sqrt{n^2-2n}\right).$$

Therefore

$$f(n+1) < f(n) < f(n-1) < \cdots < f(14) < f(13) = \sqrt{11}\left[\frac{1}{\sqrt{12}} + \frac{1}{\sqrt{30}} + \frac{1}{6}\right] < \frac{3}{\sqrt{2}}.$$

□

Theorem 8. *For $k \geq 2$,*

$$ABC(S(\underbrace{2,2,\ldots,2}_{k})) < ABC_{GG}(S(\underbrace{2,2,\ldots,2}_{k})) \qquad (5)$$

$$ABC(S(\underbrace{3,3,\ldots,3}_{k})) < ABC_{GG}(S(\underbrace{3,3,\ldots,3}_{k})). \qquad (6)$$

Proof. Consider first the starlike tree $S(\underbrace{2,2,\ldots,2}_{k})$, which has $n = 2k+1$ vertices and

$$ABC(S(2,2,\ldots,2)) = \frac{n-1}{\sqrt{2}} = \frac{2k}{\sqrt{2}}$$

$$ABC_{GG}(S(2,2,\ldots,2)) = k\sqrt{\frac{n-2}{1\cdot(n-1)}} + k\sqrt{\frac{n-2}{2\cdot(n-2)}} = k\sqrt{\frac{n-2}{n-1}} + \frac{k}{\sqrt{2}}.$$

If $k \geq 2$, then $n \geq 5$ and

$$\sqrt{\frac{n-2}{n-1}} > \frac{1}{\sqrt{2}}$$

and therefore

$$k\sqrt{\frac{n-2}{n-1}} + \frac{k}{\sqrt{2}} > \frac{2k}{\sqrt{2}}$$

implying inequality (5).

The starlike tree $S(\underbrace{3,3,\dots,3}_{k})$ has $n = 3k+1$ vertices and

$$\begin{aligned} ABC(S(3,3,\dots,3)) &= \frac{n-1}{\sqrt{2}} = \frac{3k}{\sqrt{2}} \\ ABC_{GG}(S(3,3,\dots,3)) &= k\sqrt{\frac{n-2}{1\cdot(n-1)}} + k\sqrt{\frac{n-2}{2\cdot(n-2)}} + k\sqrt{\frac{n-2}{3\cdot(n-3)}} \\ &= k\left(\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{n-2}{3(n-3)}}\right) + \frac{k}{\sqrt{2}}\,. \end{aligned}$$

Note now that since $n \geq 7$,

$$\sqrt{\frac{n-2}{n-1}} \geq \sqrt{\frac{7-2}{7-1}} = \sqrt{\frac{5}{6}}$$

whereas

$$\sqrt{\frac{n-2}{3(n-3)}} > \lim_{n\to\infty}\sqrt{\frac{n-2}{3(n-3)}} = \sqrt{\frac{1}{3}}\,.$$

Therefore

$$\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{n-2}{3(n-3)}} > \sqrt{\frac{5}{6}} + \sqrt{\frac{1}{3}} > \sqrt{2}$$

and therefore

$$k\left(\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{n-2}{3(n-3)}}\right) + \frac{k}{\sqrt{2}} > \frac{3k}{\sqrt{3}}$$

from which inequality (6) follows. $\square$

In contrast to Theorem 8, we have the following result:

Theorem 9. *Let $S(n_1, n_2, \dots, n_k)$ be a starlike tree of order n, such that $n_1 \geq n_2 \geq \cdots \geq n_k \geq 4$. Then*

$$ABC(S) > ABC_{GG}(S)\,.$$

Proof. For a starlike tree S, we have either $d_i = 2$ or $d_j = 2$ for any edge $v_iv_j \in E(S)$. Therefore

$$\sqrt{\frac{d_i + d_j - 2}{d_i\, d_j}} = \frac{1}{\sqrt{2}} \qquad \text{for any edge } \; v_iv_j \in E(S)\,.$$

Therefore

$$ABC(S) = \frac{n-1}{\sqrt{2}}\,. \tag{7}$$

By the definition of ABC_{GG}, we have

$$ABC_{GG}(S) = \sum_{i=1}^{k}\sum_{j=1}^{n_i}\sqrt{\frac{n-2}{j\,(n-j)}} \leq \sum_{i=1}^{k}\left[\sum_{j=1}^{4}\sqrt{\frac{n-2}{j\,(n-j)}}+\frac{n_i-4}{\sqrt{2}}\right]$$
$$= \sum_{i=1}^{k}\left[\sqrt{\frac{n-2}{(n-1)}}+\frac{1}{\sqrt{2}}+\sqrt{\frac{n-2}{3\,(n-3)}}+\sqrt{\frac{n-2}{4\,(n-4)}}\right]+\frac{n-4\,k-1}{\sqrt{2}}\,.$$

Applying Lemma 7 and Eq. (7), from the above, we get

$$ABC_{GG}(S)-ABC(S) = k\,\sqrt{n-2}\left[\frac{1}{\sqrt{n-1}}+\frac{1}{\sqrt{3\,(n-3)}}+\frac{1}{\sqrt{4\,(n-4)}}\right]-\frac{3\,k}{\sqrt{2}} < 0\,.$$

This completes the proof. □

Let Γ be the class of (connected) graphs such that all neighbors of any vertex of degree greater than two are vertices of degree two. In particular, $S(\underbrace{2,2,\ldots,2}_{k}) \in \Gamma$.

Theorem 10. *Let $G \in \Gamma$. If G has no pendent vertex, then $ABC(G) > ABC_{GG}(G)$.*

Proof. From the definition of Γ, we have $d_i = 2$ or $d_j = 2$ for any edge $v_iv_j \in E(G)$, $G \in \Gamma$. Moreover, G has no pendent edge. Thus we have

$$\frac{1}{n_i}+\frac{1}{n_j}-\frac{2}{n_i\,n_j} \leq \frac{1}{2} = \frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_i\,d_j} \quad \text{for any edge } \; v_iv_j \in E(G), G \in \Gamma.$$

Hence the theorem. □

3 Comparing *ABC* indices of hexagonal systems

Hexagonal systems provide the graph representation of benzenoid hydrocarbons. Their theory has been extensively studied; for details see [9, 16–18].

Theorem 11. *Let H be a hexagonal system. Then*

$$ABC(H) > ABC_{GG}(H)\,.$$

Proof. Let H be a hexagonal system with n vertices and m edges. Then $n \geq 6$ and $m \geq 6$, with equality if and only if H possesses a single hexagon, i.e., if $H \cong C_6$.

From the definition of the hexagonal systems [17], one can easily see that $(d_i, d_j) = (2,2)$ or $(2,3)$ or $(3,3)$ for any edge $v_iv_j \in E(H)$. Moreover, as shown in [19] (see also [9,24]), $n_i \geq 3$ and $n_j \geq 3$ for any edge $v_iv_j \in E(H)$ and $n_i + n_j = n$ as H is bipartite. For any edge $v_iv_j \in E(H)$,

$$\frac{d_i + d_j - 2}{d_i\, d_j} = \begin{cases} \dfrac{1}{2} & \text{if } d_i = 2 \text{ or } d_j = 2 \\ \\ \dfrac{4}{9} & \text{if } d_i = 3 \text{ and } d_j = 3 \end{cases}$$

implying that

$$\min_{v_iv_j \in E(H)} \sqrt{\frac{d_i + d_j - 2}{d_i\, d_j}} = \sqrt{\frac{4}{9}} = \frac{2}{3}\,. \tag{8}$$

Moreover,

$$\frac{n_i + n_j - 2}{n_i\, n_j} \leq \frac{n-2}{3\,(n-3)} \tag{9}$$

for any edge $v_iv_j \in E(H)$. In fact,

$$\frac{n_i + n_j - 2}{n_i\, n_j} = \frac{n-2}{3\,(n-3)}$$

holds for all edges of H if and only if $H \cong C_6$. In all other cases, H possesses edges for which the inequality (9) is strict.

Hexagonal systems possess at least 6 vertices. For $n \geq 6$,

$$\frac{2}{3} > \sqrt{\frac{n-2}{3(n-3)}}\,. \tag{10}$$

In view of Eqs. (1) and (8), and since H has m edges,

$$ABC(H) > \frac{2m}{3}\,. \tag{11}$$

Inequality (11) is strict because any hexagonal system possesses (at least six) vertices of degree 2.

Combining relations (9), (10), and (11), we obtain

$$ABC(H) > \frac{2m}{3} > m\sqrt{\frac{n-2}{3(n-3)}} \geq \sum_{v_iv_j \in E(G)} \sqrt{\frac{n_i + n_j - 2}{n_i\, n_j}} = ABC_{GG}(H)\,.$$

$\square$

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