MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **85** (2021) 161-180

ISSN 0340 - 6253

Chemical Trees with Extremal Mostar Index

Kecai Deng[a], Shuchao Li[b,1]

[a]*School of Mathematical Sciences, Huaqiao University,*

Quanzhou 362000, Fujian, P.R. China

kecaideng@126.com

[b]*Faculty of Mathematics and Statistics, Central China Normal University,*

Wuhan 430079, PR China

lscmath@mail.ccnu.edu.cn

(Received April 15, 2020)

Abstract

For a given graph G, the Mostar index $Mo(G)$ is the sum of absolute values of the differences between $n_u(e)$ and $n_v(e)$ over all edges $e = uv$ of G, where $n_u(e)$ and $n_v(e)$ are, respectively, the number of vertices of G lying closer to u than to v and the number of vertices of G lying closer to v than to u. A chemical tree is a tree with the maximum degree at most 4. In this paper, the chemical trees of order n with the greatest Mostar index are determined. And the chemical trees of order n and diameter d with the greatest Mostar index are also determined. What is more, general trees of order n and diameter d with the least Mostar index are identified.

1 Introduction

In this paper, all the graphs we considered are simple and undirected. Let $G = (V_G, E_G)$ be a graph with vertex set V_G and edge set E_G. If $H = (V_H, E_H)$ satisfies $V_H \subseteq V_G$ and $E_H \subseteq E_G$ (resp. $V_H \subseteq V_G$ and $E_H \subsetneqq E_G$), then denote by $H \leqslant G$ (resp. $H < G$) the relation between H and G. For a set X, denote by $|X|$ its cardinality. Thus, $|G| = |V_G|$ is called the *order* of G. For $v \in V_G$, denote by $d_G(v)$ (or $d(v)$ for short) the degree of v. Denote by $N(v)$ the set of vertices adjacent to v. And denote by $E(v)$ the set of

[1]Corresponding author

edges incident to v. A *k-vertex* is a vertex of degree k. Let V_k be the set of k-vertices in G. A *d-path* is a path of length d (a path with d edges). The *distance* between u, v in G is the least length among all u-v paths in G, which is denoted by $d_G(u, v)$ (or $d(u, v)$ for short). The *distance* between $e = uv$ and w in G is defined as $\min\{d(u, w), d(v, w)\}$, which is denoted by $d_G(e, w)$ or $d_G(w, e)$ (or $d(e, w)$, $d(w, e)$ for short). The *diameter* of G is defined as $dia(G) := \max\{d(u, v)|u, v \in V_G\}$. For each edge $e = uv \in E_G$, let

$$N^u_G(e) = \{x \in V_G|d_G(x, u) < d_G(x, v)\}, \quad N^v_G(e) = \{x \in V_G|d_G(x, v) < d_G(x, u)\},$$

$$N^0_G(e) = \{x \in V_G|d_G(x, v) = d_G(x, u)\}.$$

And let $n^y_G(e) = |N^y_G(e)|$ (or put $n_y := n^y_G(e)$ for short), for $y = u, v, 0$. Note that $V_G = N^u_G(e) \cup N^v_G(e) \cup N^0_G(e)$. And $N^0_G(e) = \emptyset$ for each $e \in E_G$ if and only if G is bipartite. Specially, a graph G is called *distance-balanced* if $n_u = n_v$ for each edge $uv \in E_G$. One may be referred to [1, 5, 12, 14, 15] and the references cited therein, for the study on distance-balanced graph invariants. Since there exist many graphs which are not distance-balanced, to measure how far is a graph from being distance-balanced is a natural problem. However, such measuring invariant was proposed only recently, in 2018, by Došlić et al. [6], and was named by *Mostar index*, which is defined as

$$Mo(G) = \sum_{uv \in E_G} \phi(uv)\,, \tag{1}$$

where $\phi(uv) = |n_u - n_v|$ is called the *contribution* of the edge uv for $Mo(G)$.

Clearly, a graph G is distance-balanced if and only if $Mo(G) = 0$. The Mostar index produces a global measure of peripherality of G by calculating the sum of peripherality contributions over all edges in G. In [6], Došlić et al. determined the extremal values of the Mostar index among trees and unicyclic graphs, respectively. And they stated some extremal problems on Mostar index. After that, Tepeh [17] characterized the bicyclic graphs with extremal Mostar index. Hayat and Zhou [7] gave a sharp upper bound of the Mostar index for cacti of order n with k cycles, and characterized all the cacti that achieve this bound. And in [8], Hayat and Zhou studied the Mostar index of trees with parameters. For example, they identified those trees with the least Mostar index with fixed order and fixed maximum degree, and those trees with the greatest Mostar index with fixed order and with fixed diameter.

This paper focuses on the following extremal problem proposed in [6] which involves chemical graphs and trees.

Problem 1.1 ([6]). *Find extremal chemical graphs and trees with respect to the Mostar index.*

A *chemical graph* is a connected graph with the maximum degree at most 4. A chemical graph without any cycle is called a *chemical tree*. The study on the graph invariants of chemical trees attracts much attention. One may be referred to [2–4, 10, 11, 13, 16, 18] for detailed information.

For convenience, in this context, we denote by $\mathcal{T}_n$ (resp. $\mathcal{T}_n^G$) the set of chemical trees (resp. general trees) with n vertices. Let $\mathcal{T} = \cup_{n=1}^{\infty}\mathcal{T}_n$ and $\mathcal{T}^G = \cup_{n=1}^{\infty}\mathcal{T}_n^G$. And denote by $\mathcal{T}_{n,d} \subseteq \mathcal{T}_n$ (resp. $\mathcal{T}_{n,d}^G \subseteq \mathcal{T}_n^G$) the set of chemical trees (resp. general trees) of order n and diameter d.

Let $T \in \mathcal{T}_n^G$. If there exits a vertex v^*, such that each component of $T - v^*$ contains less than $n/2$ vertices, then T is called v^*-*central* (or *central* for short) and v^* is called the *center* of T; see Fig. 1(a) for example. If there exits an edge $e^* = v_1^*v_2^*$, such that each of the two components of $T - e^*$ contains exactly $n/2$ vertices (so n is even), then T is called e^*-*edge central* (or *edge central* for short), e^* is called the *edge center* of T and v_1^*, v_2^* are called the *twin centers* of T; see Fig. 1(b) for example. Note that each tree is either central or edge central [9].

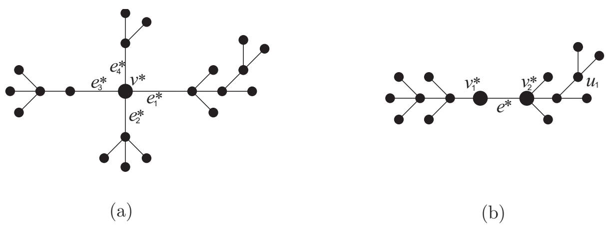

Figure 1. (a) An example of v^*-central chemical tree; (b) An example of e^*-edge central chemical tree.

Let $T \in \mathcal{T}$. Each 1-vertex (resp. 4-vertex) in T is called a *leaf* (resp. *full vertex*). A vertex is called *hungry* if it is not full. An edge $e = uv$ is called a *pendent edge* if either u or v is a leaf. Denote by e_v the pendent edge incident to v if v is a leaf. T is *complete* if each vertex is either a leaf or a full vertex. T is *symmetry* (resp. *edge symmetry*) if it is central (resp. edge central) and all leaves have the same distance from the center (resp. edge center).

Denote by $T^{cs}(r)$ (resp. $T^{ces}(r)$) the complete symmetry (resp. complete edge symmetry) chemical tree where the distance from each leaf to the center (resp. edge center) is r ($r \geqslant 1$). Let $\mathcal{T}^{cs}(r) = \{T | T^{cs}(r-1) < T \leqslant T^{cs}(r)\}$.

Denote by $T^{cs}(r,d)$ (where $d \geqslant 2r$) the graph obtained from $T^{cs}(r)$ and $P = x_1 \cdots x_{d+1}$, by identifying a $2r$-path of $T^{cs}(r)$ and the path $x_{\lceil (d+1)/2 \rceil - r} x_{\lceil (d+1)/2 \rceil - r+1} \cdots x_{\lceil (d+1)/2 \rceil + r}$. Denote by $T^{ces}(r,d)$ (where $d \geqslant 2r+1$) the graph obtained from $T^{ces}(r)$ and $P = x_1 x_2 \cdots x_d x_{d+1}$, by identifying a $(2r+1)$-path of $T^{ces}(r)$ and the path $x_{\lfloor d/2 \rfloor - r} x_{\lfloor d/2 \rfloor - r+1} \cdots x_{\lfloor d/2 \rfloor + r+1}$. $T^{cs}(r,d)$ (resp. $T^{ces}(r,d)$) is called a *d-path complete symmetry* (resp. *d-path complete edge symmetry*) chemical tree. Let $\mathcal{T}^{cs}(r,d) = \{T | T^{cs}(r-1,d) < T \leqslant T^{cs}(r,d)\}$ where $d \geqslant 2r$.

Let $\mathcal{X}^{\min}$ and $\mathcal{X}^{\max}$ be the set of graphs among $\mathcal{X}$ with the least and the greatest Mostar index, respectively, for $\mathcal{X} \in \{\mathcal{T}_n, \mathcal{T}_n^G, \mathcal{T}_{n,d}, \mathcal{T}_{n,d}^G\}$. For short, denote by $Mo(\mathcal{X}')$ the Mostar index of each graph in $\mathcal{X}'$ for $\mathcal{X}' \in \{\mathcal{X}^{\min}, \mathcal{X}^{\max} | \mathcal{X} = \mathcal{T}_n, \mathcal{T}_n^G, \mathcal{T}_{n,d}, \mathcal{T}_{n,d}^G\}$.

In [6], it was shown that paths (denoted by P_n) and stars (denoted by S_n) are extremal graphs among $\mathcal{T}_n^G$ with respect to the Mostar index. And $\mathcal{T}_{n,d}^{G\max}$ was determined in [8].

Theorem 1.2 ([6]). *For $n \geqslant 1$, one has $\mathcal{T}_n^{G\min} = \{P_n\}$ and $\mathcal{T}_n^{G\max} = \{S_n\}$, where $Mo(P_n) = (n-1)^2/2$ and $Mo(S_n) = (n-1)(n-2)$.*

Let $P(n,d)$ ($n \geqslant d+1$) be the graph obtained from the path $P_d = x_1 x_2 \cdots x_{d+1}$ by attaching $n-d-1$ pendent edges at $x_{\lfloor (d+1)/2 \rfloor}$.

Theorem 1.3 ([8]). *For $n \geqslant 2$, one has $\mathcal{T}_{n,d}^{G\max} = \{P(n,d)\}$.*

The first aim of this paper is to determine $T_n^{\max}$ for $n \geqslant 6$. Note that, since P_n ($n \geqslant 1$) and S_m ($1 \leqslant m \leqslant 5$) are also chemical trees, by Theorems 1.2, one has $\mathcal{T}_n^{\min} = \{P_n\}$ ($n \geqslant 1$) and $\mathcal{T}_m^{\max} = \{S_m\}$ ($1 \leqslant m \leqslant 5$). However, if $n \geqslant 6$, then $S_n \notin \mathcal{T}_n^{\max}$ since $S_n \notin \mathcal{T}_n$.

Theorem 1.4. *Let T be in $\mathcal{T}_n$ where $n \geqslant 6$ and $2 \cdot 3^{r-1} - 1 < n \leqslant 2 \cdot 3^r - 1$ with $r \geqslant 2$. Then*

$$Mo(T) \leqslant n^2 - (2r+1)n + 2 \cdot 3^r - 2(r+1)$$

with equality if and only if $T \in \mathcal{T}^{cs}(r) \cap \mathcal{T}_n$.

The second aim of this paper is to determine $\mathcal{T}_{n,d}^{\max}$. Note that for $T \in \mathcal{T}_{n,d}$, one has $d+1 \leqslant |T| \leqslant 2 \cdot 3^{d/2} - 1$ if d is even, while $d+1 \leqslant |T| \leqslant 3^{(d+1)/2} - 1$ if d is odd. By

Theorem 1.3 one has $\mathcal{T}_{d+i,d}^{\max} = \{P(d+i,d)\}$ for $i = 1,2,3$. And it is easy to count that $Mo(P(d+2,d)) = \lfloor d^2/2 \rfloor + 2d$, $Mo(P(d+3,d)) = \lfloor d^2/2 \rfloor + 4d + 2$.

Theorem 1.5. *Let T be in $\mathcal{T}_{n,d}$ where $d \geqslant 3$ and $n \geqslant d+4$.*

(1) *If d is odd and $(2\cdot 3^{(d-1)/2}-1)+1 < n \leqslant 3^{(d+1)/2}-1$, then $\mathcal{T}_{n,d}^{\max} = \mathcal{T}^{cs}((d+1)/2) \cap \mathcal{T}_{n,d}$.*

(2) *If $(2\cdot 3^{r-1}-1) + [d-2(r-1)] < n \leqslant (2\cdot 3^r - 1) + (d-2r)$ with $2 \leqslant r \leqslant \lfloor d/2 \rfloor$, then*

$$Mo(T) \leqslant n^2 - (2r+1)n + 2\cdot 3^r - 2r^2 + 2dr - \left\lceil \frac{d^2}{2} \right\rceil - d - 2$$

with equality if and only if $T \in \mathcal{T}^{cs}(r,d) \cap \mathcal{T}_n$.

The third aim of this paper is to determine $\mathcal{T}_{n,d}^{G\min}$. Let $\widetilde{P}(n,d)$ $(n \geqslant d+1)$ be the graph obtained from the path $P_d = x_1x_2\cdots x_{d+1}$ by attaching $\lfloor (n-d-1)/2 \rfloor$ pendent edges at x_2 and $\lceil (n-d-1)/2 \rceil$ pendent edges at x_d.

Theorem 1.6. *Let T be in $\mathcal{T}_{n,d}^{G}$ with $d \geqslant 3$ and $n \geqslant 6$. Then*

$$Mo(T) \geqslant \begin{cases} (n-d+1)(n-2) + 2\lfloor \frac{d}{2} \rfloor \lfloor \frac{d-2}{2} \rfloor, & \text{if } n \text{ is even;} \\ (n-d+1)(n-2) + 2\lfloor \frac{d-1}{2} \rfloor^2, & \text{if } n \text{ is odd.} \end{cases}$$

with equality if and only if $T \cong \widetilde{P}(n,d)$.

Theorems 1.4, 1.5 and 1.6 are proved in Sections 3, 4 and 5, respectively. The proofs are based on the properties of moving operation which are stated in Section 2.

2 Properties of some graph transformations

In this section, some necessary definitions and preliminaries are given. Denote by $[i,j] = \{i, i+1, \ldots, j\}$ for integers $i \leqslant j$ for short. By the definitions of $T^{cs}(r), T^{ces}(r)$, $T^{cs}(r,d)$ and $T^{ces}(r,d)$, one has

$$T^{cs}(r-1) < T^{ces}(r-1) < T^{cs}(r), \quad T^{cs}(r-1,d) < T^{ces}(r-1,d) < T^{cs}(r,d).$$

That is, $T^{ces}(r-1) \in \mathcal{T}^{cs}(r)$ and $T^{ces}(r-1,d) \in \mathcal{T}^{cs}(r,d)$. It is also easy to count that

(1) $|T^{cs}(r))| = 2\cdot 3^r - 1$, $|T^{ces}(r)| = 3^{r+1} - 1$;

(2) $|T^{cs}(r,d)| = (2\cdot 3^r - 1) + (d-2r)$, $|T^{ces}(r,d)| = (3^{r+1}-1) + (d-2r-1)$.

For $T \in \mathcal{T}^G$ and $u, v \in V_T$, recall that there is a unique u-v path (denoted by $P_{u,v}$) in T. Let $P_{u,e} = P_{u,v}$ where $e = wv$ and $d(u, e) = d(u, v)$.

Let $T \in \mathcal{T}^G$. If T is v^*-central, let $N(v^*) = \{v_i | i \in [1, d(v^*)]\}$ and $e_i^* = v_i v^*$ for $v_i \in N(v^*)$. Then $T - v^*$ has exactly $d(v^*)$ connected components. The connected component containing v_i is called the *v_i-branch* of T, which is denoted by T_{v_i} for $v_i \in N(v^*)$. And $T_{e_i^*} = T[V_{T_{v_i}} \cup v^*]$ is called the *v_i-extended branch* of T for for $i \in [1, d(v^*)]$. If T is e^*-edge central where $e^* = v_1^* v_2^*$, then $T - e^*$ has exactly two connected components. The component containing v_i^* is called the *v_i^*-extended branch* of T, which is denoted by $T_{v_i^*}$ for $i \in \{1, 2\}$. Let $a = v^*$ if T is central or $a = e^*$ if T is edge central. Let $R_j(T)$ (or R_j for short) be the set of vertices of distance exactly j from a for $j \geqslant 0$ (where we suppose $R_0 = \{v^*\}$ if T is central or $R_0 = \{v_1^*, v_2^*\}$ if T is edge central). Let E_j be the set of edges between R_{j-1} and R_j for $j \geqslant 1$. If T is central, let $R_{i,j} = R_j \cap V_{T_{v_i}}$ and $E_{i,j} = R_j \cap E_{T_{v_i}}$ for $i \in [1, d(v^*)]$ and $j \geqslant 1$. If T is edge central, let $R_{i,j} = R_j \cap V_{T_{v_i^*}}$ and $E_{i,j} = E_j \cap E_{T_{v_i^*}}$ for $i \in \{1, 2\}$ and $j \geqslant 1$. Let u, v be in the same extended branch of T, such that $d(u, a) \geqslant d(v, a)$ and $v \in V_{P_{u,a}}$. Then each vertex (resp. edge) in $P_{v,a}$ is called an *ancestor* (resp. *ancestor edge*) of v, while each vertex (resp. edge) in $P_{u,v}$ is called a *successor* (resp. *successor edge*) of v. Denote by $A_T(v)$ and $S_T(v)$ (resp. $EA_T(v)$ and $ES_T(v)$) the set of all ancestors and successors (resp. ancestor edges and successor edges) of v, respectively (or by $A(v), S(v), EA(v)$ and $ES(v)$ for short, respectively). Let $\sigma(v) = |S(v)|$ for each $v \in V_T$ (suppose v is not the center when T is central) and $\sigma_1(v) = \sigma(v) - 1$. For an edge $e = uu_1$ with $d(u_1, a) > d(u, a)$, let $ES(e) = ES(u_1) \cup \{e\}$.

Let $T \in \mathcal{T}^G$ with a being the center or edge center. Let $e = uu_1 \in E_T$ where $d(u_1, a) > d(u, a)$. Let $v \in V_T \setminus S(u_1)$. Denote by $T(e^-, v^+)$ the graph obtained from T by deleting e and connecting u_1 to v with a new edge (also denote the new edge by e); see Fig. 2(1) for example. The operation from T to $T(e^-, v^+)$ is called a *moving operation* on (e, v). Note that if T is a chemical tree and v is hungry, then $T(e^-, v^+)$ is also a chemical tree. Denoted by $T(u^-, v^+)$ the graph obtained from T by doing moving operation on (e_i, v) for each $e_i \in E(u) \cap ES(u)$ at the same time; see Fig. 2(2) for example. The operation from T to $T(u^-, v^+)$ is called the *moving operation on* (u, v). Note that if T is a chemical tree and $d(u) + d(v) - 1 \leqslant 4$, then $T(u^-, v^+)$ is also a chemical tree. Denote by $T(ES(e)^-, v^+)$ the graph obtained by adding $\sigma(u_1)$ pendent edges to $T[V_T \setminus S(u_1)]$ (that is do moving operations inductively on (e_i, v) for $e_i \in ES(e)$ from E_α to $E_{d(u_1,v^*)}$ where

α is the greatest distance from a leaf in $S(u_1)$ to the center or edge center); see Fig. 2(3) for example. The operation from T to $T(ES(e)^-, v^+)$ is called *the moving operation on* $(ES(e), v)$.

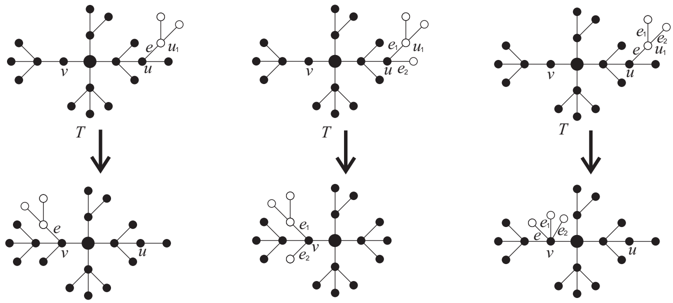

Figure 2. Examples for the moving operation from T to $T(e^-, v^+)$, $T(u^-, v^+)$ and $T(ES(e)^-, v^+)$, respectively, where the vertices in white and their incident edges are moved.

Property 2.1. *Let T be in $\mathcal{T}_n^G$ with a being the center v^* or edge center $e^* = v_1^*v_2^*$. Choose $uu_1 \in E_T, v \in V_T$ such that $v \notin S(u_1)$ and $d(u_1, a) > d(u, a)$. Let $T_1 = T(uu_1^-, v^+)$, $T_2 = T(u^-, v^+)$ and $T_3 = T(ES(uu_1)^-, v^+)$.*

(i) *If u, v are in the same extended branch, then $Mo(T_1) = Mo(T) + 2\sigma(u_1)(d(u, a) - d(v, a))$.*

(ii) *Suppose T is v^*-central and u, v are in distinct branches T_{v_1} and T_{v_2}, respectively.*
  - *If $\sigma(v_2) \leqslant \lfloor n/2 \rfloor - \sigma(u_1)$, then $Mo(T_1) = Mo(T) + 2\sigma(u_1)(d(u, v^*) - d(v, v^*))$.*
  - *If n is odd and $\sigma(v_2) = (n-1)/2 - \sigma(u_1) + 1$, then $Mo(T_1) = Mo(T) + 2\sigma(u_1)(d(u, v^*) - d(v, v^*) + 1)$.*

(iii) *If T is $v_1^*v_2^*$-edge central, $u \in V_{T_{v_1^*}}$, $v \in V_{T_{v_2^*}}$ and u_1 is a leaf, then $Mo(T_1) = Mo(T) + 2(d(u, v_1^*) - d(v, v_2^*) + 1)$.*

(iv) *If T is v^*-central, u and v are in distinct branches T_{v_1} and T_{v_2}, respectively, satisfying $\sigma(v_2) \leqslant \lfloor n/2 \rfloor - \sigma_1(u)$, then $Mo(T_2) = Mo(T) + 2\sigma_1(u)(d(u, v^*) - d(v, v^*))$.*

(v) *If T is $v_1^*v_2^*$-edge central, $u \in V_{T_{v_1^*}}$, $v \in V_{T_{v_2^*}}$, and $d(u, v_1^*) \geqslant d(v, v_2^*) - 1$, then $Mo(T_2) \geqslant Mo(T) + 2\sigma_1(u)(d(u, v_1^*) - d(v, v_2^*) + 1)$.*

(vi) *Assume that uu_1, v are in the same extended branch satisfying $d(u, a) < d(v, a)$ and $d(e, a) \leqslant d(v, a)$ for each edge in $ES(u_1)$. Then $Mo(T_3) < Mo(T)$.*

Proof. Let $\phi(e)$ (resp. $\phi_i(e)$ for $i \in \{1,2,3\}$) be the contribution of e to T (resp. T_i for $i \in \{1,2,3\}$), for $e \in E_T$ (resp. $e \in E_{T_i}$ for $i \in \{1,2,3\}$). One has $\phi_i(e) = \phi(e)$ ($i \in \{1,2,3\}$) for each $e \in E_T \setminus E_{P_{u,v}}$.

(i) Note that T_1 is also v^*-central (resp. e^*-edge central) if T is v^*-central (resp. e^*-edge central). If u, v, a are in the same path and $v \in P_{u,a}$, then $\phi_1(e) = \phi(e) + 2\sigma(u_1)$ for each $e \in E_{P_{u,v}}$. So $Mo(T_1) = Mo(T) + 2\sigma(u_1)(d(u,a) - d(v,a))$. If u, v, a are in the same path and $u \in P_{v,a}$, then $\phi_1(e) = \phi(e) - 2\sigma(u_1)$ for each $e \in E_{P_{u,v}}$. So $Mo(T_1) = Mo(T) - 2\sigma(u_1)(d(v,a) - d(u,a)) = Mo(T) + 2\sigma(u_1)(d(u,a) - d(v,a))$. If u, v, a are not in the same path, then $V_{P_{u,a}} \cap V_{P_{v,a}} = V_{P_{w,a}}$ for some w in the same extended branch. Then $\phi(e_1) = \phi(e) + 2\sigma(u_1)$ for each $e \in E_{P_{u,w}}$. And $\phi_1(e) = \phi(e) - 2\sigma(u_1)$ for each $e \in E_{P_{v,w}}$. One also has $Mo(T_1) = Mo(T) + 2\sigma(u_1)(d(u,a) - d(v,a))$. Thus, (i) holds.

(ii) Note that T_1 is v^*-central when n is odd or $\sigma(v_2) \leqslant \lfloor n/2 \rfloor - \sigma(u_1) - 1$, while T_1 is v_2v^*-edge central when n is even and $\sigma(v_2) = n/2 - \sigma(u_1)$. Then $\phi_1(e) = \phi(e) + 2\sigma(u_1)$ for each $e \in E_{P_{u,v^*}}$. And $\phi_1(e) = \phi(e) - 2\sigma(u_1)$ for each $e \in E_{P_{v,v^*}}$. So $Mo(T_1) = Mo(T) + 2\sigma(u_1)(d(u,v^*) - d(v,v^*))$. Thus, the first part of (ii) holds.

Note that T_1 is v_2-central. Then $\phi_1(e) = \phi(e) + 2\sigma(u_1)$ for each $e \in E_{P_{u,v^*}}$; $\phi_1(e) = \phi(e) - 2\sigma(u_1)$ for each $e \in E_{P_{v,v_2}}$. And $\phi_1(v^*v_2) = \phi(v^*v_2)$. So $Mo(T_1) = Mo(T) + 2\sigma(u_1)(d(u,v^*) - d(v,v_2) + 1)$. Thus, the second part of (ii) holds.

(iii) Note that T_1 is v_2^*-central if $d_T(v_2^*) \geqslant 3$, or T_1 is $v_2^*w_2$-edge central if $d_T(v_2^*) = 2$ (where w_2 is the neighbor of v_2^* other than v_1^*). Then $\phi_1(e) = \phi(e) + 2$ for each $e \in E_{P_{u,v_2^*}}$. And $\phi_1(e) = \phi(e) - 2$ for each $e \in E_{P_{v,v_2^*}}$. So $Mo(T_1) = Mo(T) + 2(d(u,v_1^*) - d(v,v_2^*) + 1)$. Thus, (iii) holds.

(iv) Recall the moving operation on (u,v) is the combination of moving operations on (e_i,v)'s over all e_i's in $E(u) \cap ES(u)$. So (iv) holds since (ii) holds and $\sigma_1(u) = \sum_{w \in N(u) \cap S(u)} \sigma(w)$.

(v) Note that the center or edge center of T_2 is in P_{v,v_2^*}. Then $\phi_2(e) = \phi(e) + 2\sigma_1(u)$ for each $e \in E_{P_{u,v_2^*}}$. And $\phi_2(e) = |\phi(e) - 2\sigma_1(u)| \geqslant \phi(e) - 2\sigma_1(u)$ for each $e \in E_{P_{v,v_2^*}}$. So $Mo(T_2) \geqslant Mo(T) + 2\sigma_1(u)(d(u,v_1^*) - d(v,v_2^*) + 1)$. Thus, (v) holds.

(vi) The conclusion in (vi) holds since (i) holds, by the definition of $T_3 = T(S(uu_1)^-, v^+)$ and by the fact that $d(uu_1) < d(v)$ and $d(e,v^*) \leqslant d(v,v^*)$ for each edge in $ES(u_1)$.

■

If the moving operation in (i), (ii), (iii) or (iv) of Property 2.1 does no change the

Mostar index, then it is called an *equivalent moving operation.* Two trees are *equivalent* if they can be obtained from each other by some equivalent moving operations.

3 Greatest Mostar index in $\mathcal{T}_n$

In this section, we prove our first main result, which characterizes all the chemical trees of order n having the largest Mostar index. At first we need some preliminary lemmas.

Lemma 3.1. *Let T be a v^*-central tree in $\mathcal{T}_n^{\max}$ where $n \geqslant 6$. Let α be the greatest distance from a leaf in T to v^*. Then $T \in \mathcal{T}^{cs}(\alpha)$.*

Proof. Let $e \in E_\alpha$. Suppose there exits a hungry vertex v in $\cup_{j=0}^{\alpha-2} R_j$. Then we can do moving operation on (e, v) to increase the Mostar index by Property 2.1(i) or Property 2.1(ii), a contradiction. So each vertex in $\cup_{j=0}^{\alpha-2} R_j$ is full. Thus, $T \in \mathcal{T}^{cs}(\alpha)$. ■

Lemma 3.2. *Let T be a $v_1^* v_2^*$-edge central tree in $\mathcal{T}_n^{\max}$ with $n \geqslant 6$. Let α be the greatest distance from a leaf to $v_1^* v_2^*$. Then $T \cong T^{ces}(\alpha)$.*

Proof. Let α_i be the greatest distance from a leaf in $T_{v_i^*}$ to v_i^* for $i \in \{1, 2\}$. Without loss of generality, suppose $\alpha = \alpha_1 \geqslant \alpha_2$. Suppose there exits a hungry vertex $v \in \cup_{j=0}^{\alpha-1} R_{2,j}$. Let $e \in E_{1,\alpha}$. Then we can do moving operation on (e, v) to increase the Mostar index by Property 2.1(iii), a contradiction. So each vertex in $\cup_{j=0}^{\alpha-1} R_{2,j}$ is full, and $\alpha_2 = \alpha = \alpha_1$. Similarly, suppose there exits a hungry vertex $v \in \cup_{j=0}^{\alpha-1} R_{1,j}$. Let $e \in E_{2,\alpha}$. Then we can do moving operation on (e, v) to increase the Mostar index by Property 2.1(iii), a contradiction. So each vertex in $\cup_{j=0}^{\alpha-1} R_{1,j}$ is also full. Thus, $T \cong T^{ces}(\alpha)$. ■

We are now in the position to prove our first main result.

Proof of Theorem 1.4. Let $T \in \mathcal{T}_n^{\max}$, where

$$|T^{cs}(r-1)| = 2 \cdot 3^{r-1} - 1 < n \leqslant 2 \cdot 3^r - 1 = |T^{cs}(r)|$$

for some $r \geqslant 2$. If T is v^*-central, then let α be the greatest distance from a leaf to v^*. By Lemma 3.1, one has $T \in \mathcal{T}^{cs}(\alpha)$. So $T \in \mathcal{T}^{cs}(r)$, since $|T^{cs}(r-1)| < n \leqslant |T^{cs}(r)|$. Recall that $T^{ces}(r-1)$ is the unique complete edge symmetry tree with the number of vertices in $[|T^{cs}(r-1)| + 1, |V_{T^{cs}(r)}|]$. If T is $v_1^* v_2^*$-edge central, then by Lemma 3.2 one also has $T \cong T^{ces}(r-1) \in \mathcal{T}^{cs}(r)$. On the other hand, note that the trees in $\mathcal{T}^{cs}(r) \cap \mathcal{T}_n$ are equivalent to each other. So $\mathcal{T}_n^{\max} = \mathcal{T}^{cs}(r) \cap \mathcal{T}_n$.

Let $T_1 = T^{cs}(r-1)$. Suppose $n = |T_1| + t$ where $1 \leqslant t \leqslant 4 \cdot 3^{r-1}$. Let w^* be the center of T_1. Let x_1 and x_2 be two leaves in distinct branches of T_1. Let T_2 be the graph obtained from T_1 by attaching $\lfloor t/2 \rfloor$ pendent edges $\{e_i | i \in [1, \lfloor t/2 \rfloor]\}$ to x_1 and attaching $\lceil t/2 \rceil$ pendent edges $\{e'_j | j \in [1, \lceil t/2 \rceil]\}$ to x_2. Then T_2 is w^*-central which is equivalent to T.

Let $\phi_i(e)$ be the contribution of e to T_i for $i \in \{1, 2\}$. Then $\phi_2(e) = \phi_1(e) + t$ for each $e \in E_{T_1} \setminus E_{P_{x_1,x_2}}$; $\phi_2(e) = \phi_1(e) + \lceil t/2 \rceil - \lfloor t/2 \rfloor$ for each $e \in E_{P_{x_1,w^*}}$; $\phi_2(e) = \phi_1(e) - \lceil t/2 \rceil + \lfloor t/2 \rfloor$ for each $e \in E_{P_{x_2,w^*}}$. And $\phi_2(e_i) = \phi_2(e'_j) = n - 2$ for each $i \in [1, \lfloor t/2 \rfloor]$ and $j \in [1, \lceil t/2 \rceil]$. So

$$\begin{aligned} Mo(T_2) &= Mo(T_1) + t \cdot (|E_{T_1}| - |E_{P_{x_1,x_2}}|) + t \cdot (n-2) \\ &= Mo(T_1) + t \cdot (2 \cdot 3^{r-1} + n - 2r - 2) \ . \end{aligned}$$

Note that for each edge $uv \in E_j(T_1)$, where $u \in R_j(T_1), v \in R_{j-1}(T_1)$, $1 \leqslant j \leqslant r-1$, the contribution of uv equals to $|T_1| - 2\sigma(u)$. And recall $\sigma(u) = \sum_{l=1}^{r-j} 3^{l-1} = (3^{r-j} - 1)/2$ and $|E_j(T_1)| = 4 \cdot 3^{j-1}$ for $1 \leqslant j \leqslant r-1$. Then

$$Mo(T_1) = \sum_{j=1}^{r-1} |E_j(T_1)| \cdot (|T_1| - 2\sigma(u)) = 4(9^{r-1} - r \cdot 3^{r-1}) \ .$$

Thus,

$$\begin{aligned} Mo(T) = Mo(T_2) &= Mo(T_1) + t \cdot (3^{r-1} + n - r - 2) \\ &= 4(9^{r-1} - r \cdot 3^{r-1}) + t \cdot (2 \cdot 3^{r-1} + n - 2r - 2) \\ &= n^2 - (2r+1)n + 2 \cdot 3^r - 2(r+1) \end{aligned}$$

since $t = n - (2 \cdot 3^{r-1} - 1)$. This completes our proof. ∎

4 Greatest Mostar index in $\mathcal{T}_{n,d}$

In this section, we prove our second main result, which characterizes all the chemical trees of order n and diameter d having the largest Mostar index. At first we give some preliminary lemmas.

Lemma 4.1. *Let T be in $\mathcal{T}_{n,d}^{\max}$ with $d \geqslant 4$ and $n \geqslant d+4$. Then the center or edge center of T is in some path length of d.*

Proof. Let $a = v^*$ if T is v^*-central and $a = e^* = v_1^*v_2^*$ if T is e^*-edge central. Suppose a is not in any path of length d. Consider a path, say $P_{x,y}$, of length d in T. Then $P_{x,y}$ is in some extended branch of T (suppose it is in T_{v_1} if T is central or it is in $T_{v_1^*}$ if T is edge central). Let $\xi = v_1$ or v_1^*. Then $(d+1) \leqslant |T_\xi| \leqslant n/2$ and there are at least $n/2 \geqslant 4$ vertices in $V_T \setminus V_{T_\xi}$.

If T is central, then $d(v^*) = 4$. For otherwise, there exists a pendent edge $e \in E_T \setminus E_{P_{x,y}}$ where $d(e, v^*) \geqslant 1$. And we can do moving operation on (e, v^*) to increase the Mostar index by Property 2.1(i), with the diameter unchanged, a contradiction. When T is central, let $N(v^*) = \{v_1, v_2, v_3, v_4\}$ and suppose T_{v_2} is the branch containing the least vertices among the three branches other than T_{v_1}.

Let z be the vertex in $P_{x,y}$ which has the least distance from ξ. Let $x_1 \in V_{P_{z,x}} \cap N(z)$ and $y_1 \in V_{P_{z,y}} \cap N(z)$. Without loss of generality, suppose $d(x,z) \geqslant d(y,z)$. Then $d(x,z) \geqslant d(v,z)$ for each $v \in S(x_1)$; $d(y,z) \geqslant d(v,z)$ for each $v \in V_{T_\xi} \setminus S(x_1)$. And $d(y,z) > d(v,z)$ for each $v \in V_T \setminus V_{T_\xi}$ by our assumption. So $d(x,a) \geqslant d(v,a)$ for each $v \in S(x_1)$; $d(y,a) \geqslant d(v,a)$ for each $v \in S(z) \setminus S(x_1)$; $d(y,a) > d(v,a)$ for each $v \in V_{T_\xi} \setminus S(z)$ (for otherwise, $d(v,x)$ would be a path of length greater than d, a contradiction). And one also has $d(y,a) > d(v,a)$ for each v in $V_T \setminus V_{T_\xi}$. Let α be the greatest distance from a leaf in $S(y_1)$ other than y to z. Let e_1 be the pendent edge in $[(ES(y_1) \cap E_{d(z,a)+\alpha}) \setminus \{e_y\}]$.

If $d(z) = 3$, then $\alpha = 0$, for otherwise we can do operation on (e_1, z) to increase the Mostar index by Property 2.1(i), with the diameter unchanged, a contradiction. So one has $\sigma(y_1) = d(y,z) \leqslant d(x,z) \leqslant \sigma(x_1)$ which implies $\sigma(y_1) \leqslant \sigma(\xi)/2$.

If $d(z) = 4$, let z_1 be the neighbor of z other than x_1, y_1. Then each vertex z_2 in $[S(z_1) \cap (\cup_{j \leqslant d(z,a)+\alpha-2} R_j)]$ is full, for otherwise we can do moving operation on (e_1, z_2) to increase the Mostar index by Property 2.1(i), with the diameter unchanged, a contradiction. Then we can do equivalent moving operations on (e_i', v_{j_i}')'s for all e_i''s in $ES(y_1) \cap E_{d(z,a)+\alpha}$ and for some v_{j_i}''s in $S(z_1) \cap S_{d(z,a)+\alpha-1}$ until $|ES(y_1) \cap E_{d(z,a)+\alpha}| \leqslant |ES(z_1) \cap E_{d(z,a)+\alpha}|$, with the diameter unchanged. Then one has $\sigma(y_1) \leqslant \sigma(z_1) + \sigma(x_1)$ which also implies $\sigma(y_1) \leqslant \sigma(\xi)/2$ after these equivalent moving operations. So without loss of generality, we can suppose $\sigma(y_1) \leqslant \sigma(\xi)/2 \leqslant n/4$.

Let w_2 be a leaf in $S(v_2)$ if T is central and w_2 be a leaf in $S(v_2^*)$ if T is edge central. Then $d(w_2, z) < d(y,z)$ by our assumption. Choose $y_2 \in V_{P_{z,y}}$ such that $d(y_2, z) = d(w_2, z)$. Then $d(y_2, a) > d(w_2, a)$. And $\sigma_1(y_2) = \sigma(y_2) - 1 \leqslant \sigma(y_1) - 1 < \sigma(\xi)/2 \leqslant n/4$.

When T is edge central, we can do moving operation on (y_2, w_2) to increase the Mostar index by Property 2.1(v). When T is central, if $\sigma(v_1) > n/4$, then $\sigma(v_2) < n/4 \leqslant n/2 - n/4 \leqslant \lfloor n/2 \rfloor - \sigma_1(y_2)$ by our choice of T_{v_2}. So we can do moving operation on (y_2, w_2) to increase the Mostar index by Property 2.1(iv). If $\sigma(v_1) \leqslant n/4$, then $\sigma_1(y_2) < \sigma(v_1)/2 \leqslant n/8$. One has $\sigma(v_2) < n/3 = n/2 - n/6 < n/2 - n/8 \leqslant \lfloor n/2 \rfloor - \sigma_1(y_2)$. So we can also do moving operation on (y_2, w_2) to increase the Mostar index by Property 2.1(iv).

On the other hand, let $T_2 = T(y_2^-, w_2^+)$. Note that, whenever T is central or edge central, one has $d_{T_2}(v, y) \leqslant d_{T_2}(x, y) = d_T(x, y) = d$. And for each $v \in V_T \setminus V_{T_a}$, one has $d_{T_2}(v, y) \leqslant d_{T_2}(y, a) + d_{T_2}(v, a) < d_T(y, z) + d_T(y, z) \leqslant d$. So T_2 has the same diameter to T but a greater Mostar index, a contradiction. Thus, there is a choice of $P_{x,y}$ such that $v^* \in V_{P_{x,y}}$. This completes the proof. ∎

Recall that, for a v^*-central T, one has $N(v^*) = \{v_i | i \in [1, d_T(v^*)]\}$.

Lemma 4.2. *Suppose T is a v^*-central tree in $\mathcal{T}_{n,d}^{\max}$ and $P_{x,y}$ is a path of length d containing v^*, where $d \geqslant 4, n \geqslant d + 4, x \in S(v_1)$, $y \in S(v_2)$ and $d(x, v^*) \geqslant d(y, v^*)$. Let α be the greatest distance from a leaf other than x or y in T to v^*. Then $\alpha \leqslant d(y, v^*) + 1$ with equality only if $T \in \mathcal{T}^{cs}(\alpha)$ and $d = 2\alpha - 1$. Furthermore, if $\alpha \leqslant d(y, v^*)$ then $T \in \mathcal{T}^{cs}(\alpha, d)$.*

Proof. Note that $d(v^*) = 4$ since $n \geqslant d + 4$ (for otherwise, we can do moving operation to increase the Mostar index, a contradiction). Let $N(v^*) = \{v_1, v_2, v_3, v_4\}$. Let α_i be the greatest distance from a leaf other than x or y in T_{v_i} to v^* for $i \in \{1, 2, 3, 4\}$.

If $\alpha \geqslant d(y, v^*) + 1$, then $\alpha = \alpha_1 > \alpha_i$ for each $i \in \{2, 3, 4\}$. Let $e \in E_\alpha \setminus E_{P_{x,y}}$. Suppose there exits a hungry vertex v in $(\cup_{j=1}^{d(y,v^*)-1} R_j) \cup (\cup_{j=1}^{\alpha-2} R_{1,j})$. Then we can do moving operation on (e, v) to increase the Mostar index by Property 2.1(i) or Property 2.1(ii), with the diameter unchanged, a contradiction. So each vertex in $(\cup_{j=1}^{d(y,v^*)-1} R_j) \cup (\cup_{j=1}^{\alpha-2} R_{1,j})$ is full. And so $T^{cs}(d(y, v^*)) < T$. Suppose $\alpha \geqslant d(y, v^*) + 2$. Then

$$\sigma(v_1) \geqslant \sum_{j=1}^{\alpha-1} 3^{j-1} > \sum_{j=1}^{d(y,v^*)} 3^j = \sigma(v_2) + \sigma(v_3) + \sigma(v_4)$$

since $\alpha \geqslant d(y, v^*) + 2$, a contradiction to the fact that T is v^*-central. So $\alpha = d(y, v^*) + 1$. Then $T^{cs}(\alpha - 1) < T$. On the other hand, suppose $d(x, v^*) \geqslant \alpha + 1$. Then we can do moving operation on (e_x, y) to increase the Mostar index by Property 2.1(ii), with the diameter unchanged, a contradiction. So $d(x, v^*) = \alpha$ which implies $T < T^{cs}(\alpha)$. Thus, $T \in \mathcal{T}^{cs}(\alpha)$ and $d = 2\alpha - 1$.

If $\alpha \leqslant d(y, v^*)$, let $e \in E_\alpha \setminus E_{P_{x,y}}$. Suppose there exits a hungry vertex $v \in \cup_{j=1}^{\alpha-2} R_j$. Then we can do moving operation on (e, v) to increase the Mostar index by Property 2.1(i) or Property 2.1(ii), with the diameter unchanged, a contradiction. So each vertex in $\cup_{j \leqslant \alpha-2} R_j$ is full. On the other hand, suppose $d(x, v^*) \geqslant d(y, v^*)+2$. Then $d(x, v^*) \geqslant \alpha+2$. Then we can do moving operation on (e_x, y) to increase the Mostar index by Property 2.1(ii), with the diameter unchanged, a contradiction. So $d(x, v^*) \leqslant d(y, v^*) + 1$. And so $T \in \mathcal{T}^{cs}(\alpha, d)$. ■

Lemma 4.3. *Suppose T is a $v_1^* v_2^*$-edge central tree in $\mathcal{T}_{n,d}^{\max}$ and $P_{x,y}$ is a path of length d containing $v_1^* v_2^*$, where $d \geqslant 4$, $n \geqslant d+4$, $x \in S(v_1^*)$, $y \in S(v_2^*)$ and $d(x, v_1^*) \geqslant d(y, v_2^*)$. Let α be the greatest distance from a leaf other than x or y to $v_1^* v_2^*$. Then $T \cong T^{ces}(\alpha, d)$ and d is odd.*

Proof. For each vertex $u \in V_{T_{v_1^*}}$ and $v \in V_{T_{v_2^*}}$, one has $d(x, v_1^*) \geqslant d(u, v_1^*)$ and $d(y, v_2^*) \geqslant d(v, v_2^*)$. Let α_i be the greatest distance from a leaf other than x or y in $T_{v_i^*}$ to v_i^* for $i \in \{1, 2\}$. Then $d(x, v_1^*) \geqslant \alpha_1$ and $d(y, v_2^*) \geqslant \alpha_2$.

Let e be in $E_{2,\alpha_2} \setminus E_{P_{x,y}}$. Suppose there exists a hungry vertex v in $\cup_{j=0}^{\alpha_2-1} R_{1,j}$. Then we can do moving operation on (e, v) to increase the Mostar index by Property 2.1(iii) with the diameter unchanged, a contradiction. So each vertex in $\cup_{j=0}^{\alpha_2-1} R_{1,j}$ is full and $\alpha_2 \leqslant \alpha_1$. Similarly, one has each vertex in $\cup_{j=0}^{\alpha_1-1} R_{2,j}$ is full and $\alpha_1 \leqslant \alpha_2$. So $\alpha_1 = \alpha_2 = \alpha$ and each vertex in $\cup_{j=0}^{\alpha-1} R_j$ is full. Then $T[\cup_{j \geqslant \alpha+1} E_j]$ consists of two paths if $\cup_{j \geqslant \alpha+1} R_j \neq \emptyset$. And the two paths have the same length, since T is edge central. So $d(x, v_1^*) = d(y, v_2^*)$. Thus, $T \cong T^{ces}(\alpha, d)$ and d is odd. ■

Now we come back to prove Theorem 1.5.

Proof of Theorem 1.5. (1) If d is odd and $(2 \cdot 3^{(d-1)/2} - 1) + 1 < n \leqslant 3^{(d+1)/2} - 1$, then $\mathcal{T}_n^{\max} \subseteq \mathcal{T}^{cs}((d+1)/2)$ by Theorem 1.4. And $\mathcal{T}_n^{\max} \cap \mathcal{T}_{n,d} \neq \emptyset$. So $\mathcal{T}_{n,d}^{\max} = \mathcal{T}_n^{\max} \cap \mathcal{T}_{n,d} = \mathcal{T}^{cs}((d+1)/2) \cap \mathcal{T}_{n,d}$.

(2) Suppose $(2 \cdot 3^{r-1} - 1) + [d - 2(r-1)] < n \leqslant (2 \cdot 3^r - 1) + (d - 2r)$ where $2 \leqslant r \leqslant \lfloor d/2 \rfloor$. Then $n \geqslant d + 4 \geqslant 8$. Let $T \in \mathcal{T}_{n,d}^{\max}$. Let $P_{x,y}$ be a path length of d in T with two leaf ends x and y.

We first consider that T is v^*-central. By Lemma 4.1, suppose $v^* \in V_{P_{x,y}}$. Without loss of generality, suppose $d(x, v^*) \geqslant d(y, v^*)$. Let α be the greatest distance from a leaf other than x or y to v^*. By Lemma 4.2, one has $\alpha \leqslant d(y, v^*) + 1$. And when $\alpha = d(y, v^*)+1$, one has $T \in \mathcal{T}^{cs}(\alpha)$ and $d = 2\alpha - 1$, which implies $\alpha = r$ and $d = 2r - 1$, since $(2 \cdot 3^{r-1} - 1) + [d - 2(r-1)] < n \leqslant (2 \cdot 3^r - 1) + (d - 2r)$. However, this contradicts the assumption of $d \geqslant 2r$. So $\alpha \leqslant d(y, v^*)$. And by Lemma 4.2, one has $T \in \mathcal{T}^{cs}(\alpha, d)$, which implies $\alpha = r$ and $T \in \mathcal{T}^{cs}(r, d)$, since $|T^{cs}(r-1, d)| < n \leqslant |T^{cs}(r, d)|$.

Now we consider that T is $v_1^* v_2^*$-edge central. By Lemma 4.1, there is a choice such that $v_1^* v_2^*$ is in a path length of d. Note that $T^{ces}(r-1, d)$ is the unique d-path complete edge symmetry chemical tree which has a number of vertices in $[|T^{cs}(r-1, d)|+1, |T^{cs}(r, d)|]$. So by Lemma 4.3, one also has $T \cong T^{ces}(r-1, d) \in \mathcal{T}^{cs}(r, d)$, since $|T^{cs}(r-1, d)| < n \leqslant |T^{cs}(r, d)|$.

On the other hand, all trees in $\mathcal{T}^{cs}(r, d)$ are equivalent to each other. Thus, we have $\mathcal{T}_{n,d}^{\max} = \mathcal{T}^{cs}(r, d) \cap \mathcal{T}_{n,d}$.

Let $T_1 = T^{cs}(r-1, d)$. Suppose $n = |T_1| + t$ where $t \in [1, 4 \cdot 3^{r-1} - 2]$. Let w^* be the center of T_1. Let x_1, x_2, x_3, x_4 be four leaves in the four distinct branches of T_1, respectively, where P_{x_1,x_2} is a path of length d and $d(x_1) \geqslant d(x_2)$. Let T_2 be the graph obtained from T_1 by attaching $\lfloor t/2 \rfloor$ pendent edges $\{e_i | i \in [1, \lfloor t/2 \rfloor]\}$ to x_3 and attaching $\lceil t/2 \rceil$ pendent edges $\{e'_j | j \in [1, \lceil t/2 \rceil]\}$ to x_4. Then T_2 is a w^*-central tree which is equivalent to T.

Let $\phi_i(e)$ be the contribution of e to T_i for $i \in \{1, 2\}$ and $e \in E_{T_i}$. Then $\phi_2(e) = \phi_1(e) + t$ for each $e \in E_{T_1} \setminus E_{P_{x_3,x_4}}$; $\phi_2(e) = \phi_1(e) + \lceil t/2 \rceil - \lfloor t/2 \rfloor$ for each $e \in E_{P_{x_3,w^*}}$; $\phi_2(e) = \phi_1(e) - \lceil t/2 \rceil + \lfloor t/2 \rfloor$ for each $e \in E_{P_{x_4,w^*}}$ and $\phi_2(e_i) = \phi_2(e'_j) = n - 2$ for each $i \in [1, \lfloor t/2 \rfloor]$ and $j \in [1, \lceil t/2 \rceil]$. So

$$\begin{aligned} Mo(T_2) &= Mo(T_1) + t \cdot (|E_{T_1}| - |E_{P_{x_3,x_4}}|) + t \cdot (n-2) \\ &= Mo(T_1) + t \cdot (2 \cdot 3^{r-1} + n + d - 4r) \; . \end{aligned}$$

Note that for each edge $uv \in E_j(T_1)$, where $u \in R_j(T_1), v \in R_{j-1}(T_1)$ and $1 \leqslant j \leqslant \lceil d/2 \rceil$, the contribution of uv equals to $|T_1| - 2\sigma(u)$. If $v \notin V_{P_{x_1,x_2}}$, one has $\sigma(u) = (3^{r-j} - 1)/2$. If u is in P_{x_1,w^*}, one has $\sigma(u) = (3^{r-j} - 1)/2 + \lceil d/2 \rceil - (r-1)$ for $1 \leqslant j \leqslant r-1$, while $\sigma(u) = \lceil d/2 \rceil - j + 1$ for $r \leqslant j \leqslant \lceil d/2 \rceil$. If u is in P_{x_2,w^*}, one has $\sigma(u) = (3^{r-j} - 1)/2 + \lfloor d/2 \rfloor - (r-1)$ for $1 \leqslant j \leqslant r-1$, while $\sigma(u) = \lfloor d/2 \rfloor - j + 1$ for

$r \leqslant j \leqslant \lfloor d/2 \rfloor$. And one has $|E_j \setminus E_{P_{x_1,x_2}}| = 4 \cdot 3^{j-1} - 2$ for $1 \leqslant j \leqslant r-1$. So

$$\begin{aligned}
Mo(T_1) =& \sum_{j=1}^{r-1} \sum_{uv \in E_j \setminus E_{P_{x_1,x_2}}} \phi_1(uv) + \sum_{j=1}^{r-1} \sum_{uv \in E_j \cap E_{P_{x_1,x_2}}} \phi_1(uv) + \sum_{j \geqslant r} \sum_{uv \in E_j} \phi_1(uv) \\
=& \sum_{j=1}^{r-1} (4 \cdot 3^{j-1} - 2)(|T_1| - 3^{r-j} + 1) + \sum_{j=1}^{r-1} [2 \cdot |T_1| - 2(3^{r-j} - 1) - 2d + 4(r-1)] \\
&+ \sum_{j=r}^{\lceil \frac{d}{2} \rceil} \left[|T_1| - 2\left(\left\lceil \frac{d}{2} \right\rceil - j + 1 \right) \right] + \sum_{j=r}^{\lfloor \frac{d}{2} \rfloor} \left[|T_1| - 2\left(\left\lfloor \frac{d}{2} \right\rfloor - j + 1 \right) \right] \\
=& 4[9^{r-1} + (d - 3r + 2)3^{r-1} - rd + 2r - 2] + 6(r-1)^2 + \left\lfloor \frac{d^2}{2} \right\rfloor .
\end{aligned}$$

Thus,

$$\begin{aligned}
Mo(T) = Mo(T_2) &= Mo(T_1) + t \cdot (2 \cdot 3^{r-1} + n + d - 4r) \\
&= n^2 - (2r+1)n + 2 \cdot 3^r - 2r^2 + 2dr - \left\lfloor \frac{d^2}{2} \right\rfloor - d - 2
\end{aligned}$$

since $t = n - [(2 \cdot 3^{r-1} - 1) + (d - 2(r-1))]$.

This completes our proof. ■

5 The least Mostar index in $\mathcal{T}_{n,d}^G$

In this section, we determine the least Mostar index of trees in $\mathcal{T}_{n,d}^G$. All the corresponding extremal trees are characterized. In order to show our main result, we give some lemmas at first.

Lemma 5.1. *Let T be in $\mathcal{T}_{n,d}^{G\min}$ with $d \geqslant 4$. Then the center or the edge center is in some path of length d.*

Proof. Suppose to the contrary that the center or the edge center of T is not in any path length of d. Let $P_{x,y}$ be a path of length d. Then $P_{x,y}$ is in some branch of T (suppose it is in T_{v_1} if T is v^*-central or in $T_{v_1^*}$ if T is $v_1^* v_2^*$-central).

Let $a = v^*$ or $v_1^* v_2^*$. Let z be the vertex in $P_{x,y}$ which has the least distance from a. Without loss of generality, assume $d(x,z) \geqslant d(y,z)$. Then for any pendent edge e in another branch or extended branch other than T_{v_1} or $T_{v_1^*}$, one has $d(e,z) \leqslant d(y,z) - 2$ by our assumption. That is $d(e,a) \leqslant d(y,a) - 3$. Then we can do moving operation on (e, y_1) where $y_1 y \in E_T$, to decrease the Mostar index by Property 2.1(ii) or Property 2.1(iii), with the diameter unchanged, a contradiction. Thus, the center or the edge center is in a path length of d. ■

Lemma 5.2. *Let T be a v^*-central tree in $\mathcal{T}_{n,d}^{G\min}$ with $d \geqslant 4$. Then $T \cong \widetilde{P}(n,d)$.*

Proof. By Lemma 5.1, let v^* be in a path, say $P_{x,y}$, of length d. Suppose $x \in S(v_1)$ and $y \in S(v_2)$. Without loss of generality, suppose $d(x,v^*) \geqslant d(y,v^*)$. Let α_i be the greatest distance from a leaf in T_{v_i} to v^* where $v_i \in N(v^*)$ and let $\alpha = \max_{1\leqslant i\leqslant d(v^*)}\{\alpha_i\}$. Then for each $v \in V_T$ and each $w \in V_T \setminus S(v_1)$, one has $\alpha = \alpha_1 = d(x,v^*) \geqslant d(v,v^*)$ and $\alpha_2 = d(y,v^*) \geqslant d(w,v^*)$. We proceed by showing the following facts.

Fact 1. *If $\alpha_i \geqslant 3$, then each vertex in $\cup_{j=1}^{\alpha_i-2} R_{i,j}$ is a 2-vertex for $i \in [1, d(v^*)]$.*

Proof of Fact 1. Suppose $\alpha_i \geqslant 3$, $w \in R_{i,\alpha_i-1}$. If there exists $u \in \cup_{j=1}^{\alpha_i-2} R_{i,j}$ such that $d(u) \geqslant 3$, then let e be in $(E(u) \cap ES(u) \setminus E_{P_{u,w}})$. Hence, we can do moving operation on $(ES(e), w)$ to decrease the Mostar index by Property 2.1(vi), with the diameter unchanged, a contradiction. ■

Fact 2. *$\alpha_2 = \alpha$ or $\alpha - 1$ and $\alpha_2 \geqslant 2$.*

Proof of Fact 2. Note that $\alpha_2 \leqslant \alpha$. Suppose $\alpha_2 \leqslant \alpha - 2$. Let $e \in E_{2,\alpha_2}$. Then we can do moving operation on $(e, v_{1,\alpha-1})$ to decrease the Mostar index by the first part of Property 2.1(ii), with the diameter unchanged, a contradiction. So $\alpha_2 = \alpha$ or $\alpha - 1$. Together with $\alpha_2 + \alpha = d \geqslant 4$, we have $\alpha_2 \geqslant 2$. ■

Fact 3. *$d(v^*) = 2$, $\sigma(v_1) = \sigma(v_2)$ and n is odd.*

Proof of Fact 3. Suppose $d(v^*) \geqslant 3$. Let $v_3 \in N(v^*)$. By Fact 1, for each leaf w' in T_{v_i}, one has $d(w',v^*) = \alpha_i$ and there is a unique vertex in R_{i,α_i-1} (let v_{i,α_i-1} be this unique vertex).

Suppose $\alpha_3 \leqslant \alpha_2 - 1$. Let $e \in E_{3,\alpha_3}$. Note that either $\sigma(v_1) \leqslant \lfloor n/2 \rfloor - 1$ or $\sigma(v_2) \leqslant \lfloor n/2 \rfloor - 1$. Then we can do moving operation on (e, v_{2,α_2-1}) or $(e, v_{1,\alpha-1})$ to decrease the Mostar index by the first part of Property 2.1(ii), with the diameter unchanged, a contradiction. So $\alpha_3 = \alpha_2$ since $\alpha_3 \leqslant \alpha_2$.

Now we can firstly do moving operations on $(e_i, v_{1,\alpha-1})$ or (e_i, v_{2,α_2-1}) for each $e_i \in E_{3,\alpha_2}$ until until $E_{3,\alpha_2} = \emptyset$, and make sure one of the branches containing x and y has at most $\lfloor n/2 \rfloor - 1$ vertices, with the Mostar index not increasing by the first part of Property 2.1(ii), and with the diameter unchanged. And secondly do moving operation on (e, v_{2,α_2-1}) or $(e, v_{1,\alpha-1})$ for $e \in E_{3,\alpha_2-1}$ to decrease the Mostar index by the first part of Property 2.1(ii), with the diameter unchanged, a contradiction. Thus, $d(v^*) = 2$. Then n is odd and $\sigma(v_1) = \sigma(v_2) = (n-1)/2$. Therefore, Fact 3 holds. ■

Now we come back to show Lemma 5.2. By Facts 2 and 3, if $\alpha_2 = \alpha$, then $d = 2\alpha$ and $|E_{1,\alpha}| = |E_{2,\alpha}|$; if $\alpha_2 = \alpha - 1$, then $d = 2\alpha - 1$ and $|E_{1,\alpha}| = |E_{2,\alpha-1}| - 1$. Thus, $T \cong \widetilde{P}(n,d)$, as claimed. ■

Lemma 5.3. *Let T be a $v_1^*v_2^*$-edge central tree in $\mathcal{T}_{n,d}^{G\min}$ with $d \geqslant 4$. Then $T \cong \widetilde{P}(n,d)$.*

Proof. By Lemma 5.1, let $v_1^*v_2^*$ be in a path, say $P_{x,y}$, of length d. Let α_i be the greatest distance from a leaf in $T_{v_i^*}$ to v_i^* for $i \in \{1,2\}$ and let $\alpha = \max\{\alpha_1, \alpha_2\}$. Suppose $x \in S(v_1^*)$ and $y \in S(v_2^*)$. Then $\alpha_1 = d(x, v_1^*)$ and $\alpha_2 = d(y, v_2^*)$. Without loss of generality, suppose $\alpha = \alpha_1 \geqslant \alpha_2$.

Let $xx_1 \in E_T$. If $\cup_{1 \leqslant j \leqslant \alpha-2} R_{1,j} \neq \emptyset$, then one may suppose there exists $u \in \cup_{1 \leqslant j \leqslant \alpha-2} R_{1,j}$ where $d(u) \geqslant 3$. Thus, let e be in $(E(u) - EA(x))$. Then we can do moving operation on $(ES(e), x_1)$ to decrease the Mostar index by Property 2.1(i), with the diameter unchanged, a contradiction. So each vertex in $\cup_{1 \leqslant j \leqslant \alpha-2} R_{1,j}$ (if it is not empty) is a 2-vertex. Similarly, each vertex in $\cup_{1 \leqslant j \leqslant \alpha_2-2} R_{2,j}$ (if it is not empty) is a 2-vertex. So there is a unique vertex v_{i,α_i-1} in R_{i,α_i-1} for $i \in \{1,2\}$.

Suppose $\alpha \geqslant \alpha_2 + 2$. Then $|E_{2,\alpha_2}| > |E_{1,\alpha}|$ since $\sigma(v_1^*) = \sigma(v_2^*)$. Let $e \in E_{2,\alpha_2}$. Then we can do moving operation on $(e, v_{1,\alpha-1})$ to decrease the Mostar index by Property 2.1(iii), with the diameter unchanged, a contradiction. So $\alpha \leqslant \alpha_2 + 1$. If $\alpha = \alpha_2$, then $d = 2\alpha + 1$ and $|E_{1,\alpha}| = |E_{1,\alpha}|$. If $\alpha = \alpha_2 + 1$, then $d = 2\alpha$ and $|E_{1,\alpha}| = |E_{2,\alpha-1}| - 1$. Thus, $T \cong \widetilde{P}(n,d)$, as claimed. ■

Proof of Theorem 1.6. If $d = 3$ and $n \geqslant 6$, then let $P = x_1x_2x_3x_4$ be a path of length 3. If T is edge central, then x_2x_3 is the edge center and T is unique where $T \cong \widetilde{P}(n,3)$. If T is central, then $v^* = x_2$ or x_3. Without loss of generality, suppose $v^* = x_2$. Then $\sigma(x_3) \leqslant \lceil n/2 \rceil - 1$. If n is even, or n is odd and $\sigma(x_3) \leqslant (n-1)/2 - 1$, then we can do moving operation on (x_2x_2', x_3) where $x_2' \neq x_3$ to decrease the Mostar index with the diameter unchanged, a contradiction. So n is odd and $\sigma(x_3) = (n-1)/2$. Thus, $T \cong \widetilde{P}(n,3)$.

If $d \geqslant 4$, by Lemmas 5.2 and 5.3, one also has $T \cong \widetilde{P}(n,d)$. On the other hand, $Mo(\widetilde{P}(n,d)) = \sum_{e \in V_1} \phi(e) + \sum_{e \in V_T \setminus V_1} \phi(e)$ for $d \geqslant 3$.

If n is even and d is odd, one has

$$Mo(\widetilde{P}(n,d)) = (n-d+1)(n-2) + 2\sum_{j=0}^{\frac{d-3}{2}} 2j = (n-d+1)(n-2) + \frac{(d-1)(d-3)}{2}\ .$$

If n is even and d is even, one has

$$Mo(\widetilde{P}(n,d)) = (n-d+1)(n-2) + \sum_{j=1}^{\frac{d}{2}-1} 2j + \sum_{j=0}^{\frac{d}{2}-2} 2j = (n-d+1)(n-2) + \frac{(d-2)^2}{2}\ .$$

If n is odd and d is odd, one has

$$Mo(\widetilde{P}(n,d)) = (n-d+1)(n-2) + \sum_{j=0}^{\frac{d-3}{2}} 2j + \sum_{j=1}^{\frac{d-1}{2}} 2j = (n-d+1)(n-2) + \frac{(d-1)^2}{2}\ .$$

If n is odd and d is even, one has

$$Mo(\widetilde{P}(n,d)) = (n-d+1)(n-2) + 2\sum_{j=1}^{\frac{d}{2}-1} 2j = (n-d+1)(n-2) + \frac{d(d-1)}{2}\ .$$

Thus, for $d \geqslant 3$,

$$Mo(T) \geqslant \begin{cases} (n-d+1)(n-2) + 2\lfloor \frac{d}{2} \rfloor \lfloor \frac{d-2}{2} \rfloor, & \text{if } n \text{ is even;} \\ (n-d+1)(n-2) + 2\lfloor \frac{d-1}{2} \rfloor^2, & \text{if } n \text{ is odd.} \end{cases}$$

This completes our proof. ■

6 Future work

In this paper, we determine the chemical trees of order n with the greatest Mostar index. We also identify chemical trees of order n and diameter d with the greatest Mostar index. What is more, we characterize the general trees of order n and diameter d having the least Mostar index. We tried to determine chemical trees of order n and diameter d having the smallest Mostar index without complete success. Hence, this problem is still open. We will do it in the near future.

Acknowledgment: Kecai Deng is partially supported by NSFC (No. 11701195) and by Scientific Research Funds of Huaqiao University (No. 16BS808) and Shuchao Li is partially ssupported by NSFC (Nos. 11671164, 11271149).

References

[1] K. Balakrishnan, B. Brešar, M. Chagat, S. Klavžar, A. Vesel, P. Žigert Pleteršek, Equal opportunity networks, distance–balanced graphs, and Wiener game, *Discr. Opt.* **12** (2014) 150–154.

[2] T. Bıyıkoğlu, J. Leydold, Dendrimers are the unique chemical trees with maximum spectral radius, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 851–854.

[3] V. Bžović, V.Ž. Kovijanić, G. Popivoda, Chemical trees with extreme values of a few types of multiplicative Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 207–220.

[4] H. Y. Deng, On the extremal Wiener polarity index of chemical trees, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 305–314.

[5] A. A. Dobrynin, E. Estaji, Wiener index of certain families of hexagonal chains, *J. Appl. Math. Comput.* **59** (2019) 245–256.

[6] T. Došlić, I. Martinjak, R. Škrekovski, S. T. Spužević, I. Zubac, Mostar index, *J. Math. Chem.* **56** (2018) 2995–3013.

[7] F. Hayat, B. Zhou, On cacti with large Mostar index, *Filomat* **33** (2019) 4865–4873.

[8] F. Hayat, B. Zhou, On Mostar index of trees with parameters, *Filomat* **33** (2019) 6453–6458.

[9] F. Harary, *Graph Theory*, Addison–Wesley, Reading, 1969.

[10] C. Heuberger, S. G. Wagner, Chemical trees minimizing energy and Hosoya index, *J. Math. Chem.* **46** (2009) 214–230.

[11] A. Ilić, I. Gutman, Eccentric connectivity index of chemical trees, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 731–744.

[12] A. Ilić, S. Klavžar, M. Milanović, On distance–balanced graphs, *Eur. J. Comb.* **31** (2010) 733–737.

[13] A. Ilić, D. Stevanović, The Estrada index of chemical trees, *J. Math. Chem.* **47** (2010) 305–314.

[14] J. Jerebic, S. Klavžar, D. F. Rall, Distance-balanced graphs, *Ann. Comb.* **12** (2008) 71–79.

[15] K. Kutnar, A. Malnič, D. Marušič, Š. Miklavič, Distance–balanced graphs: symmetry conditions, *Discr. Math.* **306** (2006) 1881–1894.

[16] X. Li, S. Lian, Conjugated chemical trees with extremal energy, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 891–902.

[17] A. Tepeh, Extremal bicyclic graphs with respect to Mostar index, *Appl. Math. Comput.* **355** (2019) 319–324.

[18] X. Wu, L. Zhang, On structural properties of *ABC*-minimal chemical trees, *Appl. Math. Comput.* **362** (2019) #124570.