On Atom-Bond Connectivity Index

Bo Zhou and Rundan Xing

Department of Mathematics, South China Normal University, Guangzhou 510631, P. R. China

Reprint requests to B. Z.; E-mail: zhoubo@scnu.edu.cn

Z. Naturforsch. **66a,** 61 – 66 (2011); received January 23, 2010 / revised June 5, 2010

The atom-bond connectivity (ABC) index, introduced by Estrada et al. in 1998, displays an excellent correlation with the formation heat of alkanes. We give upper bounds for this graph invariant using the number of vertices, the number of edges, the Randić connectivity indices, and the first Zagreb index. We determine the unique tree with the maximum ABC index among trees with given numbers of vertices and pendant vertices, and the n-vertex trees with the maximum, and the second, the third, and the fourth maximum ABC indices for $n \geq 6$.

Key words: Atom-Bond Connectivity Index; Randić Connectivity Indices; First Zagreb Index; Trees.

1. Introduction

Topological indices are numbers reflecting certain structural features of a molecule that are derived from its molecular graph [1]. They may be used in theoretical chemistry for the design of chemical compounds with given physicochemical properties or given pharmacologic and biological activities.

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, $d_G(u)$ or d_u denotes the degree of u in G. Estrada et al. [2] proposed a topological index named the atom-bond connectivity (ABC) index. It is defined as

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

This index has proven to be a valuable predictive index in the study of the formation heat in alkanes [2]. Estrada [3] developed a basically topological approach on the basis of the ABC index which explains the differences in the energy of linear and branched alkanes both qualitatively and quantitatively. Recently, Furtula et al. [4] determined the extremal (minimum and maximum) values of this index for chemical trees and showed that the star is the unique tree with the maximum ABC index.

For a graph G, two types of Randić connectivity indices are defined as [5]

$$R_{-1/2} = R_{-1/2}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}},$$

$$R_{-1} = R_{-1}(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

The former is one of the most popular descriptors and has found countless quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) applications, see, e. g., [5 – 7], while the latter is also used to develop structure-based correlations for physical properties, see, e. g., [8]. See [9] for history and [10] for mathematical properties of $R_{-1/2}$ and R_{-1}.

Another molecular descriptor in QSPR and QSAR used here is the first Zagreb index. For a graph G, it is defined as $M_1 = M_1(G) = \sum_{u \in V(G)} d_u^2$, see [5].

In this paper, we give upper bounds for the ABC index using the number of vertices, the number of edges, the Randić connectivity indices, and the first Zagreb index, and we determine the unique tree with the maximum ABC index among trees with given numbers of vertices and pendant vertices, and the n-vertex trees with the maximum and the second maximum ABC indices for $n \geq 4$, the third maximum ABC index for $n \geq 5$, and the fourth maximum ABC index for $n \geq 6$.

2. ABC Index of Graphs

A graph is a semiregular bipartite graph of degrees r, s if it is bipartite and each vertex in one partite set has degree r and each vertex in the other partite set has degree s. Define the auxiliary value of such a graph to be $\frac{r+s-2}{rs}$.

Proposition 1 *Let G be a graph with n vertices and m edges. Then*

$$ABC(G) \leq \sqrt{m\,(n-2R_{-1})}$$

with equality if and only if one of the following conditions is satisfied:
(i) $m=0$*;*
(ii) G has no isolated vertices, and every edge is incident with a vertex of degree two;
(iii) G has no isolated vertices and no vertex of degree two, and every component of G is either a regular graph of degree, say r for all such components (if exist), or a nonregular semiregular bipartite graph and all such components (if exist) have equal auxiliary value, which is equal to $\frac{2r-2}{r^2}$ *if there exist both types of the components.*

Proof: By the Cauchy-Schwarz inequality,

$$\begin{aligned} ABC(G) &= \sum_{uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\ &\leq \sqrt{m \sum_{uv\in E(G)} \frac{d_u+d_v-2}{d_u d_v}} \\ &= \sqrt{m \sum_{uv\in E(G)} \left(\frac{1}{d_u}+\frac{1}{d_v}-\frac{2}{d_u d_v}\right)} \\ &= \sqrt{m\left(\sum_{\substack{u\in V(G)\\ d_u\geq 1}} \frac{1}{d_u}\cdot d_u - 2R_{-1}\right)} \\ &\leq \sqrt{m\,(n-2R_{-1})} \end{aligned}$$

with equalities if and only if either $m=0$ or G has no isolated vertices and for any edge uv of G, $\frac{d_u+d_v-2}{d_u d_v}$ is a constant, say c. Obviously, $c\geq 0$.

Suppose that the bound for $ABC(G)$ is attained in the proposition and $m>0$. If $c=0$, then G is a regular graph of degree one. Suppose that $c>0$, then there is at least one vertex with degree at least two. Let u be a vertex of degree at least two. For two distinct neighbours v and w of u, we have $\frac{d_u+d_v-2}{d_u d_v} = \frac{d_u+d_w-2}{d_u d_w}$ and then $\frac{d_u-2}{d_v} = \frac{d_u-2}{d_w}$, which implies that either $d_u=2$ or $d_v=d_w$. If $d_u=2$, then $c=\frac{d_u+d_v-2}{d_u d_v}=\frac{1}{2}$ for any neighbour v of u. Note that $\frac{d_u+d_v-2}{d_u d_v}=\frac{1}{2}$ if and only if $(d_u-2)(d_v-2)=0$, i. e., $d_u=2$ or $d_v=2$. If there is at least one vertex in G with degree two, then $c=\frac{1}{2}$, and thus G is a graph in which every edge is incident with a vertex of degree two.

Suppose that there is no vertex of degree two in G. Then for any vertex of degree greater than two, all of its neighbours have the same degree. Thus, every component of G is either regular or is not regular but has only two different degrees. In the latter case, the end vertices of all edges have the same two different degrees. It follows that every component of G is either a regular graph of degree, say r for all such components (if exist), or a nonregular semiregular bipartite graph and all such components (if exist) have equal auxiliary value, which is equal to $\frac{2r-2}{r^2}$ if there exist both types of the components.

Conversely, it is easily seen that the bound for $ABC(G)$ is attained if G is a graph satisfying (i), (ii) or (iii). □

We note that actually the above proof suggests a slightly sharper result: If G is a graph with n_1 vertices of degree at least one and m edges, then

$$ABC(G) \leq \sqrt{m\,(n_1-2R_{-1})}$$

with equality if and only if (i) $n_1=m=0$, or (ii) every edge is incident with a vertex of degree two, or (iii) G has no vertex of degree two, and every nontrivial component of G is either a regular graph of degree, say r for all such components (if exist), or a nonregular semiregular bipartite graph and all such components (if exist) have equal auxiliary value, which is equal to $\frac{2r-2}{r^2}$ if there exist both types of the components.

Obviously, the ABC index for any of the three graphs with one or two vertices is equal to zero.

Corollary 1 *Let G be a graph with* $n\geq 3$ *vertices. Then*

$$ABC(G) \leq n\sqrt{\frac{n-2}{2}}$$

with equality if and only if G is the complete graph.

Proof: Recall that [11] $R_{-1} \geq \frac{n}{2(n-1)}$ with equality if and only if G is the complete graph. Now the result follows from Proposition 1. □

Corollary 2 [4] *Let G be a tree with* $n\geq 2$ *vertices. Then*

$$ABC(G) \leq \sqrt{(n-1)(n-2)}$$

with equality if and only if G is the star.

Proof: Recall that from [12], $R_{-1} \geq 1$ with equality if and only if G is the star. Now the result follows from Proposition 1. □

Corollary 3 *Let G be a graph with n vertices and m ≥ 1 edges. Then*

$$ABC(G) \leq \sqrt{m\left(n - \frac{4m}{4m+1-\sqrt{8m+1}}\right)}$$

with equality if and only if G is a complete graph.

Proof: For a graph with $m \geq 1$ edges, we have [13] $R_{-1} \geq \frac{2m}{4m+1-\sqrt{8m+1}}$ with equality if and only if G consists of a complete graph and possibly isolated vertices. Now the result follows from Proposition 1. □

The complete bipartite graph with a vertices in one partite set and b vertices in the other partite set is denoted by $K_{a,b}$.

Proposition 2 *Let G be a triangle-free graph with n ≥ 3 vertices.*

$$ABC(G) \leq \sqrt{n-2}R_{-1/2},$$

$$ABC(G) \leq \frac{n}{2}\sqrt{n-2}$$

with equality in the first inequality if and only if G is a complete bipartite graph, and with equality in the second inequality if and only if $G = K_{n/2,n/2}$.

Proof: Note that for any $uv \in E(G)$, $d_u + d_v \leq n$. Then

$$ABC(G) \leq \sum_{uv \in E(G)} \frac{\sqrt{n-2}}{\sqrt{d_u d_v}} = \sqrt{n-2}R_{-1/2}$$

with equality if and only if for any $uv \in E(G)$, $d_u + d_v = n$, i. e., G is a complete bipartite graph.

Then the second inequality follows and equality holds if and only if G is a regular complete bipartite graph, i. e., $G = K_{n/2,n/2}$. □

The result in previous proposition may be improved by using better lower bound for $R_{-1/2}$. An example is as follows: If G is a connected triangle-free graph with $n \geq 2$ vertices, m edges, maximum vertex degree Δ, and minimum vertex degree $\delta \geq 1$, then [14] $R_{-1/2} \leq \frac{n}{2} - \frac{1}{2m}\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right)^2$, and thus

$$ABC(G) \leq \frac{n}{2}\sqrt{n-2} - \frac{\sqrt{n-2}}{2m}\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right)^2.$$

Corollary 4 *Let G be a bipartite graph with n ≥ 3 vertices. Then*

$$ABC(G) \leq \sqrt{(n-2)\left\lfloor\frac{n}{2}\right\rfloor\left\lceil\frac{n}{2}\right\rceil}$$

with equality if and only if $G = K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.

Proof: Let X and Y be the two partite sets of G with $|X| \leq |Y|$. From [15], we have $R_{-1/2} \leq \sqrt{|X||Y|}$, implying that $R_{-1/2} \leq \sqrt{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}$, and if equality holds, then $|X| = \lfloor \frac{n}{2} \rfloor$ and $|Y| = \lceil \frac{n}{2} \rceil$. Now the result follows from Proposition 2. □

Proposition 3 *Let G be a graph with m edges. Then*

$$ABC(G) \leq \sqrt{(M_1 - 2m)R_{-1}}$$

with equality if and only if either m = 0, or every component of G is either a regular graph of degree, say r for all such components (if exist), or a nonregular semiregular bipartite graph of degrees, say s and t (depending on the component) and all such components (if exist) have equal $st(s+t-2)$*-value, which is equal to* $r^2(2r-2)$ *if there exist both types of the components.*

Proof: Note that $M_1 = \sum_{uv \in E(G)}(d_u + d_v)$. By the Cauchy-Schwarz inequality,

$$ABC(G) \leq \sqrt{\sum_{uv \in E(G)}(d_u + d_v - 2) \sum_{uv \in E(G)} \frac{1}{d_u d_v}} = \sqrt{(M_1 - 2m)R_{-1}}$$

with equality if and only if either $m = 0$ or for any edge uv of G, $d_u d_v (d_u + d_v - 2)$ is a constant. Now the result follows easily by similar arguments as in the proof of Proposition 1. □

The clique number of a graph is the number of vertices in a largest complete subgraph of the graph. A particular case of Theorem 1 in [16] says that if G is a graph with clique number ω, then $R_{-1} \leq$

$\frac{\omega-1}{2\omega}\left(\sum_{u\in V(G)}\frac{1}{d_u}\right)^2$ with equality if and only if G is the regular complete ω-partite graph. By Proposition 3, we have:

Corollary 5 *Let G be a graph with m edges and clique number ω. Then*

$$ABC(G) \le \sqrt{\frac{\omega-1}{2\omega}(M_1-2m)}\sum_{u\in V(G)}\frac{1}{d_u}$$

with equality if and only if G is the regular complete ω-partite graph.

Note that there are relations between Randić indices $R_{-1/2}$, R_{-1} and some other graph parameters, which, together with Propositions 1–3 may be used possibly to find relations between ABC index and these graph parameters.

3. ABC Index of Trees

In this section we consider ABC index of trees in more detail.

Let a, x be positive integers with $a \ge 2$. Let $f_a(x) = \sqrt{\frac{x+a-2}{ax}} - \sqrt{\frac{x+a-3}{(a-1)x}}$, i. e.,

$$f_a(x) = \frac{2-x}{\sqrt{a(a-1)x}\sqrt{(a-1)(x+a-2)}+\sqrt{a(x+a-3)}}.$$

Thus $f_a(x) \le f_a(1)$ with equality if and only if $x = 1$, and if $x \ge 2$, then $f_a(x) \le f_a(2) = 0$ with equality if and only if $x = 2$. Obviously, $f_a(2) < f_a(1)$.

Let $S_{n,p}$ be the tree formed from the path on $n-p+1$ vertices by attaching $p-1$ pendant vertices to an end vertex, where $2 \le p \le n-1$. Obviously, $S_{n,2} = P_n$ and $S_{n,n-1} = S_n$. For a tree T and its pendant vertex u, $T-u$ denotes the tree formed from T by deleting the vertex u and its incident edge.

Lemma 1 *Let T be a tree with n vertices and p pendant vertices, where $2 \le p \le n-2$. If u is a pendant vertex being adjacent to the vertex v, then*

$$ABC(T) - ABC(T-u) \le \sqrt{\frac{p-1}{p}}(p-1) - \sqrt{\frac{p-2}{p-1}}(p-2)$$

with equality if and only if $T = S_{n,p}$ and $d_v = p$.

Proof: Let $\Gamma(v)$ be the set of neighbours of v in T. Since $p \le n-2$, $\Gamma(v)\setminus\{u\}$ contains at least one vertex of degree at least two. Note that $d_v \ge 2$. Thus

$$\begin{aligned}
ABC(T) - ABC(T-u) &= \sqrt{\frac{d_v-1}{d_v}} \\
&+ \sum_{w\in\Gamma(v)\setminus\{u\}}\left(\sqrt{\frac{d_w+d_v-2}{d_wd_v}} - \sqrt{\frac{d_w+d_v-3}{d_w(d_v-1)}}\right) \\
&= \sqrt{\frac{d_v-1}{d_v}} + \sum_{w\in\Gamma(v)\setminus\{u\}} f_{d_v}(d_w) \\
&\le \sqrt{\frac{d_v-1}{d_v}} + f_{d_v}(2) + (d_v-2)f_{d_v}(1) \\
&= \sqrt{\frac{d_v-1}{d_v}} + (d_v-2)\left(\sqrt{\frac{d_v-1}{d_v}} - \sqrt{\frac{d_v-2}{d_v-1}}\right) \\
&= \sqrt{\frac{d_v-1}{d_v}}(d_v-1) - \sqrt{\frac{d_v-2}{d_v-1}}(d_v-2)
\end{aligned}$$

with equality if and only if of the d_v neighbours of v, one has degree two, and the others are all pendant vertices. Since $d_v \le p$, and the function $g(x) = \sqrt{\frac{x-1}{x}}(x-1) - \sqrt{\frac{x-2}{x-1}}(x-2)$ is increasing for $x \ge 2$, we have

$$\begin{aligned}
&ABC(T) - ABC(T-u) \\
&\le \sqrt{\frac{p-1}{p}}(p-1) - \sqrt{\frac{p-2}{p-1}}(p-2)
\end{aligned}$$

with equality if and only if of the $d_v = p$ neighbours of v, one has degree two, and the others are all pendant vertices, i. e., $T = S_{n,p}$ and $d_v = p$. □

Proposition 4 *Let T be a tree with n vertices and p pendant vertices, where $2 \le p \le n-2$. Then*

$$ABC(T) \le \sqrt{\frac{p-1}{p}}(p-1) + \frac{\sqrt{2}}{2}(n-p)$$

with equality if and only if $T = S_{n,p}$.

Proof: We argue by induction on n. It is trivial for $n = 4$. Suppose that $n \ge 5$ and it holds for all trees with $n-1$ vertices. Let T be a tree with n vertices and p pendant vertices. Let u be a pendant vertex being adjacent to the vertex v in T. First suppose that $d_v = 2$. Such u and v

always exist if $p = 2$, 3. Then $d_w \geq 2$ for the unique neighbour w of v different from u, and thus

$$ABC(T) - ABC(T-u) = \frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2} - \sqrt{\frac{d_w - 1}{d_w}} \leq \frac{\sqrt{2}}{2}$$

with equality if and only if $d_w = 2$. In this case, $T-u$ possesses p pendant vertices. If $p = n-2$, then $T-u$ is a star, and thus $T = S_{n,n-2}$. If $p \leq n-3$, then by the induction hypothesis, we have

$$\begin{aligned} ABC(T) &\leq ABC(T-u) + \frac{\sqrt{2}}{2} \\ &\leq \sqrt{\frac{p-1}{p}}(p-1) + \frac{\sqrt{2}}{2}(n-1-p) + \frac{\sqrt{2}}{2} \\ &= \sqrt{\frac{p-1}{p}}(p-1) + \frac{\sqrt{2}}{2}(n-p) \end{aligned}$$

with equalities if and only if $T-u = S_{n-1,p}$ and $d_w = 2$, i.e., $T = S_{n,p}$.

Now we suppose that $d_v \geq 3$ and $p > 3$. Then $T-u$ possesses $p-1$ pendant vertices. By Lemma 1 and the induction hypothesis, we have

$$\begin{aligned} &ABC(T) \leq \\ &ABC(T-u) + \sqrt{\tfrac{p-1}{p}}(p-1) - \sqrt{\tfrac{p-2}{p-1}}(p-2) \\ &\leq \sqrt{\tfrac{p-2}{p-1}}(p-2) + \tfrac{\sqrt{2}}{2}(n-p) \\ &+ \quad \sqrt{\tfrac{p-1}{p}}(p-1) - \sqrt{\tfrac{p-2}{p-1}}(p-2) \\ &= \sqrt{\tfrac{p-1}{p}}(p-1) + \tfrac{\sqrt{2}}{2}(n-p) \end{aligned}$$

with equality in the second inequality if and only if $T-u = S_{n-1,p-1}$ and the degree of v in $T-u$ is $p-1$, for which equality holds also in the first inequality. These are just satisfied for $T = S_{n,p}$. □

Note that $h(p) = \sqrt{\frac{p-1}{p}}(p-1) + \frac{\sqrt{2}}{2}(n-p)$ is increasing for $2 \leq p \leq n-2$. By Proposition 4, $S_{n,n-d+1}$ is the unique tree among trees with n vertices and diameter d with $3 \leq d \leq n-1$.

Let $D_{n,a}$ be the tree formed by adding an edge between the centers of the stars S_a and S_{n-a}, where $2 \leq a \leq \lfloor \frac{n}{2} \rfloor$. Then $S_{n,n-2} = D_{n,2}$.

Corollary 6 *Among the trees with $n \geq 4$ vertices, S_n is the unique tree with the maximum ABC index, which is equal to $\sqrt{(n-1)(n-2)}$, $S_{n,n-2} = D_{n,2}$ is the unique tree with the second maximum ABC index, which is equal to $\sqrt{\frac{n-3}{n-2}}(n-3) + \sqrt{2}$, $S_{5,2} = P_5$ and $D_{n,3}$ for $n \geq 6$ are the unique trees with the third maximum ABC index, where $ABC(S_{5,2}) = 2\sqrt{2}$ and $ABC(D_{n,3}) = \sqrt{\frac{n-4}{n-3}}(n-4) + \sqrt{\frac{n-2}{3(n-3)}} + \frac{2\sqrt{6}}{3}$, $D_{n,4}$ for $8 \leq n \leq 25$ and $S_{n,n-3}$ for $n = 6,7$ and $n \geq 26$ are the unique trees with the fourth maximum ABC index, where $ABC(D_{n,4}) = \sqrt{\frac{n-5}{n-4}}(n-5) + \frac{1}{2}\sqrt{\frac{n-2}{n-4}} + \frac{3\sqrt{3}}{2}$ and $ABC(S_{n,n-3}) = \sqrt{\frac{n-4}{n-3}}(n-4) + \frac{3\sqrt{2}}{2}$.*

Proof: Recall that $h(p) = \sqrt{\frac{p-1}{p}}(p-1) + \frac{\sqrt{2}}{2}(n-p)$ is increasing for $2 \leq p \leq n-2$.

Let T be a tree with n vertices. Let p be the number of pendant vertices of T. If $T \neq S_n$, then $2 \leq p \leq n-2$, and thus by Proposition 4, $ABC(T) \leq h(n-2)$ with equality if and only if $T = S_{n,n-2}$. Obviously, $\frac{n-3}{n-2} < \frac{n-2}{n-1}$ and then

$$\begin{aligned} h(n-2) &= \sqrt{\frac{n-3}{n-2}}(n-3) + \sqrt{2} \\ &< \sqrt{\frac{n-2}{n-1}}(n-1) = ABC(S_n). \end{aligned}$$

Thus S_n is the unique tree with the maximum ABC index and $S_{n,n-2}$ is the unique tree with the second maximum ABC index among trees with $n \geq 4$ vertices.

There are only three trees with five vertices: S_5, $S_{5,3}$, and P_5. Thus P_5 is the unique tree with the third maximum ABC index among trees with five vertices.

Suppose that $n \geq 6$, and $T \neq S_n, S_{n,n-2}$. If $p = n-2$, then T is of the form $D_{n,a}$ for $3 \leq a \leq \lfloor \frac{n}{2} \rfloor$. For $F(x) = \frac{(2x+1)\sqrt{x-1}}{2x\sqrt{x}} = \sqrt{1-\frac{1}{x}} + \frac{1}{2x}\sqrt{1-\frac{1}{x}}$ with $x > 1$, we have $F'(x) = \frac{1}{2x^2}\left(\left(1+\frac{1}{2x}\right)\sqrt{\frac{x}{x-1}} - \sqrt{\frac{x-1}{x}}\right) > 0$. Thus, for $H(x) = \sqrt{\frac{x-1}{x}}(x-1) + \sqrt{\frac{n-x-1}{n-x}}(n-x-1)$ with $1 < x \leq \lfloor \frac{n}{2} \rfloor$, $H'(x) = F(x) - F(n-x) \leq 0$. Note that $\sqrt{\frac{n-2}{x(n-x)}}$ is decreasing for $1 < x \leq \lfloor \frac{n}{2} \rfloor$. Then

$$\begin{aligned} &ABC(D_{n,a}) = \sqrt{\frac{a-1}{a}}(a-1) + \sqrt{\frac{n-a-1}{n-a}}(n-a-1) \\ &+ \sqrt{\frac{n-2}{a(n-a)}} = H(a) + \sqrt{\frac{n-2}{a(n-a)}} \end{aligned}$$

is decreasing for $3 \le a \le \lfloor \frac{n}{2} \rfloor$. Thus $ABC(T) \le ABC(D_{n,3})$ with equality if and only if $T = D_{n,3}$. If $p \le n-3$, then by Proposition 4, $ABC(T) \le h(n-3)$ with equality if and only if $T = S_{n,n-3}$. Note that

$$ABC(D_{n,3}) - h(n-3) = \sqrt{\frac{n-4}{n-3}}(n-4) + \sqrt{\frac{n-2}{3(n-3)}} + \frac{2\sqrt{6}}{3} - \left(\sqrt{\frac{n-4}{n-3}}(n-4) + \frac{3\sqrt{2}}{2}\right)$$
$$= \sqrt{\frac{n-2}{3(n-3)}} + \frac{2\sqrt{6}}{3} - \frac{3\sqrt{2}}{2} > \sqrt{\frac{1}{3}} + \frac{2\sqrt{6}}{3} - \frac{3\sqrt{2}}{2} > 0.$$

Thus $D_{n,3}$ is the unique tree with the third maximum ABC index among trees with $n \ge 6$ vertices.

Finally, we determine the tree(s) with the fourth maximum ABC index. The cases $n = 6, 7$ are easy to check. Suppose that $n \ge 8$. By arguments above, the fourth maximum ABC index of trees with n vertices is precisely achieved by $D_{n,4}$ and/or $S_{n,n-3}$. Note that

$$ABC(D_{n,4}) - h(n-3) = \sqrt{\tfrac{n-5}{n-4}}(n-5) + \frac{1}{2}\sqrt{\frac{n-2}{n-4}} + \frac{3\sqrt{3}}{2} - \left(\sqrt{\frac{n-4}{n-3}}(n-4) + \frac{3\sqrt{2}}{2}\right)$$
$$= \sqrt{\frac{n-5}{n-4}}(n-5) + \frac{1}{2}\sqrt{\frac{n-2}{n-4}} - \sqrt{\frac{n-4}{n-3}}(n-4) + \frac{3}{2}\left(\sqrt{3} - \sqrt{2}\right),$$

which is positive for $8 \le n \le 25$ and negative for $n \ge 26$. Thus $D_{n,4}$ for $8 \le n \le 25$ and $S_{n,n-3}$ for $n = 6, 7$ and $n \ge 26$ are the unique trees with the fourth maximum ABC index among trees with $n \ge 6$ vertices. □

The fact that S_n is the unique tree with the maximum ABC index among trees with n vertices also follows from Corollary 2.

Acknowledgement

This work was supported by the National Natural Science Foundation of China (no. 11071089) and the Guangdong Provincial Natural Science Foundation of China (no. 8151063101000026).

[1] N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton 1992.
[2] E. Estrada, L. Torres, L. Rodríguez, and I. Gutman, Indian J. Chem. **37A**, 849 (1998).
[3] E. Estrada, Chem. Phys. Lett. **463**, 422 (2008).
[4] B. Furtula, A. Graovac, and D. Vukičević, Discr. Appl. Math. **157**, 2828 (2009).
[5] R. Todeschini and V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim 2000.
[6] L. B. Kier and L. H. Hall, Molecular Connectivity in Structure-Activity Analysis, Wiley, Chichester 1986.
[7] R. García-Domenech, J. Gálvez, J. V. de Julián-Ortiz, and L. Pogliani, Chem. Rev. **108**, 1127 (2008).
[8] S. Siddhaye, K. Camarda, M. Southard, and E. Topp, Comput. Chem. Eng. **28**, 425 (2004).
[9] M. Randić, J. Mol. Graph. Model. **20**, 19 (2001).
[10] X. Li and I. Gutman, Mathematical Aspects of Randić-type Molecular Structure Descriptors, Univ. Kragujevac, Kragujevac 2006.
[11] X. Li and Y. Yang, MATCH Commun. Math. Comput. Chem. **51**, 155 (2004).
[12] L. H. Clark and J. W. Moon, Ars Combin. **54**, 223 (2000).
[13] B. Bollobás and P. Erdős, Ars Combin. **50**, 225 (1998).
[14] B. Zhou and W. Luo, MATCH Commun. Math. Comput. Chem. **62**, 155 (2009).
[15] P. Hansen and D. Vukičević, Discr. Math. **309**, 4228 (2009).
[16] B. Zhou and D. Vukičević, MATCH Commun. Math. Comput. Chem. **62**, 189 (2009).