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Maximum Atom Bond Sum Connectivity Index of Molecular Trees with a Perfect Matching

Fangxia Wang[a], Yaoyao Zhang[b*], Xiangyu Ren[c], Bo Zhang[d]

[a] *School of Mathematical Science, Xinjiang Normal University Urumqi 830054, P.R.China*

[b] *College of Mathematics and System Science, Xinjiang University Urumqi, Xinjiang, 830046, P.R.China*

[c] *School of Mathematical Sciences, Shanxi University Taiyuan, Shanxi, 030006, P.R.China*

[d] *School of Mathematics and Computer Sciences, Shanxi Normal University, Taiyuan, Shanxi 030031, P.R.China*

fangxwangxj@163.com, yoyoyame@126.com, renxy@sxu.edu.cn, 20230015@sxnu.edu.cn

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Abstract

Ali et al. [3] introduced a new type of vertex-degree-based topological indices of a graph which is called as atom-bond sum-connectivity (ABS) index. For a graph $G = (V(G), E(G))$, the ABS index of G is defined as

$$ABS(G) = \sum_{uv \in E(G)} \sqrt{1 - \frac{2}{d_G(u) + d_G(v)}},$$

where $d_G(u)$ denotes the degree of the vertex u in G. Recall that G is a molecular graph if $d_G(u) \le 4$ for all $u \in V(G)$. In this paper, we characterize molecular trees with a perfect matching attaining the maximum ABS index.

*Corresponding author.

1 Introduction

Recently, Ali et al. [3] defined a new topological index which is called as *atom-bond sum-connectivity (ABS) index*. For a graph G, its ABS index is defined as follows:

$$ABS(G) = \sum_{uv \in E(G)} \sqrt{1 - \frac{2}{d_G(u) + d_G(v)}}.$$

Ali et al. [2] showed that the ABS index performs somewhat better than the other topological indices for some physico-chemical properties. Moreover, they [3] characterized the graphs which attains the extreme values of the ABS index over the classes of (molecular) trees and general graphs of a fixed order. Alraqad et al. [5] determined the extremal graphs with respect to the ABS index with chromatic number, independence number, number of pendant vertices. People may refer to [1,4,6,11–14,16] for more relevant works.

There are many researches on the extremal value of topological indices of molecular graphs. Cruza et al. [8] determined the graphs extremal with respect to the Sombor index over (connected) chemical graphs, chemical trees, and hexagonal systems. Deng et al. [9] gave the sharp upper bound for the reduced Sombor index among all molecular trees of given order n. Wang et al. [15] gave the maximum value of the reduced Sombor index among all molecular trees of order n with perfect matching and show that the maximum molecular trees of exponential reduced Sombor index. Ali et al. [3] determined the graphs which attain the extreme values of the ABS index over the classes of (molecular) trees and general graphs of a fixed order. Du and Su [10] showed extremal results on bond incident degree indices of molecular trees with a fixed order and a fixed number of leaves. Motivated by known results, in this paper, we aim to characterize molecular trees with a perfect matching attaining the maximum ABS index.

The paper is organized as follows. In Section 2, some fundamental definitions used in this paper are given. Section 3 shows the process of characterizing molecular trees with a perfect matching attaining the maximum ABS index.

2 Terminologies and Notations

All graphs considered in this paper are simple, undirected and finite, and we refer to [7] for undefined terminology and notation. For a graph G, denote $V(G)$ and $E(G)$ as the vertex set and the edge set, respectively. Denote the number of vertices and edges of G as n and m. For a vertex $v \in V(G)$, the *degree* of v, denoted by $d_G(v)$, is the number of edges incident with v in G. If $d_G(v) = 1$, then v is called a *pendant vertex.* Denote $N_G(v)$ as the neighborhood of a vertex v in G.

For $S \subseteq E(G)$, denote $G-S$ as the graph obtained from G by removing the edges in S. Similarly, if S is a subset of the edge set of the complement of G, then $G+S$ denotes the graph obtained from G by adding the edges in S. In particular, if $S = \{uv\}$, then $G-S$ and $G+S$ are simply denoted as $G-uv$ and $G+uv$, respectively.

A *matching* in a graph is a set of pairwise nonadjacent edges. A *perfect matching* is one which covers every vertex of the graph. As usual, the path and the complete graph of order n are denoted by P_n and K_n, respectively. An *acyclic* graph is one that it contains no cycles. A connected acyclic graph is called a *tree*. Recall that G is a *molecular graph* if $d_G(u) \leq 4$ for all $u \in V(G)$. Let G be a molecular graph. Denote n_i as the number of vertices of degree i in G for each $i \in \{1,2,3,4\}$ and $m_{i,j}$ be the number of edges of G connecting a vertex of degree i with a vertex of degree j. Denote $Q = \{(i,j) \in N \times N : 1 \leq i \leq j \leq 4\}$, Thus, the ABS index of G can be rewritten as

$$ABS(G) = \sum_{(i,j)\in Q} \sqrt{1 - \frac{2}{i+j}} m_{i,j}.$$

3 Maximum *ABS* index of molecular trees with a perfect matching

In this section, we give the characterization for molecular trees which have maximum ABS index in the class of molecular trees of order n ($n \geq 14$) with a perfect matching. For molecular trees of $n < 14$ which have a perfect matching, due to the size is small, it is easy to find the ones which has maximum ABS index by simple calculation, see Figure 1.

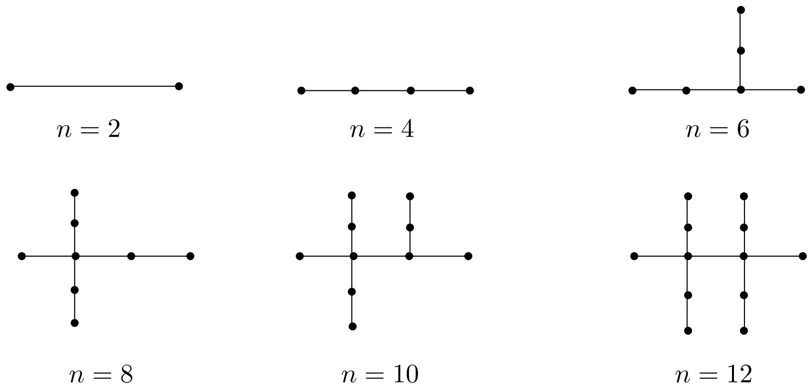

Figure 1. Trees with a perfect matching of order $n(n \leq 12)$

Thus, we prepare to give useful lemmas to describe properties of molecular trees which have maximum ABS index in the class of molecular trees of order n ($n \geq 14$) with a perfect matching.

Lemma 1. *(i) The function f by*

$$f(x,y) = \sqrt{1 - \frac{2}{x+y}} - \sqrt{1 - \frac{2}{x+y+1}}$$

with $\min\{x,y\} \geq 1$ *and* $x+y \geq 3$*, is strictly increasing in* x.

(ii) The function f by

$$f(x,y) = \sqrt{1 - \frac{2}{x+y+1}} + \sqrt{1 - \frac{2}{x+y-1}} - 2\sqrt{1 - \frac{2}{x+y}}$$

with $\min\{x,y\} \geq 1$ *and* $x+y \geq 3$*, is strictly increasing in* x.

Lemma 2. *Let T be a molecular tree that has maximum ABS index in the class of molecular trees of order n ($n \geq 14$) with a perfect matching M. For any $u \in V(T)$ with $d_T(u) \geq 2$, there exists $v \in N_T(u)$ such that v is a pendent vertex.*

Proof. We prove by contradiction. Suppose there exists $u \in V(T)$ with $d_T(u) \geq 2$ such that for any $v \in N_T(u)$, $d_T(v) \geq 2$. We consider the following cases.

Case 1. $d_T(u) = 2$.

Let $v_1, v_2 \in N_T(u)$ and $uv_2 \in M$. Let P be a maximal path which starts from v_1 and contains uv_2. Without loss of generality, suppose x is another end-point of P. Obviously, x is a pendant vertex. Let y be the neighbor of x. Since T has a perfect matching, then $d_T(y) = 2$. Let z be the another neighbor of y. Next, we distinguish the following two subcases.

Case 1.1. $z = v_2$.

Let $T' = T - uv_1 + yv_1$. Clearly, T' is also in the class of molecular trees of order n ($n \geq 14$) with a perfect matching. In the following, we aim to obtain a contradiction by showing $ABS(T') > ABS(T)$. Therefore

$$\begin{aligned}
&ABS(T') - ABS(T) \\
=&\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(v_1)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_1)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(x)}} \\
&-\sqrt{1-\frac{2}{d_T(y)+d_T(x)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(v_2)}}-\sqrt{1-\frac{2}{d_T(y)+d_T(v_2)}} \\
&+\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(v_2)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_2)}} \\
=&\sqrt{1-\frac{2}{3+d_T(v_1)}}-\sqrt{1-\frac{2}{2+d_T(v_1)}}+\sqrt{\frac{1}{2}}-\sqrt{\frac{1}{3}}+\sqrt{1-\frac{2}{3+d_T(v_2)}} \\
&-\sqrt{1-\frac{2}{2+d_T(v_2)}}+\sqrt{1-\frac{2}{1+d_T(v_2)}}-\sqrt{1-\frac{2}{2+d_T(v_2)}}. \qquad (1)
\end{aligned}$$

According to (i) of Lemma 1, the right side of (1) is decreasing with $d_T(v_1)$. And according to (ii) of Lemma 1, the right side of (1) is increasing with $d_T(v_2)$. Replace $d_T(v_2)=2$ and $d_T(v_1)=4$ in the right side of (1), thus $ABS(T')-ABS(T)\geq\sqrt{\frac{5}{7}}+\sqrt{\frac{3}{5}}-\sqrt{\frac{2}{3}}-\sqrt{\frac{1}{2}}>0$, a contradiction to the fact that ABS index of T is maximum in the class of molecular trees of order n ($n\geq 14$) with a perfect matching.

Case 1.2. $z\neq v_2$.

Let $T'=T-uv_1+yv_1$. Thus

$$\begin{aligned}
&ABS(T')-ABS(T)\\
&=\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(v_1)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_1)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(x)}}\\
&\quad-\sqrt{1-\frac{2}{d_T(y)+d_T(x)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(z)}}-\sqrt{1-\frac{2}{d_T(y)+d_T(z)}}\\
&\quad+\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(v_2)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_2)}}\\
&=\sqrt{1-\frac{2}{3+d_T(v_1)}}-\sqrt{1-\frac{2}{2+d_T(v_1)}}+\sqrt{\frac{1}{2}}-\sqrt{\frac{1}{3}}\\
&\quad+\sqrt{1-\frac{2}{3+d_T(z)}}-\sqrt{1-\frac{2}{2+d_T(z)}}+\sqrt{1-\frac{2}{1+d_T(v_2)}}-\sqrt{1-\frac{2}{2+d_T(v_2)}} \qquad (2)
\end{aligned}$$

According to (i) of Lemma 1, the right side of (2) is decreasing with both $d_T(v_1)$ and $d_T(z)$, and increasing with $d_T(v_2)$. Replace $d_T(v_2)=2$ and $d_T(v_1)=d_T(z)=4$ in the right side of (2), thus $ABS(T')-ABS(T)\geq 2\sqrt{\frac{5}{7}}-2\sqrt{\frac{2}{3}}>0$, a contradiction to the definition of T.

Case 2. $d_T(u)=3$.

Let $v_1,v_2,v_3\in N_T(u)$ and $uv_2\in M$. Let us say that $d_T(v_2)\geq 3$, otherwise, by Case 1, v_2 is adjacent to a pendant vertex, a contradiction to $uv_2\in M$. Let P be a maximal path which starts from v_1 and contains uv_2. Without loss of generality, suppose x is another end-point of P. Obviously, x is a pendant vertex. Let y be the neighbor of x. Since T has a perfect matching, then $d_T(y)=2$. Let z be another neighbor of y. Next, we distinguish the following two subcases.

Case 2.1. $z=v_2$.

Let $T' = T - uv_1 + yv_1$. Therefore,

$$
\begin{aligned}
&ABS(T') - ABS(T) \\
=&\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(v_1)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_1)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(x)}} \\
&-\sqrt{1-\frac{2}{d_T(y)+d_T(x)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(v_2)}}-\sqrt{1-\frac{2}{d_T(y)+d_T(v_2)}} \\
&+\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(v_2)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_2)}} \\
&+\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(v_3)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_3)}} \\
=&\sqrt{1-\frac{2}{3+d_T(v_1)}}-\sqrt{1-\frac{2}{3+d_T(v_1)}}+\sqrt{\frac{1}{2}}-\sqrt{\frac{1}{3}} \\
&+\sqrt{1-\frac{2}{3+d_T(v_2)}}-\sqrt{1-\frac{2}{2+d_T(v_2)}}+\sqrt{1-\frac{2}{2+d_T(v_2)}}-\sqrt{1-\frac{2}{3+d_T(v_2)}} \\
&+\sqrt{1-\frac{2}{2+d_T(v_3)}}-\sqrt{1-\frac{2}{3+d_T(v_3)}} \\
=&\sqrt{\frac{1}{2}}-\sqrt{\frac{1}{3}}+\sqrt{1-\frac{2}{2+d_T(v_3)}}-\sqrt{1-\frac{2}{3+d_T(v_3)}} \qquad (3)
\end{aligned}
$$

According to (i) of Lemma 1, the right side of (3) is increasing with $d_T(v_3)$. Replace $d_T(v_3) = 2$ in the right side of (3), thus $ABS(T') - ABS(T) \geq 2\sqrt{\frac{1}{2}} - \sqrt{\frac{1}{3}} - \sqrt{\frac{3}{5}} > 0$, a contradiction to the definition of T.

Case 2.2. $z \neq v_2$.

Let $T' = T - uv_1 + yv_1$. Since $d_T(v_2) \geq 3$, then

$$
\begin{aligned}
&ABS(T') - ABS(T) \\
=&\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(v_1)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_1)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(x)}}
\end{aligned}
$$

$$-\sqrt{1-\frac{2}{d_T(y)+d_T(x)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(z)}}-\sqrt{1-\frac{2}{d_T(y)+d_T(z)}}$$
$$+\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(v_2)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_2)}}$$
$$+\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(v_3)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_3)}}$$
$$=\sqrt{\frac{1}{2}}-\sqrt{\frac{1}{3}}+\sqrt{1-\frac{2}{3+d_T(z)}}-\sqrt{1-\frac{2}{2+d_T(z)}}+\sqrt{1-\frac{2}{2+d_T(v_2)}}$$
$$-\sqrt{1-\frac{2}{3+d_T(v_2)}}+\sqrt{1-\frac{2}{2+d_T(v_3)}}-\sqrt{1-\frac{2}{3+d_T(v_3)}} \tag{4}$$

According to (i) of Lemma 1, the right side of (4) is increasing with $d_T(v_i)$ where $i \in \{2,3\}$ and decreasing with $d_T(z)$. Replace $d_T(v_3)=2$, $d_T(v_2)=3$ and $d_T(z)=4$ in the right side of (4), thus $ABS(T')-ABS(T) \geq 2\sqrt{\frac{1}{2}}-2\sqrt{\frac{2}{3}}+\sqrt{\frac{5}{7}}-\sqrt{\frac{1}{3}}>0$, a contradiction to the definition of T.

Case 3. $d_T(u)=4$.

Let $v_1, v_2, v_3, v_4 \in N_T(u)$ and $uv_2 \in M$. Let us say that $d_T(v_2)=4$, otherwise, by Case 2, v_2 is adjacent to a pendant vertex, a contradiction to $uv_2 \in M$. Let P be a maximal path which starts from v_1 and contains uv_2. Without loss of generality, suppose x is another end-point of P. Obviously, x is a pendant vertex. Let y be the neighbor of x. Since T has a perfect matching, then $d_T(y)=2$. Let z be another neighbor of y. Next, we distinguish the following two subcases.

Case 3.1. $z=v_2$.

Let $T'=T-uv_1+yv_1$. Note $d_T(v_2)=4$, then

$$ABS(T')-ABS(T)$$
$$=\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(v_1)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_1)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(x)}}$$
$$-\sqrt{1-\frac{2}{d_T(y)+d_T(x)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(v_2)}}-\sqrt{1-\frac{2}{d_T(y)+d_T(v_2)}}$$

$$+\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(v_2)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_2)}}$$

$$+\sum_{i=3}^{4}\left[\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(v_i)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_i)}}\right]$$

$$=\sqrt{1-\frac{2}{3+d_T(v_1)}}-\sqrt{1-\frac{2}{4+d_T(v_1)}}+\sqrt{\frac{1}{2}}-\sqrt{\frac{1}{3}}+\sqrt{\frac{5}{7}}$$

$$-\sqrt{\frac{2}{3}}+\sqrt{\frac{5}{7}}-\sqrt{\frac{3}{4}}+\sum_{i=3}^{4}\left[\sqrt{1-\frac{2}{3+d_T(v_i)}}-\sqrt{1-\frac{2}{4+d_T(v_i)}}\right] \quad (5)$$

According to (i) of Lemma 1, the right side of (5) is increasing with $d_T(v_i)$ where $i\in\{1,3,4\}$. Replace $d_T(v_1)=d_T(v_3)=d_T(v_4)=2$ in the right side of (5), thus $ABS(T')-ABS(T)\geq\sqrt{\frac{1}{2}}+3\sqrt{\frac{3}{5}}+2\sqrt{\frac{5}{7}}-\sqrt{\frac{1}{3}}-4\sqrt{\frac{2}{3}}-\sqrt{\frac{3}{4}}>0$, a contradiction to the definition of T.

Case 3.2. $z\neq v_2$.

Let $T'=T-uv_1+yv_1$. Since $d_T(v_2)=4$, we have

$$ABS(T')-ABS(T)$$

$$=\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(v_1)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_1)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(x)}}$$

$$-\sqrt{1-\frac{2}{d_T(y)+d_T(x)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(z)}}-\sqrt{1-\frac{2}{d_T(y)+d_T(z)}}$$

$$+\sum_{i=2}^{4}\left[\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(v_i)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_i)}}\right]$$

$$=\sqrt{\frac{1}{2}}-\sqrt{\frac{1}{3}}+\sqrt{\frac{5}{7}}-\sqrt{\frac{3}{4}}+\sqrt{1-\frac{2}{3+d_T(z)}}-\sqrt{1-\frac{2}{2+d_T(z)}}$$

$$+\sum_{i\in\{1,3,4\}}\left[\sqrt{1-\frac{2}{3+d_T(v_i)}}-\sqrt{1-\frac{2}{4+d_T(v_i)}}\right] \quad (6)$$

According to (i) of Lemma 1, the right side of (6) is increasing with $d_T(v_i)$ where $i\in\{1,3,4\}$, and decreasing with $d_T(z)$. Replace $d_T(v_1)=d_T(v_3)=d_T(v_4)=2$ and $d_T(z)=4$ in the right side of (5), thus $ABS(T')-ABS(T)\geq\sqrt{\frac{1}{2}}+3\sqrt{\frac{3}{5}}+2\sqrt{\frac{5}{7}}-\sqrt{\frac{1}{3}}-4\sqrt{\frac{2}{3}}-\sqrt{\frac{3}{4}}>0$, a contradiction to the definition of T.

The proof is completed. ■

Lemma 3. *Let T be a molecular tree which has maximum ABS index in the class of molecular trees of order n ($n \geq 14$) with a perfect matching M. If T has vertices of degree 4, then*

(i) for each vertex u of degree 4 in T, there exists vertex of degree 2 adjacent to u.

(ii) for each vertex u of degree 2 in T, there exists a neighbor v of u of degree 4.

Proof. (i) We prove by contradiction. Suppose that u is a vertex of degree 4. By Lemma 2, let $N_T(u) = \{v_1, v_2, v_3, v\}$ where $d_T(v_i) \geq 3$ for $i \in \{1, 2, 3\}$ and $d_T(v) = 1$. Hence, uv is a matched edge. Let P be a maximal path which starts from v and contains uv_2. Without loss of generality, suppose x is another end-point of P. Obviously, x is a pendant vertex. Let y be the neighbor of x. Since T has a perfect matching, then $d_T(y) = 2$. Let z be another neighbor of y. Consider $T' = T - uv_1 + yv_1$. Clearly, T' is also in the class of molecular trees of order n ($n \geq 14$) with a perfect matching. In the following, we aim to obtain a contradiction by showing $ABS(T') > ABS(T)$. We proceed with the proof by cases.

Case 1. $z = v_2$.

$$
\begin{aligned}
&ABS(T') - ABS(T) \\
&= \sqrt{1 - \frac{2}{d_{T'}(y) + d_{T'}(v_1)}} - \sqrt{1 - \frac{2}{d_T(u) + d_T(v_1)}} + \sqrt{1 - \frac{2}{d_{T'}(x) + d_{T'}(y)}} \\
&\quad - \sqrt{1 - \frac{2}{d_T(x) + d_T(y)}} + \sqrt{1 - \frac{2}{d_{T'}(y) + d_{T'}(v_2)}} - \sqrt{1 - \frac{2}{d_T(y) + d_T(v_2)}} \\
&\quad + \sqrt{1 - \frac{2}{d_{T'}(u) + d_{T'}(v_2)}} - \sqrt{1 - \frac{2}{d_T(u) + d_T(v_2)}} + \sqrt{1 - \frac{2}{d_{T'}(u) + d_{T'}(v)}} \\
&\quad - \sqrt{1 - \frac{2}{d_T(u) + d_T(v)}} + \sqrt{1 - \frac{2}{d_{T'}(u) + d_{T'}(v_3)}} - \sqrt{1 - \frac{2}{d_T(u) + d_T(v_3)}} \\
&= \sqrt{1 - \frac{2}{3 + d_T(v_1)}} - \sqrt{1 - \frac{2}{4 + d_T(v_1)}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{1}{3}}
\end{aligned}
$$

$$+\sqrt{1-\frac{2}{3+d_T(v_2)}}-\sqrt{1-\frac{2}{2+d_T(v_2)}}+\sqrt{1-\frac{2}{3+d_T(v_2)}}-\sqrt{1-\frac{2}{4+d_T(v_2)}}$$
$$+\sqrt{\frac{1}{2}}-\sqrt{\frac{3}{5}}+\sqrt{1-\frac{2}{3+d_T(v_3)}}-\sqrt{1-\frac{2}{4+d_T(v_3)}} \tag{7}$$

According to (i) of Lemma 1, the right side of (7) is increasing with $d_T(v_i)$ where $i \in \{1,3\}$. And according to (ii) of Lemma 1, the right side of (7) is decreasing with $d_T(v_2)$. Replace $d_T(v_1) = d_T(v_3) = 3$ and $d_T(v_2) = 4$ in the right side of (7), thus $ABS(T') - ABS(T) \geq 2\sqrt{\frac{1}{2}} + \sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}} - \sqrt{\frac{3}{5}} - \sqrt{\frac{3}{4}} > 0$, a contradiction to the definition of T.

Case 2. $z \neq v_2$.

$$\begin{aligned}
&ABS(T') - ABS(T)\\
&=\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(v_1)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_1)}}+\sqrt{1-\frac{2}{d_{T'}(x)+d_{T'}(y)}}\\
&\quad-\sqrt{1-\frac{2}{d_T(x)+d_T(y)}}+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(z)}}-\sqrt{1-\frac{2}{d_T(y)+d_T(z)}}\\
&\quad+\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(v)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v)}}\\
&\quad+\sum_{i=2}^{3}\left[\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(v_i)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v_i)}}\right]\\
&=\sqrt{\frac{1}{2}}-\sqrt{\frac{1}{3}}+\sqrt{1-\frac{2}{3+d_T(z)}}-\sqrt{1-\frac{2}{2+d_T(z)}}+\sqrt{\frac{1}{2}}-\sqrt{\frac{3}{5}}\\
&\quad+\sum_{i\in\{1,2,3\}}\left[\sqrt{1-\frac{2}{3+d_T(v_i)}}-\sqrt{1-\frac{2}{4+d_T(v_i)}}\right]
\end{aligned} \tag{8}$$

According to (i) of Lemma 1, the right side of (8) is increasing with $d_T(v_i)$ where $i \in \{1,2,3\}$, and decreasing with $d_T(z)$. Replace $d_T(v_i) = 3$ for $i \in \{1,2,3\}$ and $d_T(z) = 4$ in the right side of (8), thus $ABS(T') - ABS(T) \geq 2\sqrt{\frac{1}{2}} + 2\sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}} - \sqrt{\frac{3}{5}} - 2\sqrt{\frac{5}{7}} > 0$, a contradiction to the definition of T.

The proof is competed.

(ii) We prove by contradiction. Suppose there exists $u \in V(T)$ such that $N_T(u) = \{x, v\}$ where $N_T(v) = \{v_1, u, y\}$ and $d_T(x) = 1$. According to Lemma 2, we may say that vv_1 is the pendent edge incident with v. Thus $d_T(v_1) = 1$. Since $n \geq 14$, so $d_T(y) \geq 3$. We proceed with the proof by cases.

Case 1. $d_T(y) = 3$.

Without loss of generality, denote $N_T(y) = \{v, y_1, y_2\}$ with $d_T(y_1) = 1$ and $d_T(y_2) \geq 3$. Let $T' = T - y_2y + y_2v$. Thus

$$\begin{aligned}
&ABS(T') - ABS(T)\\
&= \sqrt{1-\frac{2}{d_{T'}(v)+d_{T'}(y_2)}} - \sqrt{1-\frac{2}{d_T(y)+d_T(y_2)}} + \sqrt{1-\frac{2}{d_{T'}(v)+d_{T'}(v_1)}}\\
&\quad - \sqrt{1-\frac{2}{d_T(v)+d_T(v_1)}} + \sqrt{1-\frac{2}{d_{T'}(v)+d_{T'}(u)}} - \sqrt{1-\frac{2}{d_T(v)+d_T(u)}}\\
&\quad + \sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(y_1)}} - \sqrt{1-\frac{2}{d_T(y)+d_T(y_1)}}\\
&= \sqrt{1-\frac{2}{4+d_T(y_2)}} - \sqrt{1-\frac{2}{3+d_T(y_2)}} + \sqrt{\frac{3}{5}} - \sqrt{\frac{1}{2}} + \sqrt{\frac{2}{3}} - \sqrt{\frac{3}{5}}\\
&\quad + \sqrt{\frac{1}{3}} - \sqrt{\frac{1}{2}} \qquad (9)
\end{aligned}$$

According to (i) of Lemma 1, the right side of (9) is decreasing with $d_T(y_2)$. Replace $d_T(y_2) = 4$ in the right side of (9), thus $ABS(T') - ABS(T) \geq \sqrt{\frac{2}{3}} + \sqrt{\frac{1}{3}} + \sqrt{\frac{3}{4}} - 2\sqrt{\frac{1}{2}} - \sqrt{\frac{5}{7}} > 0$, a contradiction to the definition of T.

Case 2. $d_T(y) = 4$.

Without loss of generality, denote $N_T(y) = \{v, y_1, y_2, y_3\}$. By Lemma 3 and (i), without loss of generality, let $d_T(y_1) = 1$ and $d_T(y_2) = 2$. Therefore $d_T(y_3) \geq 3$ for $n \geq 14$. Let $T' = T - yy_2 + uy_2$, thus

$$\begin{aligned}
&ABS(T') - ABS(T)\\
&= \sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(y_2)}} - \sqrt{1-\frac{2}{d_T(y)+d_T(y_2)}}
\end{aligned}$$

$$+\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(x)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(x)}}$$
$$+\sqrt{1-\frac{2}{d_{T'}(u)+d_{T'}(v)}}-\sqrt{1-\frac{2}{d_T(u)+d_T(v)}}$$
$$+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(v)}}-\sqrt{1-\frac{2}{d_T(y)+d_T(v)}}$$
$$+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(y_1)}}-\sqrt{1-\frac{2}{d_T(y)+d_T(y_1)}}$$
$$+\sqrt{1-\frac{2}{d_{T'}(y)+d_{T'}(y_3)}}-\sqrt{1-\frac{2}{d_T(y)+d_T(y_3)}}$$
$$=\sqrt{\frac{3}{5}}-\sqrt{\frac{2}{3}}+\sqrt{\frac{1}{2}}-\sqrt{\frac{1}{3}}+\sqrt{\frac{2}{3}}-\sqrt{\frac{3}{5}}+\sqrt{\frac{2}{3}}-\sqrt{\frac{5}{7}}+\sqrt{\frac{1}{2}}-\sqrt{\frac{3}{5}}$$
$$+\sqrt{1-\frac{2}{3+d_T(y_3)}}-\sqrt{1-\frac{2}{4+d_T(y_3)}}$$
$$=2\sqrt{\frac{1}{2}}+\sqrt{\frac{2}{3}}-\sqrt{\frac{1}{3}}-\sqrt{\frac{3}{5}}-\sqrt{\frac{5}{7}}+\sqrt{1-\frac{2}{3+d_T(y_3)}}-\sqrt{1-\frac{2}{4+d_T(y_3)}} \quad (10)$$

According to (i) of Lemma 1, the right side of (10) is increasing with $d_T(y_3)$. Replace $d_T(y_3)=3$ in the right side of (10), thus $ABS(T')-ABS(T)\geq 2\sqrt{\frac{1}{2}}+2\sqrt{\frac{2}{3}}-\sqrt{\frac{1}{3}}-\sqrt{\frac{3}{5}}-2\sqrt{\frac{5}{7}}>0$, a contradiction to the definition of T.

The proof is competed. ■

Lemma 4. *Let T be a molecular tree which has maximum ABS index in the class of molecular trees of order n ($n\geq 14$) with a perfect matching M. If T has vertices of degree 4, then*

(i) for each vertex u of degree 4 in T, there exists a pair of vertices of degree 2 adjacent to u.

(ii) there are exactly two vertices of degree 4 and four vertices of degree 2 in T.

Proof. (i) Combine Lemma 2 and (i) of Lemma 3, it is enough to prove that there exists no vertex of degree 4 neighboring exactly one vertex of degree 2. We prove by contradiction. Suppose there exists $u\in V(T)$ such that $N_T(u) = \{v_1, v_2, v_3, v_4\}$ where $d_T(v_1) = 1$, $d_T(v_2) = 2$ and $d_T(v_i) \geq 3$ where $i \in \{3, 4\}$. Let another neighbor of v_2 be x. Since lemma 2, we have $d_T(x) = 1$. Let $T' = T - uv_4 + v_2v_4$. Thus, by lemma 1, we abtain

$$\begin{aligned}
&ABS(T') - ABS(T)\\
&= \sqrt{1 - \frac{2}{d_{T'}(v_2)+d_{T'}(v_4)}} - \sqrt{1 - \frac{2}{d_T(u)+d_T(v_4)}} + \sqrt{1 - \frac{2}{d_{T'}(v_2)+d_{T'}(x)}}\\
&\quad - \sqrt{1 - \frac{2}{d_T(v_2)+d_T(x)}} + \sqrt{1 - \frac{2}{d_{T'}(u)+d_{T'}(v_1)}} - \sqrt{1 - \frac{2}{d_T(u)+d_T(v_1)}}\\
&\quad + \sqrt{1 - \frac{2}{d_{T'}(u)+d_{T'}(v_3)}} - \sqrt{1 - \frac{2}{d_T(u) + d_T(v_3)}}\\
&= \sqrt{1 - \frac{2}{3 + d_T(v_4)}} - \sqrt{1 - \frac{2}{4 + d_T(v_4)}} + \sqrt{\frac{1}{2}} - \sqrt{\frac{1}{3}}\\
&\quad + \sqrt{\frac{1}{2}} - \sqrt{\frac{3}{5}} + \sqrt{1 - \frac{2}{3 + d_T(v_3)}} - \sqrt{1 - \frac{2}{4 + d_T(v_3)}} \qquad (11)
\end{aligned}$$

According to (i) of Lemma 1, the right side of (11) is increasing with $d_T(v_i)$ where $i \in \{3, 4\}$. Replace $d_T(v_3) = d_T(v_4) = 3$ in the right side of (11), thus $ABS(T') - ABS(T) \geq 2\sqrt{\frac{1}{2}} + 2\sqrt{\frac{2}{3}} - \sqrt{\frac{1}{3}} - \sqrt{\frac{3}{5}} - 2\sqrt{\frac{5}{7}} > 0$, a contradiction to the definition of T.

The proof is competed.

(ii) Let $u \in V(T)$ with $N_T(u) = \{v_1, v_2, v_3, v_4\}$. Without loss of generality, according to Lemma 2 and (i) of Lemma 4, let us say that $d_T(v_1) = 1$ and $d_T(v_2) = d_T(v_3) = 2$. Let P be a maximal path which starts from u and contains uv_4. Without loss of generality, suppose x is another endpoint of P. Obviously, x is a pendant vertex. Let y be the neighbor of x. Since T has a perfect matching, then $d_T(y) = 2$. According to (ii) of Lemma 3, let v be another neighbor of y with $d_T(v) = 4$. Denote the unique path between u, v in T as P_1. According to Lemma 2, (i) of Lemma 4 and the fact that $n \geq 14$, it can be obtained that all internal vertices of P_1 are of degree 3. Combine that with Lemma 2 and (i) of Lemma 4, it is easy to know that there are exactly two vertices of degree 4 and four vertices of degree 2 in T. ■

Figure 2. T_1

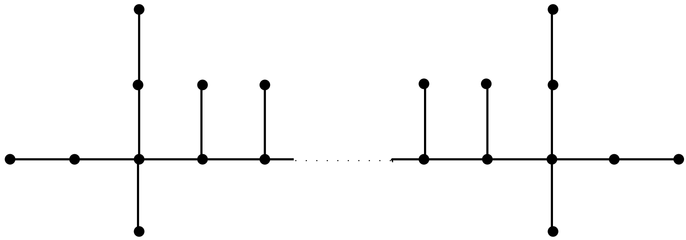

Figure 3. T_2

Theorem 1. *Let T be a molecular tree that has maximum ABS index in the class of molecular trees of order $n(n \geq 14)$ with a perfect matching. Then*

$$ABS(T) \leq \frac{n-6}{2}\sqrt{\frac{2}{3}} + 4\sqrt{\frac{1}{3}} + 2\sqrt{\frac{3}{5}} + 2\sqrt{\frac{5}{7}} + \frac{n-12}{2}\sqrt{\frac{1}{2}}.$$

The equality holds if and only if T is isomorphic to T_2 shown in Figure 3.

Proof. Let n_i be the number of vertices of degree i in T for each $i \in 1, 2, 3, 4$. According to the number of the vertex of degree 4, we distinguish the following two cases.

Case 1. $n_4 = 0$

According to Lemma 2, then T is isomorphic to T_1 shown in Figure 2. And there are $m_{1,2} = m_{3,2} = 2$, $m_{3,1} = \frac{n-4}{2}$ and $m_{3,3} = \frac{n-6}{2}$ in T_1. So

$$ABS(T_1) = 2\sqrt{\frac{1}{3}} + 2\sqrt{\frac{3}{5}} + \frac{n-4}{2}\sqrt{\frac{1}{2}} + \frac{n-6}{2}\sqrt{\frac{2}{3}}. \tag{12}$$

Case 2. $n_4 \geq 1$

According to Lemmas 2, 3 and 4, then T is isomorphic to T_2 shown in Figure 3. And there are $m_{4,2} = m_{1,2} = 4$, $m_{4,1} = m_{4,3} = 2$, $m_{1,3} = \frac{n-12}{2}$ and $m_{3,3} = \frac{n-14}{2}$ in T_2. Thus by a simple calculation,

$$ABS(T_2) = \frac{n-6}{2}\sqrt{\frac{2}{3}} + 4\sqrt{\frac{1}{3}} + 2\sqrt{\frac{3}{5}} + 2\sqrt{\frac{5}{7}} + \frac{n-12}{2}\sqrt{\frac{1}{2}}\,. \qquad (13)$$

Combine (12) and (13), thus

$$\begin{aligned} ABS(T_2) - ABS(T_1) &= \left(\frac{n-6}{2}\sqrt{\frac{2}{3}} + 4\sqrt{\frac{1}{3}} + 2\sqrt{\frac{3}{5}} + 2\sqrt{\frac{5}{7}} + \frac{n-12}{2}\sqrt{\frac{1}{2}}\right) \\ &\quad - \left(2\sqrt{\frac{1}{3}} + 2\sqrt{\frac{3}{5}} + \frac{n-4}{2}\sqrt{\frac{1}{2}} + \frac{n-6}{2}\sqrt{\frac{2}{3}}\right) \\ &= 2\sqrt{\frac{1}{3}} + 2\sqrt{\frac{5}{7}} - 4\sqrt{\frac{1}{2}} > 0. \end{aligned}$$

Therefore, we have that T_2 has maximum ABS index in the class of molecular trees of order $n (n \geq 14)$ with a perfect matching. Thus

$$ABS(T) \leq \frac{n-6}{2}\sqrt{\frac{2}{3}} + 4\sqrt{\frac{1}{3}} + 2\sqrt{\frac{3}{5}} + 2\sqrt{\frac{5}{7}} + \frac{n-12}{2}\sqrt{\frac{1}{2}},$$

the equality holds if and only if T is isomorphic to T_2 shown in Figure 3.

The proof is competed. ■

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