Atom-bond connectivity index of unicyclic graphs with perfect matchings

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Abstract

The atom-bond connectivity (ABC) index of a graph G is defined in mathematical chemistry as $ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_u d_v}}$, where $E(G)$ is the edge set of G and d_u is the degree of vertex u in G. In this paper, we determine the unique graphs with the largest and the second largest ABC indices respectively in the class of unicyclic graphs on $2m$ vertices with perfect matchings.

1 Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, $N(u)$ denotes the set of neighbors of u in G. Then $d_u = |N(u)|$ is the degree of vertex u in G. The atom-bond connectivity (ABC) index of G is defined as [3]

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

The ABC index displays an excellent correlation with the heat of information of alkanes [2, 3], and thus may be used as a molecular descriptor. Its mathematical properties have also received attention, see [1, 4–8]. In particular, Furtula et al. [4] determined the minimum and maximum ABC

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indices for n-vertex trees with maximum degree at most four and showed that the star is the unique n-vertex tree with the maximum ABC index, and Xing et al. [5] gave the sharp upper bound for the ABC index of trees with a perfect matching.

In this paper, we determine the unicyclic graphs on $2m$ vertices of perfect matchings for $m \geq 2$ with the largest and the second largest ABC indices respectively. Recall that in mathematical chemistry a unicyclic graph with perfect matchings is known as a conjugated unicyclic graph.

2 Preliminaries

A matching M of a graph G is a subset of $E(G)$ such that no two edges in M share a common vertex. If every vertex of G is incident with an edge of M, then M is a perfect matching.

For a graph G with $u, v \in V(G)$, $G - u$ denotes the graph formed from G by deleting vertex u (and its incident edges), $G + uv$ denotes the graph formed from G by adding the edge uv if $uv \notin E(G)$, and $G - uv$ denotes the graph formed from G by deleting the edge uv if $uv \in E(G)$.

For $x, y \geq 1$, let $f(x,y) = \sqrt{\frac{x+y-2}{xy}}$.

Lemma 1 [5] *If $y \geq 2$ is fixed, then $f(x,y)$ is decreasing in x.*

Let $\mathbb{U}(m)$ be the class of unicyclic graphs on $2m$ vertices with perfect matchings, where $m \geq 2$. Let C_r be the cycle on r vertices, where $r \geq 3$. Let U_m with $m \geq 3$ be the graph obtained from C_m by attaching a pendent vertex to each vertex of C_m, and U_m^* with $m \geq 2$ the graph obtained from C_{m+1} by attaching a pendent vertex to each vertex of C_{m+1} except two fixed adjacent vertices.

3 Results

In the following we show that U_m and U_m^* are the unique graphs with the largest and the second largest ABC indices respectively in $\mathbb{U}(m)$ for $m \geq 3$.

Theorem 1 *Let $G \in \mathbb{U}(m) \setminus \{U_m\}$, where $m \geq 2$. Then*

$$ABC(G) \leq \frac{3}{\sqrt{2}} + \sqrt{\frac{2}{3}}(m-1) + \frac{2}{3}(m-2)$$

with equality if and only if $G \cong U_m^*$.

Proof. Let $\mathbb{U}^*(m) = \mathbb{U}(m) \backslash \{U_m\}$. Let $\varphi(m) = ABC(U_m^*) = \frac{3}{\sqrt{2}} + \sqrt{\frac{2}{3}}(m-1) + \frac{2}{3}(m-2)$.

We prove the result by induction on m.

If $m = 2$, then $G \cong U_2^*$ or C_4. By direct calculation, we have $\varphi(2) = \frac{3}{\sqrt{2}} + \sqrt{\frac{2}{3}} > ABC(C_4) = \frac{4}{\sqrt{2}}$. The result follows for $m = 2$. If $m = 3$, then $G \cong U_3^*$, C_6 or G_i ($i = 1, 2, \ldots, 5$, see Fig. 1). By direct calculation, we have $\varphi(3) = ABC(U_3^*) = 4.4210$, $ABC(C_6) = \frac{6}{\sqrt{2}} = 4.2426$, $ABC(G_1) = 4.4016$, $ABC(G_2) = 4.3116$, $ABC(G_3) = 4.2426$, $ABC(G_4) = 4.2426$, and $ABC(G_5) = 4.3520$ (up to four decimal places). Thus the result follows for $m = 3$.

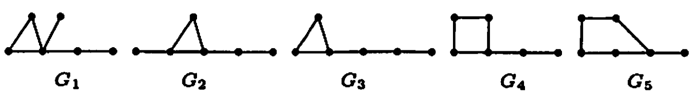

Fig. 1 Graphs in $\mathbb{U}^*(3) \setminus \{U_3^*, C_6\}$.

Suppose that $m \geq 4$ and the result follows for the uncyclic graphs in $\mathbb{U}^*(k)$ with $k \leq m-1$. Let $G \in \mathbb{U}^*(m)$. If $G \cong C_{2m}$, then

$$\begin{aligned}
\varphi(m) - ABC(G) &= \varphi(m) - \sqrt{2}m \\
&= \left(\sqrt{\tfrac{2}{3}} + \tfrac{2}{3} - \sqrt{2}\right) m - \sqrt{\tfrac{2}{3}} - \tfrac{4}{3} + \tfrac{3}{\sqrt{2}} \\
&> \left(\sqrt{\tfrac{2}{3}} + \tfrac{2}{3} - \sqrt{2}\right) - \sqrt{\tfrac{2}{3}} - \tfrac{4}{3} + \tfrac{3}{\sqrt{2}} \\
&> 0,
\end{aligned}$$

and thus $ABC(G) < \varphi(m)$. Suppose that $G \ncong C_{2m}$. Let M be a perfect matching of G. There are two cases.

Case 1. G has a pendent vertex u whose unique neighbor w has degree two. Obviously, $uw \in M$. Let $G_1 = G - u - w$. Then $M \setminus \{uw\}$ is a perfect matching of G_1. Let v be the neighbor of w different from u in G. Obviously, v has at most one pendent neighbor.

Suppose first that v is not adjacent to a pendent vertex. Then for any $v' \in N(v)$, $d_{v'} \geq 2$. If $G_1 \cong U_{m-1}$, then $d_v = 2$ and by direct calculation, $ABC(G) = \varphi(m) - \sqrt{\frac{2}{3}} + \frac{2}{3} < \varphi(m)$. If $G_1 \in \mathbb{U}^*(m-1)$, then by Lemma 1 and the induction hypothesis, we have

$$\begin{aligned}
ABC(G) &= ABC(G_1) + \tfrac{2}{\sqrt{2}} \\
&\quad + \sum_{v' \in N(v) \backslash \{w\}} \left(\sqrt{\tfrac{d_v + d_{v'} - 2}{d_v d_{v'}}} - \sqrt{\tfrac{(d_v - 1) + d_{v'} - 2}{(d_v - 1) d_{v'}}} \right) \\
&\leq ABC(G_1) + \tfrac{2}{\sqrt{2}} \leq \varphi(m-1) + \tfrac{2}{\sqrt{2}} \\
&= \varphi(m) - \tfrac{2}{3} - \sqrt{\tfrac{2}{3}} + \tfrac{2}{\sqrt{2}} < \varphi(m).
\end{aligned}$$

Now suppose that v is adjacent to a pendent vertex v_1. Then $vv_1 \in M$, $d_v \geq 3$ and for any $v' \in N(v) \setminus \{v_1\}$, $d_{v'} \geq 2$. Suppose that $d_v \geq 4$. If $G_1 \cong U_{m-1}$, then $d_v = 4$ and by direct calculation, $ABC(G) = \varphi(m) - \sqrt{\frac{2}{3}} - \frac{2}{3} - \frac{1}{\sqrt{2}} + \sqrt{\frac{3}{4}} + 2 \cdot \sqrt{\frac{5}{12}} < \varphi(m)$. If $G_1 \in \mathbb{U}^*(m-1)$, then by Lemma 1 and the induction hypothesis, and noting $g(x) = \sqrt{\frac{x-1}{x}} - \sqrt{\frac{x-2}{x-1}}$ is decreasing for $x \geq 2$, we have

$$\begin{aligned}
ABC(G) &= ABC(G_1) + \tfrac{2}{\sqrt{2}} + \sqrt{\tfrac{d_v-1}{d_v}} - \sqrt{\tfrac{d_v-2}{d_v-1}} \\
&\quad + \sum_{v' \in N(v)\setminus\{w,v_1\}} \left(\sqrt{\tfrac{d_v+d_{v'}-2}{d_v d_{v'}}} - \sqrt{\tfrac{(d_v-1)+d_{v'}-2}{(d_v-1)d_{v'}}} \right) \\
&\leq ABC(G_1) + \tfrac{2}{\sqrt{2}} + g(d_v) \\
&\leq \varphi(m-1) + \tfrac{2}{\sqrt{2}} + \sqrt{\tfrac{3}{4}} - \sqrt{\tfrac{2}{3}} \\
&= \varphi(m) - \tfrac{2}{3} - 2 \cdot \sqrt{\tfrac{2}{3}} + \tfrac{2}{\sqrt{2}} + \sqrt{\tfrac{3}{4}} < \varphi(m).
\end{aligned}$$

Suppose that $d_v = 3$. Let $N(v) \setminus \{w, v_1\} = \{v_2\}$. Then $d_{v_2} \geq 2$, $G_1 \in \mathbb{U}^*(m-1)$ and $G_1 \ncong U^*_{m-1}$. Suppose that $d_{v_2} \geq 3$. Then

$$\begin{aligned}
ABC(G) &= ABC(G_1) + \sqrt{\tfrac{2}{3}} + \sqrt{\tfrac{d_{v_2}+1}{3d_{v_2}}} \\
&< \varphi(m-1) + \sqrt{\tfrac{2}{3}} + \sqrt{\tfrac{d_{v_2}+1}{3d_{v_2}}} \\
&= \varphi(m) - \tfrac{2}{3} + \sqrt{\tfrac{d_{v_2}+1}{3d_{v_2}}} \leq \varphi(m).
\end{aligned}$$

Suppose that $d_{v_2} = 2$. Denote $N(v_2) = \{v, z\}$. Then $d_z \geq 2$. Let $G_2 = G - u - w - v - v_1$. Then $M \setminus \{uw, vv_1\}$ is a perfect matching of G_2. If $G_2 \cong U_{m-2}$, then by direct calculation, $ABC(G) = \varphi(m) - \sqrt{\frac{2}{3}} + \frac{1}{\sqrt{2}} < \varphi(m)$. If $G_2 \in \mathbb{U}^*(m-2)$, then by the induction hypothesis and noting that $h(x) = \sqrt{\frac{x-1}{x}}$ is increasing for $x \geq 1$, we have

$$\begin{aligned}
ABC(G) &= ABC(G_2) + \tfrac{4}{\sqrt{2}} + \sqrt{\tfrac{2}{3}} - \sqrt{\tfrac{d_z-1}{d_z}} \\
&\leq \varphi(m-2) + \tfrac{3}{\sqrt{2}} + \sqrt{\tfrac{2}{3}} + \tfrac{1}{\sqrt{2}} - h(d_z) \\
&\leq \varphi(m-2) + \tfrac{3}{\sqrt{2}} + \sqrt{\tfrac{2}{3}} \\
&= \varphi(m) - \sqrt{\tfrac{2}{3}} - \tfrac{4}{3} + \tfrac{3}{\sqrt{2}} < \varphi(m).
\end{aligned}$$

Case 2. No neighbor of a pendent vertex has degree two in G. Let C be the unique cycle of G. Since G has a perfect matching and a pendent vertex is incident to an edge in M, the graph obtained from G by deleting the edges of C consists of isolated edges. Thus G is a cycle C together with some pendent vertices each attached to a vertex of C. Let $C = u_1 u_2 \ldots u_p u_1$.

Since $G \ncong U_m$, there is at least one vertex of degree two on C. Since $G \ncong C_{2m}$, there are adjacent vertices on C, one of degree two and the other of degree three. Assume that $d_{u_2} = 3$ and $d_{u_3} = 2$. Denote by w_2 the pendent neighbor of u_2, then $u_2w_2 \in M$. Since $u_3u_4 \in M$, we have $d_{u_4} = 2$. Suppose first that $d_{u_1} = 3$. Let $G_3 = G - u_2 - w_2 + u_1u_3$. Then $M \setminus \{u_2w_2\}$ is a perfect matching of G_3 and $G_3 \in \mathbb{U}^*(m-1)$. By the induction hypothesis, we have

$$ABC(G) = ABC(G_3) + \sqrt{\frac{2}{3}} + \frac{2}{3} \leq \varphi(m-1) + \sqrt{\frac{2}{3}} + \frac{2}{3} = \varphi(m)$$

with equality if and only if $G_3 \cong U^*_{m-1}$, i.e., $G \cong U^*_m$. Suppose that $d_{u_1} = 2$. Similarly, we have $d_{u_p} = 2$ and $u_1u_p \in M$. Note that $u_4u_p \notin E(G)$ since $m \geq 4$. Let $G_4 = G - u_1 - u_2 - u_3 - w_2 + u_4u_p$. Then $(M \setminus \{u_2w_2, u_3u_4, u_1u_p\}) \cup \{u_4u_p\}$ is a perfect matching of G_4 and $G_4 \in \mathbb{U}^*(m-2)$. By the induction hypothesis, we have

$$ABC(G) = ABC(G_4) + \frac{3}{\sqrt{2}} + \sqrt{\frac{2}{3}} \leq \varphi(m-2) + \frac{3}{\sqrt{2}} + \sqrt{\frac{2}{3}} < \varphi(m).$$

By combining Cases 1 and 2, the result follows. □

Theorem 2 *Let $G \in \mathbb{U}(m)$, where $m \geq 3$. Then*

$$ABC(G) \leq \left(\sqrt{\frac{2}{3}} + \frac{2}{3}\right) m$$

with equality if and only if $G \cong U_m$.

Proof. If $G \ncong U_m$, then by Theorem 1,

$$ABC(G) \leq \frac{3}{\sqrt{2}} + \sqrt{\frac{2}{3}}(m-1) + \frac{2}{3}(m-2)$$

with equality if and only if $G \cong U^*_m$. Then the result follows since $ABC(U_m) - ABC(U^*_m) = \left(\sqrt{\frac{2}{3}} + \frac{2}{3}\right) m - \left[\frac{3}{\sqrt{2}} + \sqrt{\frac{2}{3}}(m-1) + \frac{2}{3}(m-2)\right] = \sqrt{\frac{2}{3}} + \frac{4}{3} - \frac{3}{\sqrt{2}} > 0.$ □

Note that $\mathbb{U}(2) = \{U^*_2, C_4\}$. By Theorems 1 and 2, U^*_2 for $m = 2$ and U_m for $m \geq 3$ are the unique graphs with the largest ABC index in $\mathbb{U}(m)$, while C_4 for $m = 2$ and U^*_m for $m \geq 3$ are the unique graphs with the second largest ABC index in $\mathbb{U}(m)$.

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