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On atom bond sum connectivity index of chemical unicyclic graphs with a perfect matching

Jianwei Du[a,*], Xiaoling Sun[a], Yinzhen Mei[a]

[a] *School of Mathematics, North University of China, Taiyuan 030051, China*

Abstract. The atom bond sum connectivity (ABS) index of a graph $\Gamma = (V(\Gamma), E(\Gamma))$ is formulated by $ABS(\Gamma) = \sum_{xy \in E(\Gamma)} \sqrt{\frac{d_\Gamma(x)+d_\Gamma(y)-2}{d_\Gamma(x)+d_\Gamma(y)}}$, where $d_\Gamma(x)$ denotes the degree of vertex x in Γ. In this work, we determine the maximum value of atom bond sum connectivity index of chemical unicyclic graphs with a perfect matching and identify the corresponding extremal graphs. Our discoveries extend the results of the recent paper [Wang et al., MATCH Commun. Math. Comput. Chem. 92 (2024) 653-669] from chemical trees with a perfect matching to chemical unicyclic graphs with a perfect matching.

1. Introduction

In this paper, we are only concerned with simple, undirected and connected graphs. For such a graph Γ, the vertex and edge sets of Γ are denoted by $V(\Gamma)$ and $E(\Gamma)$, respectively. Let $N_\Gamma(x) = \{y \in V(\Gamma) : xy \in E(\Gamma)\}$ and $d_\Gamma(x) = |N_\Gamma(x)|$. Generally, a pendent vertex is a vertex with degree 1, and a pendent edge is an edge incident to a pendent vertex. Let $\Gamma - uv$ and $\Gamma + uv$ be the graphs obtained from Γ by deleting the edge $uv \in E(\Gamma)$ and by connecting two vertices $u, v \in V(\Gamma)$ ($uv \notin E(\Gamma)$), respectively. We use $\Gamma - v$ to denote the subgraph of Γ obtained by deleting the vertex $v \in V(\Gamma)$ and the edges incident with v. Recall that a chemical graph is a graph Γ with $d_\Gamma(x) \leq 4$ for all $x \in V(\Gamma)$. A unicyclic graph is a graph with exactly one cycle.

A set of pairwise nonadjacent edges of a graph Γ is called a matching in Γ. A perfect matching is defined as a set of edges that cover every vertex of the graph. Let $\boldsymbol{C\Gamma}_{2m}$ be the set of $2m$-vertex chemical unicyclic graphs with perfect matchings. For undefined notations and terminologies, one can see [8, 16, 17].

In the realm of mathematical chemistry and chemoinformatics, topological indices have emerged as indispensable tools for characterizing molecular structures and predicting physicochemical, biological, or pharmacological properties of compounds [11, 12]. The atom-bond sum connectivity (ABS) index, a recently

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* Corresponding author: Jianwei Du
Email addresses: jianweidu@nuc.edu.cn (Jianwei Du), sunxiaoling@nuc.edu.cn (Xiaoling Sun), myzmath@nuc.edu.cn (Yinzhen Mei)
ORCID iDs: https://orcid.org/0000-0002-9415-6852 (Jianwei Du), https://orcid.org/0000-0001-9215-2340 (Xiaoling Sun), https://orcid.org/0000-0001-8289-9053 (Yinzhen Mei)

proposed topological descriptor by Ali et al. [6], has attracted great attention and has been widely studied. For a graph Γ, ABS index is defined as

$$ABS(\Gamma) = \sum_{xy\in E(\Gamma)} \sqrt{\frac{d_\Gamma(x) + d_\Gamma(y) - 2}{d_\Gamma(x) + d_\Gamma(y)}} = \sum_{xy\in E(\Gamma)} \sqrt{1 - \frac{2}{d_\Gamma(x) + d_\Gamma(y)}}.$$

Ali et al. [5] showed that the ABS index has good predictive potential for some physico-chemical properties. For recent mathematical investigations on the ABS index, we refer the readers to [1–4, 7, 9, 10, 13–15, 18, 19] and the references therein. Motivated by these works, in this paper, we aim to determine the maximum ABS index of chemical unicyclic graphs with a perfect matching.

The paper is structured as follows: Section 2 gives useful lemmas which will be used in the proof of our main results. Section 3 shows the process of characterizing chemical unicyclic graphs with a perfect matching achieving the maximum ABS index. Our discoveries extend the results of the recent paper [18] from chemical trees with a perfect matching to chemical unicyclic graphs with a perfect matching.

2. Preliminaries

Let $A(a, b) = \sqrt{\frac{a+b-2}{a+b}}$, where $a, b \geq 1$ are positive integers and $a+b \geq 3$. Clearly, $A(a, b)$ is strictly increasing with respect to a or b. Next, we provide two lemmas which are specifically used in our main results.

Lemma 2.1. *[18] Let* $f(x) = A(x, \alpha) - A(x, \alpha - 1) = \sqrt{\frac{x+\alpha-2}{x+\alpha}} - \sqrt{\frac{x+\alpha-3}{x+\alpha-1}}$, *where* $\alpha \geq 2$ *and* $x \geq 1$. *Then* $f(x)$ *is decreasing with respect to* x.

Lemma 2.2. *Let* $\Gamma \in \boldsymbol{C\Gamma}_{2m}$ $(m \geq 4)$ *and* M *be a perfect matching of* Γ. *If* Γ *has the maximum ABS index and* $uv \in M$, *then* uv *must be a pendent edge of* Γ.

Proof. On the contrary, we assume that uv is a non-pendent edge. Therefore, $2 \leq d_\Gamma(u), d_\Gamma(v) \leq 4$. Let C be the unique cycle of Γ. Next, we consider the following six cases.

Case 1. $d_\Gamma(u) = 2$ and $d_\Gamma(v) = 2$.

Denote $N_\Gamma(u) \setminus \{v\} = \{u_1\}$ and $N_\Gamma(v) \setminus \{u\} = \{v_1\}$.

Case 1.1. $u \notin V(C)$.

Case 1.1.1. u is the vertex that is situated closer to C than v.

Notice that $d_\Gamma(v_1) \geq 2$ since $uv \in M$. Let $\Gamma_1 = U - vv_1 + uv_1$. Then $\Gamma_1 \in \boldsymbol{C\Gamma}_{2m}$ and one has

$$\begin{aligned}
&ABS(\Gamma_1) - ABS(\Gamma)\\
=&A(3, d_\Gamma(u_1)) + A(3, d_\Gamma(v_1)) + A(3, 1) - A(2, d_\Gamma(u_1)) - A(2, d_\Gamma(v_1)) - A(2, 2)\\
=&(A(3, d_\Gamma(u_1)) - A(2, d_\Gamma(u_1))) + (A(3, d_\Gamma(v_1)) - A(2, d_\Gamma(v_1))) + A(3, 1) - A(2, 2)\\
>&A(3, 1) - A(2, 2)\\
=&0.
\end{aligned}$$

Thus $ABS(\Gamma_1) > ABS(\Gamma)$, which contradicts the assumption that Γ has the maximum ABS index.

Case 1.1.2. v is the vertex that is situated closer to C than u.

Note that $v \notin V(C)$ otherwise $d_\Gamma(v) \geq 3$. Let $\Gamma_2 = U - uu_1 + vu_1$. Then $\Gamma_2 \in \boldsymbol{C\Gamma}_{2m}$ and we derive

$$\begin{aligned}
&ABS(\Gamma_2) - ABS(\Gamma)\\
=&A(3, d_\Gamma(u_1)) + A(3, d_\Gamma(v_1)) + A(3, 1) - A(2, d_\Gamma(u_1)) - A(2, d_\Gamma(v_1)) - A(2, 2)\\
>&0.
\end{aligned}$$

Hence $ABS(\Gamma_2) > ABS(\Gamma)$, a contradiction.

Case 1.2. $u \in V(C)$.

Now, $v \in V(C)$, otherwise $d_\Gamma(u) \geq 3$. So $u_1, v_1 \in V(C)$.

Case 1.2.1. $u_1 \neq v_1$.

Let $\Gamma_3 = U - vv_1 + uv_1$. Then $\Gamma_3 \in \boldsymbol{C\Gamma}_{2m}$ and we derive

$$
\begin{aligned}
&ABS(\Gamma_3) - ABS(\Gamma)\\
=&A(3, d_\Gamma(u_1)) + A(3, d_\Gamma(v_1)) + A(3, 1) - A(2, d_\Gamma(u_1)) - A(2, d_\Gamma(v_1)) - A(2, 2)\\
>&0.
\end{aligned}
$$

Therefore, $ABS(\Gamma_3) > ABS(\Gamma)$, which is a contradiction.

Case 1.2.2. $u_1 = v_1$.

Observe that $C = uvu_1u$ is the only cycle of Γ. Since $uv \in M$ and $m \geq 4$, there exist a neighbor u_1' of u_1 other than u and v such that $u_1u_1' \in M$ and $d_\Gamma(u_1') \geq 2$, or there exist a pendent neighbor and a non-pendent neighbor u_1' of u_1 other than u and v such that $d_\Gamma(u_1') \geq 2$. Suppose P is a maximal path from u_1 to x and containing u_1u_1'. It is obvious that $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_4 = U - uu_1 + yu_1$. Then $\Gamma_4 \in \boldsymbol{C\Gamma}_{2m}$ and it can be concluded that

$$
\begin{aligned}
&ABS(\Gamma_4) - ABS(\Gamma)\\
=&A(3, d_\Gamma(u_1)) + A(3, d_\Gamma(y_1)) + A(3, 1) + A(2, 1)\\
&- A(2, d_\Gamma(u_1)) - A(2, d_\Gamma(y_1)) - A(2, 2) - A(2, 1)\\
>&A(3, 1) + A(2, 1) - A(2, 2) - A(2, 1)\\
=&0.
\end{aligned}
$$

So $ABS(\Gamma_4) > ABS(\Gamma)$, a contradiction.

Case 2. $d_\Gamma(u) = 2$ and $d_\Gamma(v) = 3$.

Denote $N_\Gamma(u) \setminus \{v\} = \{u_1\}$ and $N_\Gamma(v) \setminus \{u\} = \{v_1, v_2\}$.

Case 2.1. $u \notin V(C)$.

Case 2.1.1. u is the vertex that is situated nearer to C than v.

Let $\Gamma_5 = U - \{vv_1, vv_2\} + \{uv_1, uv_2\}$. Then $\Gamma_5 \in \boldsymbol{C\Gamma}_{2m}$ and it follows that

$$
\begin{aligned}
&ABS(\Gamma_5) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(v_1)) + A(4, d_\Gamma(v_2)) + A(4, 1)\\
&- A(2, d_\Gamma(u_1)) - A(3, d_\Gamma(v_1)) - A(3, d_\Gamma(v_2)) - A(2, 3)\\
>&A(4, 1) - A(2, 3)\\
=&0.
\end{aligned}
$$

As a result, $ABS(\Gamma_5) > ABS(\Gamma)$, which contradicts the fact that Γ has the maximum ABS index.

Case 2.1.2. v is the vertex that is situated nearer to C than u.

We have $d_\Gamma(u_1) \geq 2$ since $uv \in M$. Let $\Gamma_6 = U - uu_1 + vu_1$. Then $\Gamma_6 \in \boldsymbol{C\Gamma}_{2m}$ and it can be concluded that

$$
\begin{aligned}
&ABS(\Gamma_6) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(v_1)) + A(4, d_\Gamma(v_2)) + A(4, 1)\\
&- A(2, d_\Gamma(u_1)) - A(3, d_\Gamma(v_1)) - A(3, d_\Gamma(v_2)) - A(2, 3)\\
>&A(4, 1) - A(2, 3)\\
=&0.
\end{aligned}
$$

Thus $ABS(\Gamma_6) > ABS(\Gamma)$, a contradiction.

Case 2.2. $u \in V(C)$.

Since $v \in V(C)$, we suppose that $v_1 \in V(C)$ and $v_2 \notin V(C)$. So $d_\Gamma(v_2) \geq 2$.

Case 2.2.1. $u_1 \neq v_1$.

Let $\Gamma_7 = U - uu_1 + vu_1$. Then $\Gamma_7 \in \boldsymbol{C\Gamma}_{2m}$ and we derive

$$\begin{aligned}
&ABS(\Gamma_7) - ABS(\Gamma) \\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(v_1)) + A(4, d_\Gamma(v_2)) + A(4, 1) \\
&- A(2, d_\Gamma(u_1)) - A(3, d_\Gamma(v_1)) - A(3, d_\Gamma(v_2)) - A(2, 3) \\
>&A(4, 1) - A(2, 3) \\
=&0.
\end{aligned}$$

So $ABS(\Gamma_7) > ABS(\Gamma)$, which is a contradiction.

Case 2.2.2. $u_1 = v_1$.

Note that $C = uvu_1u$ is the only cycle of Γ. Suppose P is a maximal path from v to x and containing vv_2. So $d_\Gamma(x) = 1$ and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_8 = U - uu_1 + yu_1$. Then $\Gamma_8 \in \boldsymbol{C\Gamma}_{2m}$ and one has

$$\begin{aligned}
&ABS(\Gamma_8) - ABS(\Gamma) \\
=&A(3, d_\Gamma(y_1)) + A(3, d_\Gamma(u_1)) + A(3, 1) + A(3, 1) \\
&- A(2, d_\Gamma(y_1)) - A(2, d_\Gamma(u_1)) - A(3, 2) - A(2, 1) \\
>&A(3, 1) + A(3, 1) - A(3, 2) - A(2, 1) \\
=&\sqrt{2} - \sqrt{\frac{3}{5}} - \sqrt{\frac{1}{3}} \\
\approx&0.0623 > 0.
\end{aligned}$$

Therefore, $ABS(\Gamma_8) > ABS(\Gamma)$, a contradiction.

Case 3. $d_\Gamma(u) = 2$ and $d_\Gamma(v) = 4$.

Denote $N_\Gamma(u) \setminus \{v\} = \{u_1\}$ and $N_\Gamma(v) \setminus \{u\} = \{v_1, v_2, v_3\}$.

Case 3.1. $u \notin V(C)$.

Case 3.1.1. u is the vertex that is situated closer to C than v.

Since $uv \in M$, then $d_\Gamma(u_1), d_\Gamma(v_1), d_\Gamma(v_2), d_\Gamma(v_3) \geq 2$. Suppose P is a maximal path from v to x and containing vv_2. It is clear that $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_9 = U - \{uu_1, vv_3\} + \{u_1v, yv_3\}$. Then $\Gamma_9 \in \boldsymbol{C\Gamma}_{2m}$ and by Lemma 2.1, we have

$$\begin{aligned}
&ABS(\Gamma_9) - ABS(\Gamma) \\
=&A(4, d_\Gamma(u_1)) + A(3, d_\Gamma(y_1)) + A(3, d_\Gamma(v_3)) + A(4, 1) + A(3, 1) \\
&- A(2, d_\Gamma(u_1)) - A(2, d_\Gamma(y_1)) - A(4, d_\Gamma(v_3)) - A(2, 4) - A(2, 1) \\
>&A(3, d_\Gamma(v_3)) - A(4, d_\Gamma(v_3)) + A(4, 1) + A(3, 1) - A(2, 4) - A(2, 1) \\
\geq&A(3, 2) - A(4, 2) + A(4, 1) + A(3, 1) - A(2, 4) - A(2, 1) \\
=&2\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - 2\sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}} \\
\approx&0.0460 > 0.
\end{aligned}$$

Hence $ABS(\Gamma_9) > ABS(\Gamma)$, which is a contradiction.

Case 3.1.2. v is the vertex that is situated closer to C than u.

Without loss of generality, we suppose that v_1 is the vertex that is situated nearer to C than v_2, v_3 when $v \notin V(C)$, and $v_1, v_3 \in V(C)$ when $v \in V(C)$. Suppose P is a maximal path from v to x and containing vv_2. We know that $d_\Gamma(x) = 1$ and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote

$N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_{10} = U - uu_1 + yu_1$. Then $\Gamma_{10} \in \boldsymbol{C\Gamma}_{2m}$ and we have

$$
\begin{aligned}
&ABS(\Gamma_{10}) - ABS(\Gamma)\\
=&A(3, d_\Gamma(u_1)) + A(3, d_\Gamma(y_1)) + A(4,1) + A(3,1)\\
&- A(2, d_\Gamma(u_1)) - A(2, d_\Gamma(y_1)) - A(2,4) - A(2,1)\\
>&A(4,1) + A(3,1) - A(2,4) - A(2,1)\\
=&\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}}\\
\approx&0.0879 > 0.
\end{aligned}
$$

Thus $ABS(\Gamma_{10}) > ABS(\Gamma)$, a contradiction.

Case 3.2. $u \in V(C)$.

Since $v \in V(C)$, we suppose that $v_1 \in V(C)$ and $v_2, v_3 \notin V(C)$. So $d_\Gamma(v_2), d_\Gamma(v_3) \geq 2$.

Case 3.2.1. $u_1 \neq v_1$.

Suppose P is a maximal path from v to x and containing vv_2. We see that $d_\Gamma(x) = 1$ and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_{11} = U - \{uu_1, vv_3\} + \{u_1v, yv_3\}$. Then $\Gamma_{11} \in \boldsymbol{C\Gamma}_{2m}$ and by Lemma 2.1, we dereive

$$
\begin{aligned}
&ABS(\Gamma_{11}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(3, d_\Gamma(y_1)) + A(3, d_\Gamma(v_3)) + A(4,1) + A(3,1)\\
&- A(2, d_\Gamma(u_1)) - A(2, d_\Gamma(y_1)) - A(4, d_\Gamma(v_3)) - A(2,4) - A(2,1)\\
>&A(3, d_\Gamma(v_3)) - A(4, d_\Gamma(v_3)) + A(4,1) + A(3,1) - A(2,4) - A(2,1)\\
\geq&A(3,2) - A(4,2) + A(4,1) + A(3,1) - A(2,4) - A(2,1)\\
=&2\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - 2\sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}
$$

So $ABS(\Gamma_{11}) > ABS(\Gamma)$, which is a contradiction.

Case 3.2.2. $u_1 = v_1$.

Note that $C = uvu_1u$ is the only cycle of Γ. Suppose P is a maximal path from v to x and containing vv_2. It is clear that $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_{12} = U - uu_1 + yu_1$. Then $\Gamma_{12} \in \boldsymbol{C\Gamma}_{2m}$ and we have

$$
\begin{aligned}
&ABS(\Gamma_{12}) - ABS(\Gamma)\\
=&A(3, d_\Gamma(u_1)) + A(3, d_\Gamma(y_1)) + A(4,1) + A(3,1)\\
&- A(2, d_\Gamma(u_1)) - A(2, d_\Gamma(y_1)) - A(2,4) - A(2,1)\\
>&A(4,1) + A(3,1) - A(2,4) - A(2,1)\\
=&\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}
$$

As a result, $ABS(\Gamma_{12}) > ABS(\Gamma)$, a contradiction.

Case 4. $d_\Gamma(u) = 3$ and $d_\Gamma(v) = 3$.

Denote $N_\Gamma(u) \setminus \{v\} = \{u_1, u_2\}$ and $N_\Gamma(v) \setminus \{u\} = \{v_1, v_2\}$.

Case 4.1. $u \notin V(C)$.

Case 4.1.1. u is the vertex that is situated nearer to C than v.

Since $uv \in M$, then $d_\Gamma(u_1), d_\Gamma(u_2), d_\Gamma(v_1), d_\Gamma(v_2) \geq 2$. Suppose u_1 is the vertex that is situated nearer to C than u_2 and P is a maximal path from u to x and containing uu_2. So $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$.

Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_{13} = U - \{vv_1, vv_2\} + \{yv_1, yv_2\}$. Then $\Gamma_{13} \in \boldsymbol{C\Gamma}_{2m}$ and we have

$$\begin{aligned}
&ABS(\Gamma_{13}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(v_1)) + A(4, d_\Gamma(v_2)) + A(4, d_\Gamma(y_1)) + A(4, 1) + A(3, 1)\\
&- A(3, d_\Gamma(v_1)) - A(3, d_\Gamma(v_2)) - A(2, d_\Gamma(y_1)) - A(3, 3) - A(2, 1)\\
>&A(4, 1) + A(3, 1) - A(3, 3) - A(2, 1)\\
=&\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

Thus $ABS(\Gamma_{13}) > ABS(\Gamma)$, which is a contradiction.

Case 4.1.2. v is the vertex that is situated nearer to C than u.

Without loss of generality, we assume that v_1 is the vertex that is situated nearer to C than v_2 when $v \notin V(C)$, and $v_1, v_2 \in V(C)$ when $v \in V(C)$.

If $v \notin V(C)$, suppose P is a maximal path from v to x and containing vv_2. It is obvious that $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_{14} = U - \{uu_1, uu_2\} + \{yu_1, yu_2\}$. Then $\Gamma_{14} \in \boldsymbol{C\Gamma}_{2m}$ and we have

$$\begin{aligned}
&ABS(\Gamma_{14}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(u_2)) + A(4, d_\Gamma(y_1)) + A(4, 1) + A(3, 1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(u_2)) - A(2, d_\Gamma(y_1)) - A(3, 3) - A(2, 1)\\
>&A(4, 1) + A(3, 1) - A(3, 3) - A(2, 1)\\
=&\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

Hence $ABS(\Gamma_{14}) > ABS(\Gamma)$, which is a contradiction.

If $v \in V(C)$, suppose P is a maximal path from u to x and containing uu_2. We can see that $d_\Gamma(x) = 1$ and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_{15} = U - \{uu_1, uu_2\} + \{vu_2, yu_1\}$. Then $\Gamma_{15} \in \boldsymbol{C\Gamma}_{2m}$. If $y \neq u_2$, we have

$$\begin{aligned}
&ABS(\Gamma_{15}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(v_1)) + A(4, d_\Gamma(v_2)) + A(4, d_\Gamma(u_2)) + A(3, d_\Gamma(y_1)) + A(4, 1) + A(3, 1)\\
&- A(3, d_\Gamma(v_1)) - A(3, d_\Gamma(v_2)) - A(3, d_\Gamma(u_2)) - A(2, d_\Gamma(y_1)) - A(3, 3) - A(2, 1)\\
>&A(4, 1) + A(3, 1) - A(3, 3) - A(2, 1)\\
=&\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

If $y = u_2$, i.e. $u = y_1$, we have

$$\begin{aligned}
&ABS(\Gamma_{15}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(v_1)) + A(4, d_\Gamma(v_2)) + A(4, 3) + A(4, 1) + A(3, 1)\\
&- A(3, d_\Gamma(v_1)) - A(3, d_\Gamma(v_2)) - A(3, 2) - A(3, 3) - A(2, 1)\\
>&A(4, 1) + A(3, 1) - A(3, 3) - A(2, 1)\\
=&\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

As a result, $ABS(\Gamma_{15}) > ABS(\Gamma)$, a contradiction.

Case 4.2. $u \in V(C)$.

Case 4.2.1. $v \notin V(C)$.

Since $uv \in M$, then $d_\Gamma(v_1), d_\Gamma(v_2) \geq 2$. Suppose P is a maximal path from v to x and containing vv_2. Thus, $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y)\backslash\{x\} = \{y_1\}$. Let $\Gamma_{16} = U - \{vv_1, vv_2\} + \{uv_2, yv_1\}$. Then $\Gamma_{16} \in \boldsymbol{C\Gamma}_{2m}$. If $y \neq v_2$, we have

$$\begin{aligned}
&ABS(\Gamma_{16}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(u_2)) + A(4, d_\Gamma(v_2)) + A(3, d_\Gamma(y_1)) + A(4, 1) + A(3, 1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(u_2)) - A(3, d_\Gamma(v_2)) - A(2, d_\Gamma(y_1)) - A(3, 3) - A(2, 1)\\
>&A(4, 1) + A(3, 1) - A(3, 3) - A(2, 1)\\
=&\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

If $y = v_2$, i.e. $v = y_1$, we have

$$\begin{aligned}
&ABS(\Gamma_{16}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(u_2)) + A(4, 3) + A(4, 1) + A(3, 1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(u_2)) - A(3, 2) - A(3, 3) - A(2, 1)\\
>&A(4, 1) + A(3, 1) - A(3, 3) - A(2, 1)\\
=&\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

As a result, $ABS(\Gamma_{16}) > ABS(\Gamma)$, which is a contradiction.

Case 4.2.2. $v \in V(C)$.

Without loss of generality, we assume that $u_1, v_1 \in V(C)$ and $u_2, v_2 \notin V(C)$. Since $uv \in M$, then $d_\Gamma(u_2), d_\Gamma(v_2) \geq 2$. Suppose P is a maximal path from v to x and containing vv_2. It can be seen that $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Let $N_\Gamma(y) \setminus \{x\} = \{y_1\}$.

Case 4.2.2.1. $u_1 \neq v_1$.

Let $\Gamma_{17} = U - \{uu_1, uu_2\} + \{u_1v, yu_2\}$. Then $\Gamma_{17} \in \boldsymbol{C\Gamma}_{2m}$. If $y \neq v_2$, we have

$$\begin{aligned}
&ABS(\Gamma_{17}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(v_1)) + A(4, d_\Gamma(v_2)) + A(4, d_\Gamma(u_1)) + A(3, d_\Gamma(y_1)) + A(4, 1) + A(3, 1)\\
&- A(3, d_\Gamma(v_1)) - A(3, d_\Gamma(v_2)) - A(3, d_\Gamma(u_1)) - A(2, d_\Gamma(y_1)) - A(3, 3) - A(2, 1)\\
>&A(4, 1) + A(3, 1) - A(3, 3) - A(2, 1)\\
=&\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

If $y = v_2$, i.e. $v = y_1$, we have

$$\begin{aligned}
&ABS(\Gamma_{17}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(v_1)) + A(4, 3) + A(4, 1) + A(3, 1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(v_1)) - A(3, 2) - A(3, 3) - A(2, 1)\\
>&A(4, 1) + A(3, 1) - A(3, 3) - A(2, 1)
\end{aligned}$$

$$=\sqrt{\frac{3}{5}}+\sqrt{\frac{1}{2}}-\sqrt{\frac{2}{3}}-\sqrt{\frac{1}{3}}$$
$$>0.$$

Thus $ABS(\Gamma_{17}) > ABS(\Gamma)$, which is a contradiction.

Case 4.2.2.2. $u_1 = v_1$.

Note that $C = uvu_1u$ is the only cycle of Γ. Let $\Gamma_{18} = U - \{uu_1, uu_2\} + \{vu_2, yu_1\}$. Then $\Gamma_{18} \in \mathbf{C\Gamma}_{2m}$. If $y \neq v_2$, we have

$$\begin{aligned}
&ABS(\Gamma_{18}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(u_2)) + A(3, d_\Gamma(y_1)) + A(4, 1) + A(3, 1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(u_2)) - A(2, d_\Gamma(y_1)) - A(3, 3) - A(2, 1)\\
>&A(4, 1) + A(3, 1) - A(3, 3) - A(2, 1)\\
=&\sqrt{\frac{3}{5}}+\sqrt{\frac{1}{2}}-\sqrt{\frac{2}{3}}-\sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

If $y = v_2$, i.e. $v = y_1$, we have

$$\begin{aligned}
&ABS(\Gamma_{18}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(u_2)) + A(4, 3) + A(4, 1) + A(3, 1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(u_2)) - A(3, 2) - A(3, 3) - A(2, 1)\\
>&A(4, 1) + A(3, 1) - A(3, 3) - A(2, 1)\\
=&\sqrt{\frac{3}{5}}+\sqrt{\frac{1}{2}}-\sqrt{\frac{2}{3}}-\sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

Hence $ABS(\Gamma_{18}) > ABS(\Gamma)$, a contradiction.

Case 5. $d_\Gamma(u) = 3$ and $d_\Gamma(v) = 4$.

Denote $N_\Gamma(u) \setminus \{v\} = \{u_1, u_2\}$ and $N_\Gamma(v) \setminus \{u\} = \{v_1, v_2, v_3\}$.

Case 5.1. $u \notin V(C)$.

Case 5.1.1. u is the vertex that is situated closer to C than v.

Since $uv \in M$, then $d_\Gamma(u_1), d_\Gamma(u_2), d_\Gamma(v_1), d_\Gamma(v_2), d_\Gamma(v_3) \geq 2$. Suppose u_1 is the vertex that is situated nearer to C than u_2 and P is a maximal path from u to x and containing uu_2. It is obvious that $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_{19} = U - \{vv_1, vv_2, vv_3\} + \{uv_1, yv_2, yv_3\}$. Then $\Gamma_{19} \in \mathbf{C\Gamma}_{2m}$. If $y \neq u_2$, we get

$$\begin{aligned}
&ABS(\Gamma_{19}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(u_2)) + A(4, d_\Gamma(y_1)) + A(4, 1) + A(4, 1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(u_2)) - A(2, d_\Gamma(y_1)) - A(4, 3) - A(2, 1)\\
>&A(4, 1) + A(4, 1) - A(4, 3) - A(2, 1)\\
=&2\sqrt{\frac{3}{5}}-\sqrt{\frac{5}{7}}-\sqrt{\frac{1}{3}}\\
\approx&0.1267 > 0.
\end{aligned}$$

If $y = u_2$, i.e. $u = y_1$, we derive

$$\begin{aligned}
&ABS(\Gamma_{19}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4,4) + A(4,1) + A(4,1)\\
&- A(3, d_\Gamma(u_1)) - A(3,2) - A(4,3) - A(2,1)\\
>&A(4,1) + A(4,1) - A(4,3) - A(2,1)\\
=&2\sqrt{\frac{3}{5}} - \sqrt{\frac{5}{7}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

As a result, $ABS(\Gamma_{19}) > ABS(\Gamma)$, which is a contradiction.

Case 5.1.2. v is the vertex that is situated closer to C than u.

Without loss of generality, we assume that v_1 is the vertex that is situated closer to C than v_2, v_3 when $v \notin V(C)$, and $v_1, v_2 \in V(C)$, $v_3 \notin V(C)$ when $v \in V(C)$.

If $v \notin V(C)$, suppose P is a maximal path from v to x and containing vv_2. Obviously, $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_{20} = U - \{uu_1, uu_2\} + \{yu_1, yu_2\}$. Then $\Gamma_{20} \in \boldsymbol{C\Gamma}_{2m}$ and we have

$$\begin{aligned}
&ABS(\Gamma_{20}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(u_2)) + A(4, d_\Gamma(y_1)) + A(4,1) + A(4,1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(u_2)) - A(2, d_\Gamma(y_1)) - A(4,3) - A(2,1)\\
>&A(4,1) + A(4,1) - A(4,3) - A(2,1)\\
=&2\sqrt{\frac{3}{5}} - \sqrt{\frac{5}{7}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

So $ABS(\Gamma_{20}) > ABS(\Gamma)$, which is a contradiction.

If $v \in V(C)$, suppose P is a maximal path from v to x and containing vv_3. It is clear that $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_{21} = U - \{uu_1, uu_2\} + \{yu_1, yu_2\}$. Then $\Gamma_{21} \in \boldsymbol{C\Gamma}_{2m}$ and we have

$$\begin{aligned}
&ABS(\Gamma_{21}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(u_2)) + A(4, d_\Gamma(y_1)) + A(4,1) + A(4,1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(u_2)) - A(2, d_\Gamma(y_1)) - A(4,3) - A(2,1)\\
>&A(4,1) + A(4,1) - A(4,3) - A(2,1)\\
=&2\sqrt{\frac{3}{5}} - \sqrt{\frac{5}{7}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

Hence $ABS(\Gamma_{21}) > ABS(\Gamma)$, a contradiction.

Case 5.2. $u \in V(C)$.

Case 5.2.1. $v \notin V(C)$.

Since $uv \in M$, then $d_\Gamma(v_1), d_\Gamma(v_2), d_\Gamma(v_3) \geq 2$. Suppose P is a maximal path from v to x and containing vv_2. So $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Denote

$N_\Gamma(y) \setminus \{x\} = \{y_1\}$. Let $\Gamma_{22} = U - \{vv_1, vv_2, vv_3\} + \{uv_2, yv_1, yv_3\}$. Then $\Gamma_{22} \in \boldsymbol{C\Gamma}_{2m}$. If $y \neq v_2$, we have

$$\begin{aligned}
&ABS(\Gamma_{22}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(u_2)) + A(4, d_\Gamma(y_1)) + A(4, 1) + A(4, 1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(u_2)) - A(2, d_\Gamma(y_1)) - A(4, 3) - A(2, 1)\\
>&A(4, 1) + A(4, 1) - A(4, 3) - A(2, 1)\\
=&2\sqrt{\frac{3}{5}} - \sqrt{\frac{5}{7}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

If $y = v_2$, i.e. $v = y_1$, we derive

$$\begin{aligned}
&ABS(\Gamma_{22}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(u_2)) + A(4, 4) + A(4, 1) + A(4, 1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(u_2)) - A(2, 4) - A(4, 3) - A(2, 1)\\
>&A(4, 1) + A(4, 1) - A(4, 3) - A(2, 1)\\
=&2\sqrt{\frac{3}{5}} - \sqrt{\frac{5}{7}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

Thus $ABS(\Gamma_{22}) > ABS(\Gamma)$, which is a contradiction.

Case 5.2.2. $v \in V(C)$.

Without loss of generality, we assume that $u_1, v_1 \in V(C)$ and $u_2, v_2, v_3 \notin V(C)$. Since $uv \in M$, then $d_\Gamma(u_2), d_\Gamma(v_2), d_\Gamma(v_3) \geq 2$. Suppose P is a maximal path from v to x and containing vv_2. It is obvious that $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Let $N_\Gamma(y) \setminus \{x\} = \{y_1\}$.

Case 5.2.2.1. $u_1 \neq v_1$.

Let $\Gamma_{23} = U - \{uu_1, uu_2, vv_3\} + \{u_1v, yu_2, yv_3\}$. Then $\Gamma_{23} \in \boldsymbol{C\Gamma}_{2m}$ and it follows that

$$\begin{aligned}
&ABS(\Gamma_{23}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(u_2)) + A(4, d_\Gamma(y_1)) + A(4, 1) + A(4, 1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(u_2)) - A(2, d_\Gamma(y_1)) - A(4, 3) - A(2, 1)\\
>&A(4, 1) + A(4, 1) - A(4, 3) - A(2, 1)\\
=&2\sqrt{\frac{3}{5}} - \sqrt{\frac{5}{7}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

So $ABS(\Gamma_{23}) > ABS(\Gamma)$, which is a contradiction.

Case 5.2.2.2. $u_1 = v_1$.

Note that $C = uvu_1u$ is the only cycle of Γ. Let $\Gamma_{24} = U - \{uu_1, uu_2\} + \{yu_1, yu_2\}$. Then $\Gamma_{24} \in \boldsymbol{C\Gamma}_{2m}$ and we derive

$$\begin{aligned}
&ABS(\Gamma_{24}) - ABS(\Gamma)\\
=&A(4, d_\Gamma(u_1)) + A(4, d_\Gamma(u_2)) + A(4, d_\Gamma(y_1)) + A(4, 1) + A(4, 1)\\
&- A(3, d_\Gamma(u_1)) - A(3, d_\Gamma(u_2)) - A(2, d_\Gamma(y_1)) - A(4, 3) - A(2, 1)\\
>&A(4, 1) + A(4, 1) - A(4, 3) - A(2, 1)\\
=&2\sqrt{\frac{3}{5}} - \sqrt{\frac{5}{7}} - \sqrt{\frac{1}{3}}\\
>&0.
\end{aligned}$$

Hence $ABS(\Gamma_{24}) > ABS(\Gamma)$, a contradiction.

Case 6. $d_\Gamma(u) = 4$ and $d_\Gamma(v) = 4$.

Denote $N_\Gamma(u) \setminus \{v\} = \{u_1, u_2, u_3\}$ and $N_\Gamma(v) \setminus \{u\} = \{v_1, v_2, v_3\}$.

Case 6.1. $u \notin V(C)$.

Case 6.1.1. u is the vertex that is situated nearer to C than v.

Since $uv \in M$, then $d_\Gamma(u_1), d_\Gamma(u_2), d_\Gamma(u_3), d_\Gamma(v_1), d_\Gamma(v_2), d_\Gamma(v_3) \geq 2$. Suppose u_1 is the vertex that is situated nearer to C than u_2, u_3 and P is a maximal path from u to x and containing uu_2. So $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Let $\Gamma_{25} = U - \{vv_1, vv_2, vv_3\} + \{xv_1, xv_2, xv_3\}$. Then $\Gamma_{25} \in \boldsymbol{C\Gamma}_{2m}$ and we have

$$\begin{aligned} & ABS(\Gamma_{25}) - ABS(\Gamma) \\ =& A(4,1) + A(4,2) - A(4,4) - A(2,1) \\ =& \sqrt{\frac{3}{5}} + \sqrt{\frac{2}{3}} - \sqrt{\frac{3}{4}} - \sqrt{\frac{1}{3}} \\ \approx& 0.1477 > 0. \end{aligned}$$

Thus $ABS(\Gamma_{25}) > ABS(\Gamma)$, which is a contradiction.

Case 6.1.2. v is the vertex that is situated nearer to C than u.

Without loss of generality, we assume that v_1 is the vertex that is situated nearer to C than v_2, v_3 when $v \notin V(C)$, and $v_1, v_2 \in V(C)$, $v_3 \notin V(C)$ when $v \in V(C)$.

If $v \notin V(C)$, suppose P is a maximal path from v to x and containing vv_2. We see that $d_\Gamma(x) = 1$ and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Let $\Gamma_{26} = U - \{uu_1, uu_2, uu_3\} + \{xu_1, xu_2, xu_3\}$. Then $\Gamma_{26} \in \boldsymbol{C\Gamma}_{2m}$ and we have

$$\begin{aligned} & ABS(\Gamma_{26}) - ABS(\Gamma) \\ =& A(4,1) + A(4,2) - A(4,4) - A(2,1) \\ =& \sqrt{\frac{3}{5}} + \sqrt{\frac{2}{3}} - \sqrt{\frac{3}{4}} - \sqrt{\frac{1}{3}} \\ >& 0. \end{aligned}$$

So $ABS(\Gamma_{26}) > ABS(\Gamma)$, which is a contradiction.

If $v \in V(C)$, suppose P is a maximal path from v to x and containing vv_3. It can be seen that $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Let $\Gamma_{27} = U - \{uu_1, uu_2, uu_3\} + \{xu_1, xu_2, xu_3\}$. Then $\Gamma_{27} \in \boldsymbol{C\Gamma}_{2m}$ and one has

$$\begin{aligned} & ABS(\Gamma_{27}) - ABS(\Gamma) \\ =& A(4,1) + A(4,2) - A(4,4) - A(2,1) \\ =& \sqrt{\frac{3}{5}} + \sqrt{\frac{2}{3}} - \sqrt{\frac{3}{4}} - \sqrt{\frac{1}{3}} \\ >& 0. \end{aligned}$$

Therefore, $ABS(\Gamma_{27}) > ABS(\Gamma)$, a contradiction.

Case 6.2. $u \in V(C)$.

Case 6.2.1. $v \notin V(C)$.

Without loss of generality, we assume that $u_1, u_2 \in V(C)$ and $u_3 \notin V(C)$. Since $uv \in M$, then $d_\Gamma(u_3), d_\Gamma(v_1), d_\Gamma(v_2), d_\Gamma(v_3) \geq 2$. Suppose P is a maximal path from u to x and containing uu_3. So $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Let $\Gamma_{28} =$

$U - \{vv_1, vv_2, vv_3\} + \{xv_1, xv_2, xv_3\}$. Then $\Gamma_{28} \in \boldsymbol{C\Gamma}_{2m}$ and it follows that

$$\begin{aligned}&ABS(\Gamma_{28}) - ABS(\Gamma)\\ =&A(4,1) + A(4,2) - A(4,4) - A(2,1)\\ =&\sqrt{\frac{3}{5}} + \sqrt{\frac{2}{3}} - \sqrt{\frac{3}{4}} - \sqrt{\frac{1}{3}}\\ >&0.\end{aligned}$$

Thus $ABS(\Gamma_{28}) > ABS(\Gamma)$, which is a contradiction.

Case 6.2.2. $v \in V(C)$.

Without loss of generality, we assume that $u_1, v_1 \in V(C)$ and $u_2, u_3, v_2, v_3 \notin V(C)$. Since $uv \in M$, then $d_\Gamma(u_2), d_\Gamma(u_3), d_\Gamma(v_2), d_\Gamma(v_3) \geq 2$. Suppose P is a maximal path from v to x and containing vv_2. It is obvious that $d_\Gamma(x) = 1$, and we denote $N_\Gamma(x) = \{y\}$. Then $d_\Gamma(y) = 2$ since Γ has a perfect matching. Let $N_\Gamma(y) \setminus \{x\} = \{y_1\}$.

Case 6.2.2.1. $u_1 \neq v_1$.

Let $\Gamma_{29} = U - \{uu_1, uu_2, uu_3, vv_3\} + \{u_1v, xu_2, xu_3, xv_3\}$. Then $\Gamma_{29} \in \boldsymbol{C\Gamma}_{2m}$ and we have

$$\begin{aligned}&ABS(\Gamma_{29}) - ABS(\Gamma)\\ =&A(4,1) + A(4,2) - A(4,4) - A(2,1)\\ =&\sqrt{\frac{3}{5}} + \sqrt{\frac{2}{3}} - \sqrt{\frac{3}{4}} - \sqrt{\frac{1}{3}}\\ >&0.\end{aligned}$$

Hence $ABS(\Gamma_{29}) > ABS(\Gamma)$, which is a contradiction.

Case 6.2.2.2. $u_1 = v_1$.

Note that $C = uvu_1u$ is the only cycle of Γ and $d_\Gamma(u_1) \geq 3$. Suppose P is a maximal path from v to x' and containing vv_3. It is clear that $d_\Gamma(x') = 1$, and we denote $N_\Gamma(x') = \{y'\}$. Then $d_\Gamma(y') = 2$ since Γ has a perfect matching. Denote $N_\Gamma(y') \setminus \{x'\} = \{y'_1\}$. Let $\Gamma_{30} = U - \{uu_1, uu_2, uu_3\} + \{y'u_2, y'u_3, yu_1\}$. Then $\Gamma_{30} \in \boldsymbol{C\Gamma}_{2m}$ and by Lemma 2.1, we have

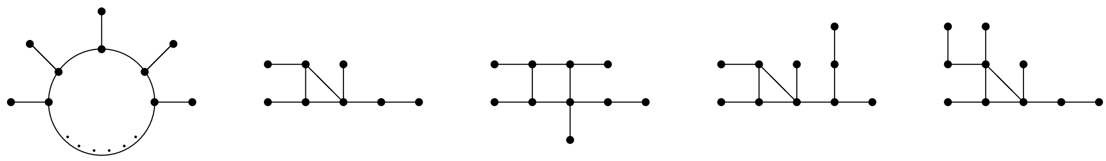
$$\begin{aligned}&ABS(\Gamma_{30}) - ABS(\Gamma)\\ =&A(3, d_\Gamma(y_1)) + A(4, d_\Gamma(y'_1)) + A(3, d_\Gamma(u_1)) + 2A(4,1) + A(3,1)\\ &- A(2, d_\Gamma(y_1)) - A(2, d_\Gamma(y'_1)) - A(4, d_\Gamma(u_1)) - A(4,4) - 2A(2,1)\\ >&A(3, d_\Gamma(u_1)) - A(4, d_\Gamma(u_1)) + 2A(4,1) + A(3,1) - A(4,4) - 2A(2,1)\\ \geq&A(3,3) - A(4,3) + 2A(4,1) + A(3,1) - A(4,4) - 2A(2,1)\\ =&\sqrt{\frac{2}{3}} - \sqrt{\frac{5}{7}} + 2\sqrt{\frac{3}{5}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{3}{4}} - 2\sqrt{\frac{1}{3}}\\ \approx&0.2069 > 0.\end{aligned}$$

As a result, $ABS(\Gamma_{30}) > ABS(\Gamma)$, a contradiction.

The proof is completed. □

3. Main results

Let $\mathscr{U}(2m)$ $(m \geq 3)$ be the $2m$-vertex chemical unicyclic graph obtained from C_m by attaching exactly one pendent edge to its each vertex (see Fig. 3.1). Observe that $ABS(\mathscr{U}(2m)) = (\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{3})m$.



$\mathscr{U}(2m),\ m \geq 3$ G_1 G_2 G_3 G_4

Fig. 3.1. The graphs $\mathscr{U}(2m), G_1, G_2, G_3$ and G_4.

Theorem 3.1. *Let $\Gamma \in \boldsymbol{C\Gamma}_{2m}$, where $m \geq 3$. Then*

$$ABS(\Gamma) \leq (\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{3})m.$$

The equality holds only when $\Gamma \cong \mathscr{U}(2m)$.

Proof. Let

$$\psi(m) = (\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{3})m.$$

Since $\Gamma \in \boldsymbol{C\Gamma}_{2m}$, every non-pendent vertex in Γ has at most one pendent neighbor. Thus, we can conclude that the number of pendent vertices of Γ is less than or equal to m. In the following, we consider two separate cases.

Case 1. The number of pendent vertices of Γ is m.

Now, every non-pendent vertex of Γ has a pendent neighbor. We prove the conclusion of this case by induction on m. If $m = 3$, $\Gamma \cong \mathscr{U}(6)$ (see Fig. 3.1) and $ABS(\mathscr{U}(6)) = \frac{3\sqrt{2}}{2} + \sqrt{6} = \psi(3)$. If $m = 4$, $\Gamma \cong \mathscr{U}(8)$ or G_1 (see Fig. 3.1) and $ABS(\mathscr{U}(8)) = 2\sqrt{2} + \frac{4\sqrt{6}}{3} = \psi(4)$, $ABS(G_1) = \sqrt{2} + \frac{2}{3}\sqrt{6} + \frac{2}{7}\sqrt{35} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{3} \approx 6.0895 < \psi(4) \approx 6.0944$. If $m = 5$, Γ contains $\mathscr{U}(10), G_2, G_3$ and G_4 (see Fig. 3.1). Notice that $ABS(\mathscr{U}(10)) = \frac{5\sqrt{2}}{2} + \frac{5\sqrt{6}}{3} = \psi(5)$, $ABS(G_2) = \frac{3}{2}\sqrt{2} + \sqrt{6} + \frac{2}{7}\sqrt{35} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{3} \approx 7.6131 < \psi(5) \approx 7.6180$, $ABS(G_3) = \frac{3}{2}\sqrt{2} + \frac{\sqrt{6}}{3} + \frac{3}{7}\sqrt{35} + \frac{2\sqrt{15}}{5} + \frac{\sqrt{3}}{3} \approx 7.5998 < \psi(5)$, $ABS(G_4) = \frac{\sqrt{2}}{2} + \frac{2\sqrt{6}}{3} + \frac{2}{7}\sqrt{35} + \frac{2\sqrt{15}}{5} + \frac{2\sqrt{3}}{3} + \frac{\sqrt{3}}{2} \approx 7.6003 < \psi(5)$. Therefore, the result follows for $m = 3, 4$ and 5.

Suppose that the result holds for $\Gamma \in \boldsymbol{C\Gamma}_{2k}$, $k < m$ and $m \geq 6$. Let M be a perfect matching of Γ. We use $x, x_1, x_2, \cdots, x_{m-1}$ to denote all pendent vertices of Γ and $y, z_1, z_2, \cdots, z_{m-1}$ are their adjacent non-pendent vertices, respectively, where $d_\Gamma(y), d_\Gamma(z_1), d_\Gamma(z_2), \cdots, d_\Gamma(z_{m-1}) \geq 2$. It can be seen easily that $M = \{xy, x_1z_1, x_2z_2, \cdots, x_{m-1}z_{m-1}\}$.

Case 1.1. Γ contains a pendent vertex x adjacent to a vertex y of degree 2.

Observe that $xy \in M$, we denote $N_\Gamma(y) \setminus \{x\} = \{z_s\}$. Since every non-pendent vertex of Γ has a pendent neighbor, so $d_\Gamma(z_s) \geq 3$.

Case 1.1.1. $d_\Gamma(z_s) = 3$.

Denote $N_\Gamma(z_s) = \{y, x_s, z_{s+1}\}$, where $d_\Gamma(x_s) = 1$ and $d_\Gamma(z_{s+1}) \geq 3$. If Γ contains no vertex of degree 4, this leads to a contradiction that Γ is a unicyclic graph since every non-pendent vertex of Γ has a pendent neighbor. Therefore, there is a vertex z_{s+t} $(t \geq 1)$ with $d_\Gamma(z_{s+t}) = 4$ such that $z_{s+1}, z_{s+2}, \cdots, z_{s+t-1}$ are vertices with degree 3 in Γ. We know that $\{xy, x_sz_s, x_{s+1}z_{s+1}, \cdots, x_{s+t-1}z_{s+t-1}\} \in M$ for $\Gamma \in \boldsymbol{C\Gamma}_{2m}$. Let $\Gamma_1 = \Gamma - \{x_s, z_s, x_{s+1}, z_{s+1}, \cdots, x_{s+t-1}, z_{s+t-1}\} + yz_{s+t}$. Then $M \backslash \{x_sz_s, x_{s+1}z_{s+1}, \cdots, x_{s+t-1}z_{s+t-1}\}$ is a perfect matching of Γ_1 and $\Gamma_1 \in \boldsymbol{C\Gamma}_{2(m-t)}$. By the induction hypothesis, we derive

$$\begin{aligned}ABS(\Gamma) =&ABS(\Gamma_1) + tA(1,3) + (t-1)A(3,3) + A(2,3) + A(3,4) - A(2,4)\\ \leq&\psi(m-t) + \frac{\sqrt{2}}{2}t + \frac{\sqrt{6}}{3}(t-1) + \frac{\sqrt{15}}{5} + \frac{\sqrt{35}}{7} - \frac{\sqrt{6}}{3}\\ =&\psi(m) - \frac{2\sqrt{6}}{3} + \frac{\sqrt{15}}{5} + \frac{\sqrt{35}}{7}\\ \approx&\psi(m) - 0.0132\\ <&\psi(m).\end{aligned}$$

Case 1.1.2. $d_\Gamma(z_s) = 4$.

Denote $N_\Gamma(z_s) = \{y, x_s, z_{s-1}, z_{s+1}\}$, where $d_\Gamma(x_s) = 1$, $d_\Gamma(z_{s-1}), d_\Gamma(z_{s+1}) \geq 2$ and at least one of z_{s-1} and z_{s+1} has degree equal to 3 or 4 since $\Gamma \in \boldsymbol{C\Gamma}_{2m}$ and every non-pendent vertex of Γ has a pendent neighbor.

Case 1.1.2.1. $d_\Gamma(z_{s-1}) = 2$ and $d_\Gamma(z_{s+1}) = 3$.

Denote $N_\Gamma(z_{s-1}) = \{x_{s-1}, z_s\}$ and $N_\Gamma(z_{s+1}) = \{x_{s+1}, z_s, z_{s+2}\}$, where $d_\Gamma(x_{s-1}) = 1$, $d_\Gamma(x_{s+1}) = 1$ and $d_\Gamma(z_{s+2}) \geq 3$. If Γ contains no vertex of degree 4 except z_s, then Γ is not a unicyclic graph, a contradiction. Therefore, there is a vertex z_{s+t} $(t \geq 2)$ with degree 4 such that $d_\Gamma(z_{s+1}) = d_\Gamma(z_{s+2}) = \cdots = d_\Gamma(z_{s+t-1}) = 3$ in Γ. We can see that $\{xy, x_s z_s, x_{s+1}z_{s+1}, \cdots, x_{s+t-1}z_{s+t-1}\} \in M$ for $\Gamma \in \boldsymbol{C\Gamma}_{2m}$. Let $\Gamma_2 = \Gamma - \{x, y, x_s, z_s, x_{s+1}, z_{s+1}, \cdots, x_{s+t-1}, z_{s+t-1}\} + z_{s-1}z_{s+t}$. Then $M \setminus \{xy, x_s z_s, x_{s+1}z_{s+1}, \cdots, x_{s+t-1}z_{s+t-1}\}$ is a perfect matching of Γ_2 and $\Gamma_2 \in \boldsymbol{C\Gamma}_{2(m-t-1)}$. By the induction hypothesis, one has

$$\begin{aligned}ABS(\Gamma) =&ABS(\Gamma_2) + (t-1)A(1,3) + (t-2)A(3,3) + A(2,1) + A(2,4)\\ &+ A(4,1) + A(3,4) + A(3,4)\\ \leq&\psi(m-t-1) + \frac{\sqrt{2}}{2}(t-1) + \frac{\sqrt{6}}{3}(t-2) + \frac{\sqrt{3}}{3} + \frac{\sqrt{6}}{3} + \frac{\sqrt{15}}{5} + \frac{2\sqrt{35}}{7}\\ =&\psi(m) - \sqrt{2} - \frac{2\sqrt{6}}{3} + \frac{\sqrt{3}}{3} + \frac{\sqrt{15}}{5} + \frac{2\sqrt{35}}{7}\\ \approx&\psi(m) - 0.0050\\ <&\psi(m).\end{aligned}$$

Case 1.1.2.2. $d_\Gamma(z_{s-1}) = 2$ and $d_\Gamma(z_{s+1}) = 4$.

Let $\Gamma_3 = \Gamma - \{x, y, x_s, z_s\} + z_{s-1}z_{s+1}$. Then $M \setminus \{xy, x_s z_s\}$ is a perfect matching of Γ_3 and $\Gamma_3 \in \boldsymbol{C\Gamma}_{2(m-2)}$. By the induction hypothesis, one has

$$\begin{aligned}ABS(\Gamma) =&ABS(\Gamma_3) + A(2,1) + A(2,4) + A(4,1) + A(4,4)\\ \leq&\psi(m-2) + \frac{\sqrt{3}}{3} + \frac{\sqrt{6}}{3} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{2}\\ =&\psi(m) - \frac{\sqrt{6}}{3} - \sqrt{2} + \frac{\sqrt{3}}{3} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{2}\\ \approx&\psi(m) - 0.0127\\ <&\psi(m).\end{aligned}$$

Case 1.1.2.3. $d_\Gamma(z_{s-1}) = 3$ and $d_\Gamma(z_{s+1}) = 3$.

Let $\Gamma_4 = \Gamma - \{x, y\}$. Then $M \setminus \{xy\}$ is a perfect matching of Γ_4 and $\Gamma_4 \in \boldsymbol{C\Gamma}_{2(m-1)}$. By the induction hypothesis, one has

$$\begin{aligned} ABS(\Gamma) =& ABS(\Gamma_4) + 2A(3,4) + A(4,2) + A(4,1) + A(2,1) - 2A(3,3) - A(3,1) \\ \le& \psi(m-1) + \frac{2\sqrt{35}}{7} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{3} - \frac{\sqrt{6}}{3} - \frac{\sqrt{2}}{2} \\ =& \psi(m) - \frac{2\sqrt{6}}{3} - \sqrt{2} + \frac{2\sqrt{35}}{7} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{3} \\ \approx& \psi(m) - 0.0050 \\ <& \psi(m). \end{aligned}$$

Case 1.1.2.4. $d_\Gamma(z_{s-1}) = 3$ and $d_\Gamma(z_{s+1}) = 4$.

Let $\Gamma_5 = \Gamma - \{x, y, x_s, z_s\} + z_{s-1}z_{s+1}$. Then $M \setminus \{xy, x_sz_s\}$ is a perfect matching of Γ_5 and $\Gamma_5 \in \boldsymbol{C\Gamma}_{2(m-2)}$. By the induction hypothesis, we derive

$$\begin{aligned} ABS(\Gamma) =& ABS(\Gamma_5) + A(2,1) + A(2,4) + A(4,1) + A(4,4) \\ \le& \psi(m-2) + \frac{\sqrt{3}}{3} + \frac{\sqrt{6}}{3} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{2} \\ =& \psi(m) - \frac{\sqrt{6}}{3} - \sqrt{2} + \frac{\sqrt{3}}{3} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{2} \\ <& \psi(m). \end{aligned}$$

Case 1.1.2.5. $d_\Gamma(z_{s-1}) = 4$ and $d_\Gamma(z_{s+1}) = 4$.

Let $\Gamma_6 = \Gamma - \{x, y, x_s, z_s\} + z_{s-1}z_{s+1}$. Then $M \setminus \{xy, x_sz_s\}$ is a perfect matching of Γ_6 and $\Gamma_6 \in \boldsymbol{C\Gamma}_{2(m-2)}$. By the induction hypothesis, it follows that

$$\begin{aligned} ABS(\Gamma) =& ABS(\Gamma_6) + A(2,1) + A(2,4) + A(4,1) + A(4,4) \\ \le& \psi(m-2) + \frac{\sqrt{3}}{3} + \frac{\sqrt{6}}{3} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{2} \\ =& \psi(m) - \frac{\sqrt{6}}{3} - \sqrt{2} + \frac{\sqrt{3}}{3} + \frac{\sqrt{15}}{5} + \frac{\sqrt{3}}{2} \\ <& \psi(m). \end{aligned}$$

Case 1.2. Γ contains no neighbor of pendent vertex of degree 2.

Now, observe that $\Gamma \cong \mathscr{U}(2m)$ since $\Gamma \in \boldsymbol{C\Gamma}_{2m}$ and every non-pendent vertex of Γ has a pendent neighbor, where $\mathscr{U}(2m)$ is displayed in Fig. 3.1. After a simple calculation, we derive $ABS(\mathscr{U}(2m)) = (\frac{\sqrt{6}}{3} + \frac{\sqrt{2}}{2})m$, as desired.

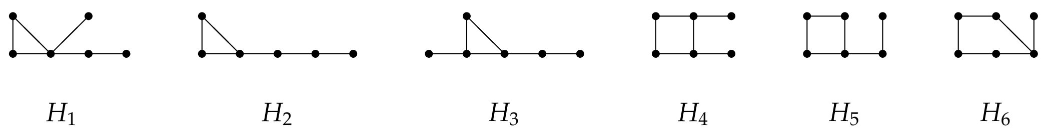


Fig. 3.2. The graphs H_1, H_2, H_3, H_4, H_5 and H_6.

Case 2. Γ contains less than m pendent vertices.

Note that Γ contains a vertex with no pendent neighbor. If $m = 3$, Γ contains $H_1, H_2, \cdots, H_6$ (see Fig. 3.2) and C_6, where C_6 is a cycle of order 6. It is easy to check that $ABS(H_i) < \psi(3)$ ($i = 1, 2, \cdots, 6$) and $ABS(C_6) < \psi(3)$. If $m \ge 4$, by Lemma 2.2 and the proof of Case 1, one can easily see that any vertex of Γ has maximum ABS index if and only if it has a pendent neighbor. Thus, $ABS(\Gamma) < \psi(m)$.

The proof is completed. □

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