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Wei Gao

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EXTREMAL TREES AND MOLECULAR TREES WITH RESPECT TO THE SOMBOR-INDEX-LIKE GRAPH INVARIANTS $\mathcal{SO}_5$ AND $\mathcal{SO}_6$

Wei Gao, Abington

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Abstract. I. Gutman (2022) constructed six new graph invariants based on geometric parameters, and named them Sombor-index-like graph invariants, denoted by $\mathcal{SO}_1, \mathcal{SO}_2, \ldots, \mathcal{SO}_6$. Z. Tang, H. Deng (2022) and Z. Tang, Q. Li, H. Deng (2023) investigated the chemical applicability and extremal values of these Sombor-index-like graph invariants, and raised some open problems, see Z. Tang, Q. Li, H. Deng (2023). We consider the first open problem formulated at the end of Z. Tang, Q. Li, H. Deng (2023). We obtain the extremal values of the graph invariants $\mathcal{SO}_5$ and $\mathcal{SO}_6$ among all trees and molecular trees of order n, and characterize the trees and molecular trees that achieve the extremal values, respectively. Thus, the problem is completely solved.

Keywords: tree; molecular tree; Sombor-index-like graph invariant; extremal value

MSC 2020: 05C50, 05C09, 05C92

1. Introduction

Let G be a simple connected graph with the vertex set $V(G)$ and edge set $E(G)$. For $v \in V(G)$, we denote the degree of v in G by $d_G(v)$. Let $\Delta(G)$ and $\delta(G)$ be the maximum degree and minimum degree of G, respectively. A tree is a connected acyclic graph, and a molecular tree is a tree of maximum degree at most four. Denote by $\mathcal{T}_n$ and $\mathcal{CT}_n$ the sets of all trees and molecular trees of order n, respectively.

The Sombor index of a graph G is defined as

$$\mathcal{SO} = \mathcal{SO}(G) = \sum_{uv \in E(G)} \sqrt{d_G^2(u) + d_G^2(v)}.$$

This index was conceived in [1] by considering a geometric representation of edges, and soon attracted much attention. For $uv \in E(G)$, we form a triangle by the

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points (a,b), (b,a) and $(0,0)$, where $a = d_G(u)$, $b = d_G(v)$. Then the distance between the point (a,b) and the origin is $\sqrt{d_G^2(u)+d_G^2(v)}$. Summing this over all edges of the graph G, one obtains the right-hand side of the Sombor index. Numerous research studies of $\mathcal{SO}$ then followed, with its geometric origin being ignored and more focused on its algebraic and combinatorial aspects. Extending this consideration, recently in [2] Gutman showed the geometry-based interpretation of some classical VDB topological indices and generated a series of new Sombor-index-like graph invariants, defined as

$$\begin{aligned}
\mathcal{SO}_1 = \mathcal{SO}_1(G) &= \frac{1}{2}\sum_{uv\in E(G)} |d_G^2(u) - d_G^2(v)|,\\
\mathcal{SO}_2 = \mathcal{SO}_2(G) &= \sum_{uv\in E(G)} \frac{|d_G^2(u) - d_G^2(v)|}{d_G^2(u) + d_G^2(v)},\\
\mathcal{SO}_3 = \mathcal{SO}_3(G) &= \sum_{uv\in E(G)} \sqrt{2}\frac{d_G^2(u) + d_G^2(v)}{d_G(u) + d_G(v)}\pi,\\
\mathcal{SO}_4 = \mathcal{SO}_4(G) &= \frac{1}{2}\sum_{uv\in E(G)} \Big(\frac{d_G^2(u) + d_G^2(v)}{d_G(u) + d_G(v)}\Big)^2\pi,\\
\mathcal{SO}_5 = \mathcal{SO}_5(G) &= \sum_{uv\in E(G)} \frac{2|d_G^2(u) - d_G^2(v)|}{\sqrt{2} + 2\sqrt{d_G^2(u) + d_G^2(v)}}\pi,\\
\mathcal{SO}_6 = \mathcal{SO}_6(G) &= \sum_{uv\in E(G)} \Big(\frac{d_G^2(u) - d_G^2(v)}{\sqrt{2} + 2\sqrt{d_G^2(u) + d_G^2(v)}}\Big)^2\pi,
\end{aligned}$$

where $\mathcal{SO}_5$ pertains to the perimeter of the circle inscribed into the triangle described before, and $\mathcal{SO}_6$ pertains to the area of the same triangle. In [4], [5], the chemical applicability of these Sombor-index-like graph invariants was investigated, and it has been shown that almost all of these six graph invariants are useful in predicting physicochemical properties with high accuracy compared to some well-established and often used indices. Also, bounds have been obtained for some of the Sombor-index-like graph invariants among all trees and molecular trees with a fixed number of vertices, and the trees and molecular trees that achieve the extremal values have been characterized. In particular, at the end of [5], the following open problems are raised.

Problem 1.1 ([5])**.** *Find the extremal values of $\mathcal{SO}_5(G)$, $\mathcal{SO}_6(G)$ in the set of trees and molecular trees with a given number of vertices.*

Problem 1.2 ([5])**.** *Find the maximum value of $\mathcal{SO}_4(G)$ in the set of trees with a given number of vertices.*

Problem 1.3 ([5]). *Find the extremal values of $\mathcal{SO}_5(G)$, $\mathcal{SO}_6(G)$ in the set of connected graphs with a given number of vertices.*

Problem 1.4 ([5]). *Find the maximum values of $\mathcal{SO}_3(G)$, $\mathcal{SO}_4(G)$ in the set of connected graphs with a given number of vertices.*

In this paper, we obtain the extremal values of $\mathcal{SO}_5(G)$, $\mathcal{SO}_6(G)$ among all trees and molecular trees of order n, and characterize the trees and molecular trees that achieve the extremal values, respectively. Thus, Problem 1.1 is completely solved.

2. The extremal values of $\mathcal{SO}_5(G)$ and $\mathcal{SO}_6(G)$ among $\mathcal{T}_n$

In this section, we obtain the extremal values of $\mathcal{SO}_5$ and $\mathcal{SO}_6$ among $\mathcal{T}_n$ with $n \geqslant 3$, and characterize the trees that achieve the extremal values.

Let T be a tree of order n. A vertex v with $d_T(v) = i$ is called an i-degree vertex of T. An edge $e = uv$ with $d_T(u) = i$ and $d_T(v) = j$ is called an (i, j)-edge of T. The symbols $n_i = n_i(T)$ and $m_{ij} = m_{ij}(T)$ denote the number of i-degree vertices and the number of (i, j)-edges of T, respectively. Put

$$\omega_{ij}^5 = \frac{|i^2 - j^2|}{\sqrt{2} + 2\sqrt{i^2 + j^2}}, \quad \omega_{ij}^6 = \Big(\frac{i^2 - j^2}{\sqrt{2} + 2\sqrt{i^2 + j^2}}\Big)^2.$$

Then

$$\mathcal{SO}_5(T) = 2\pi \sum_{\delta(T) \leqslant i < j \leqslant \Delta(T)} m_{ij}\omega_{ij}^5, \tag{2.1}$$

$$\mathcal{SO}_6(T) = \pi \sum_{\delta(T) \leqslant i < j \leqslant \Delta(T)} m_{ij}\omega_{ij}^6. \tag{2.2}$$

Lemma 2.1. *Let $n \geqslant 3$ and $f(x, y) = (y^2 - x^2)/(\sqrt{2} + 2\sqrt{x^2 + y^2})$ with $1 \leqslant x < \frac{1}{2}n$ and $x + 1 \leqslant y \leqslant n - x$. Then*

$$\frac{3}{\sqrt{2} + 2\sqrt{5}} \leqslant f(x, y) \leqslant \frac{n^2 - 2n}{\sqrt{2} + 2\sqrt{n^2 - 2n + 2}}. \tag{2.3}$$

The left equality holds if and only if $x = 1$ and $y = 2$, and the right equality holds if and only if $x = 1$ and $y = n - 1$.

Proof. Let $1 \leqslant x < \frac{1}{2}n$ and $x + 1 \leqslant y \leqslant n - x$. Since

$$\frac{\partial f(x, y)}{\partial y} = \frac{2y(3x^2 + y^2 + \sqrt{2}\sqrt{x^2 + y^2})}{\sqrt{x^2 + y^2}(\sqrt{2} + 2\sqrt{x^2 + y^2})^2} > 0,$$

we have

$$f(x, x + 1) \leqslant f(x, y) \leqslant f(x, n - x). \tag{2.4}$$

Note that

$$\frac{\mathrm{d}f(x,x+1)}{\mathrm{d}x}=\frac{\mathrm{d}}{\mathrm{d}x}\Big(\frac{2x+1}{\sqrt{2}+2\sqrt{2x^2+2x+1}}\Big)=\frac{\sqrt{2}+1/\sqrt{2x^2+2x+1}}{2\sqrt{4x^2+4x+2}+4x^2+4x+3}>0$$

and

$$\begin{aligned}\frac{\mathrm{d}f(x,n-x)}{\mathrm{d}x}&=\frac{\mathrm{d}}{\mathrm{d}x}\Big(\frac{n^2-2nx}{\sqrt{2}+2\sqrt{n^2-2nx+2x^2}}\Big)\\&=-\frac{\sqrt{2}n+n^3/\sqrt{n^2-2nx+2x^2}}{2\sqrt{2}\sqrt{n^2-2nx+2x^2}+2(n-x)^2+2x^2+1}<0.\end{aligned}$$

By (2.4), we have

$$\begin{aligned}f(x,y)&\geqslant f(x,x+1)\geqslant f(1,2)=\frac{3}{\sqrt{2}+2\sqrt{5}},\\f(x,y)&\leqslant f(x,n-x)\leqslant f(1,n-1)=\frac{n^2-2n}{\sqrt{2}+2\sqrt{n^2-2n+2}}.\end{aligned}$$

Then (2.3) holds. From the above derivation process, it is easy to see that the left equality in (2.3) holds if and only if $x=1$ and $y=x+1=2$, and the right equality in (2.3) holds if and only if $x=1$ and $y=n-x=n-1$. □

Lemma 2.2. *Let $n\geqslant 3$ and $g(x,y)=((y^2-x^2)/(\sqrt{2}+2\sqrt{x^2+y^2}))^2$ with $1\leqslant x<\frac{1}{2}n$ and $x+1\leqslant y\leqslant n-x$. Then*

$$\frac{11-2\sqrt{10}}{18}\leqslant g(x,y)\leqslant\Big(\frac{n^2-2n}{\sqrt{2}+2\sqrt{n^2-2n+2}}\Big)^2. \tag{2.5}$$

The left equality holds if and only if $x=1$ and $y=2$, and the right equality holds if and only if $x=1$ and $y=n-1$.

P r o o f. Let $1\leqslant x<\frac{1}{2}n$ and $x+1\leqslant y\leqslant n-x$. Since

$$\frac{\partial g(x,y)}{\partial y}=\frac{4y(y^2-x^2)(\sqrt{2}\sqrt{x^2+y^2}+3x^2+y^2)}{\sqrt{x^2+y^2}(2\sqrt{x^2+y^2}+\sqrt{2})^3}>0,$$

we have

$$g(x,x+1)\leqslant g(x,y)\leqslant g(x,n-x). \tag{2.6}$$

Note that

$$\begin{aligned}\frac{\mathrm{d}g(x,x+1)}{\mathrm{d}x}&=\frac{\mathrm{d}}{\mathrm{d}x}\Big(\frac{2x+1}{\sqrt{2}+2\sqrt{2x^2+2x+1}}\Big)^2\\&=\frac{4(2x+1)(\sqrt{4x^2+4x+2}+1)}{\sqrt{2x^2+2x+1}(\sqrt{2}+2\sqrt{2x^2+2x+1})^3}>0\end{aligned}$$

and

$$\frac{\mathrm{d}g(x,n-x)}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\Big(\frac{n^2-2nx}{\sqrt{2}+2\sqrt{n^2-2nx+2x^2}}\Big)^2$$
$$= -\frac{4n^2(n-2x)(n^2+\sqrt{2}\sqrt{n^2-2nx+2x^2})}{\sqrt{n^2-2nx+2x^2}(\sqrt{2}+2\sqrt{n^2-2nx+2x^2})^3} < 0.$$

Then by (2.6), we have

$$g(x,y) \geqslant g(x,x+1) \geqslant g(1,2) = \frac{11-2\sqrt{10}}{18},$$
$$g(x,y) \leqslant g(x,n-x) \leqslant g(1,n-1) = \Big(\frac{n^2-2n}{\sqrt{2}+2\sqrt{n^2-2n+2}}\Big)^2.$$

So (2.5) holds. From the above derivation process, it is easy to see that the left equality in (2.5) holds if and only if $x=1$ and $y=x+1=2$, and the right equality in (2.5) holds if and only if $x=1$ and $y=n-x=n-1$. □

Theorem 2.3. *Let $T \in \mathcal{T}_n$ with $n \geqslant 3$. Then*

$$\frac{12\pi}{\sqrt{2}+2\sqrt{5}} \leqslant \mathcal{SO}_5(T) \leqslant \frac{2n(n-2)(n-1)\pi}{\sqrt{2}+2\sqrt{n^2-2n+2}}, \tag{2.7}$$

$$\frac{(11-2\sqrt{10})\pi}{9} \leqslant \mathcal{SO}_6(T) \leqslant \frac{n^2(n-2)^2(n-1)\pi}{(\sqrt{2}+2\sqrt{(n-2)n+2})^2}. \tag{2.8}$$

The left equalities in (2.7) *and* (2.8) *hold if and only if $T \cong P_n$, and the right equalities in* (2.7) *and* (2.8) *hold if and only if $T \cong S_n$.*

P r o o f. Let $T \in \mathcal{T}_n$ and $e=uv \in E(T)$. Then $d_T(u)+d_T(v) \leqslant n$. Without loss of generality, we may assume $d_T(u) \leqslant d_T(v)$. If $d_T(u)=d_T(v)$, then

$$\frac{|d_T^2(u)-d_T^2(v)|}{\sqrt{2}+2\sqrt{d_T^2(u)+d_T^2(v)}} = \Big(\frac{|d_T^2(u)-d_T^2(v)|}{\sqrt{2}+2\sqrt{d_T^2(u)+d_T^2(v)}}\Big)^2 = 0. \tag{2.9}$$

If $d_T(u) < d_T(v)$, then $1 \leqslant d_T(u) < \frac{1}{2}n$ and $d_T(u)+1 \leqslant d_T(v) \leqslant n-d_T(u)$. So by Lemmas 2.1 and 2.2,

$$\omega_{12}^5 \leqslant \frac{|d_T^2(u)-d_T^2(v)|}{\sqrt{2}+2\sqrt{d_T^2(u)+d_T^2(v)}} \leqslant \omega_{1,n-1}^5, \tag{2.10}$$

$$\omega_{12}^6 \leqslant \Big(\frac{|d_T^2(u)-d_T^2(v)|}{\sqrt{2}+2\sqrt{d_T^2(u)+d_T^2(v)}}\Big)^2 \leqslant \omega_{1,n-1}^6. \tag{2.11}$$

Note that $|E(T)| = n-1$. Then by (2.9)–(2.11), and the definitions of $\mathcal{SO}_5$ and $\mathcal{SO}_6$, we have that

$$\mathcal{SO}_5(T) \leqslant 2\pi|E(T)|\omega_{1,n-1}^5 = \frac{2n(n-2)(n-1)\pi}{\sqrt{2}+2\sqrt{n^2-2n+2}},$$
$$\mathcal{SO}_6(T) \leqslant \pi|E(T)|\omega_{1,n-1}^6 = \frac{n^2(n-2)^2(n-1)\pi}{(\sqrt{2}+2\sqrt{(n-2)n+2})^2},$$

and the equalities in the two inequalities above hold if and only if each edge of T is a $(1,n-1)$-edge, that is, $T \cong S_n$.

Let E_1 be the set of pendant edges of T and $E_2 = E\backslash E_1$. Then $|E_1| \geqslant 2$. By (2.10) and (2.11), we have

$$\mathcal{SO}_5(T) \geqslant 2\pi \sum_{uv\in E_1} \frac{|d_T^2(u)-d_T^2(v)|}{\sqrt{2}+2\sqrt{d_T^2(u)+d_T^2(v)}} \geqslant 2\pi|E_1|\omega_{12}^5 \geqslant 4\pi\omega_{12}^5 = \frac{12\pi}{\sqrt{2}+2\sqrt{5}},$$
$$\mathcal{SO}_6(T) \geqslant \pi \sum_{uv\in E_1} \Big(\frac{d_T^2(u)-d_T^2(v)}{\sqrt{2}+2\sqrt{d_T^2(u)+d_T^2(v)}}\Big)^2 \geqslant \pi|E_1|\omega_{12}^6 \geqslant 2\pi\omega_{12}^6 = \frac{(11-2\sqrt{10})\pi}{9}.$$

It is easy to see that all equalities in the two inequalities above hold if and only if E_1 consists of two $(1,2)$-edges, and $d_T(u) = d_T(v)$ for any $e = uv \in E_2$, that is, $T \cong P_n$. □

3. The extremal values of $\mathcal{SO}_5(G)$ and $\mathcal{SO}_6(G)$ among $\mathcal{CT}_n$

In this section, we obtain the extremal values of $\mathcal{SO}_5$ and $\mathcal{SO}_6$ among $\mathcal{CT}_n$, and characterize the molecular trees that achieve the extremal values.

Note that the path P_n is a molecular tree. The following theorem is obvious from Theorem 2.3.

Theorem 3.1. *Let $T \in \mathcal{CT}_n$ with $n \geqslant 3$. Then*

$$\mathcal{SO}_5(T) \geqslant \frac{12\pi}{\sqrt{2}+2\sqrt{5}}, \tag{3.1}$$
$$\mathcal{SO}_6(T) \geqslant \frac{\left(11-2\sqrt{10}\right)\pi}{9}. \tag{3.2}$$

The equalities in (3.1) *and* (3.2) *hold if and only if $T \cong P_n$.*

In the following, we determine the maximum values of $\mathcal{SO}_5$ and $\mathcal{SO}_6$ among $\mathcal{CT}_n$ with $n \geqslant 8$, and characterize the molecular trees that achieve the maximum values. We say that a molecular tree $T \in \mathcal{CT}_n$ is a maximal $\mathcal{SO}_k$ molecular tree if T has the maximum value of $\mathcal{SO}_k$ among $\mathcal{CT}_n$ $(k = 5, 6)$.

Let $T \in \mathcal{CT}_n$ with $n \geqslant 8$. Then the following "book-keeping" relations are obeyed (see [3]):

$$\begin{aligned} n_1 + n_2 + n_3 + n_4 &= n, \\ n_1 + 2n_2 + 3n_3 + 4n_4 &= 2(n-1), \\ m_{12} + m_{13} + m_{14} &= n_1, \\ m_{12} + 2m_{22} + m_{23} + m_{24} &= 2n_2, \\ m_{13} + m_{23} + 2m_{33} + m_{34} &= 3n_3, \\ m_{14} + m_{24} + m_{34} + 2m_{44} &= 4n_4. \end{aligned} \tag{3.3}$$

Solving the system (3.3) with unknowns m_{14}, m_{24}, n_1, n_2, n_3, n_4, we can obtain

$$\begin{aligned} m_{14} &= \frac{n+3}{2} - \frac{3m_{12}}{2} - \frac{7m_{13}}{6} - \frac{m_{22}}{2} - \frac{m_{23}}{6} + \frac{m_{33}}{6} + \frac{m_{34}}{3} + \frac{m_{44}}{2}, \\ m_{24} &= \frac{n-5}{2} + \frac{m_{12}}{2} + \frac{m_{13}}{6} - \frac{m_{22}}{2} - \frac{5m_{23}}{6} - \frac{7m_{33}}{6} - \frac{4m_{34}}{3} - \frac{3m_{44}}{2}, \\ n_1 &= \frac{n+3}{2} - \frac{m_{12}}{2} - \frac{m_{13}}{6} - \frac{m_{22}}{2} - \frac{m_{23}}{6} + \frac{m_{33}}{6} + \frac{m_{34}}{3} + \frac{m_{44}}{2}, \\ n_2 &= \frac{n-5}{4} + \frac{3m_{12}}{4} + \frac{7m_{13}}{12} + \frac{3m_{22}}{4} + \frac{m_{23}}{12} - \frac{7m_{33}}{12} - \frac{2m_{34}}{3} - \frac{3m_{44}}{4}, \\ n_3 &= \frac{m_{13}}{3} + \frac{m_{23}}{3} + \frac{2m_{33}}{3} + \frac{m_{34}}{3}, \\ n_4 &= \frac{n-1}{4} - \frac{m_{12}}{4} - \frac{m_{13}}{4} - \frac{m_{22}}{4} - \frac{m_{23}}{4} - \frac{m_{33}}{4} + \frac{m_{44}}{4}. \end{aligned} \tag{3.4}$$

We now define six subsets $\mathcal{T}_0(n)$, $\mathcal{T}_1(n)$, $\mathcal{T}_2(n)$, $\mathcal{T}_2'(n)$, $\mathcal{T}_3(n)$, $\mathcal{T}_3'(n)$ of $\mathcal{CT}_n$ $(n \geqslant 8)$ that will be used in the following theorem.

(1) $\mathcal{T}_0(n)$ consists of molecular trees on $n \equiv 0 \pmod 4$ vertices with $m_{12} = m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = 0$, and $m_{44} = 1$.

(2) $\mathcal{T}_1(n)$ consists of molecular trees on $n \equiv 1 \pmod 4$ vertices with $m_{12} = m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = m_{44} = 0$.

(3) $\mathcal{T}_2(n)$ consists of molecular trees on $n \equiv 2 \pmod 4$ vertices with $m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = m_{44} = 0$, and $m_{12} = 1$.

(4) $\mathcal{T}_2'(n)$ consists of molecular trees on $n \equiv 2 \pmod 4$ vertices with $m_{12} = m_{13} = m_{23} = m_{33} = m_{34} = m_{44} = 0$, and $m_{22} = 1$.

(5) $\mathcal{T}_3(n)$ consists of molecular trees on $n \equiv 3 \pmod 4$ vertices with $m_{12} = m_{22} = m_{23} = m_{33} = m_{44} = 0$, $m_{13} = 2$, and $m_{34} = 1$.

(6) $\mathcal{T}_3'(n)$ consists of molecular trees on $n \equiv 3 \pmod 4$ vertices with $m_{12} = m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = 0$, and $m_{44} = 2$.

Note that for a molecular tree $T \in \mathcal{CT}_n$, if the values of m_{12}, m_{13}, m_{22}, m_{23}, m_{33}, m_{34}, and m_{44} are given, then the values of m_{14}, m_{24}, n_1, n_2, n_3, and n_4 can be uniquely determined by (3.4).

In Figure 1, for each of the six subsets defined above, an example is given. This means that all of these subsets are nonempty.

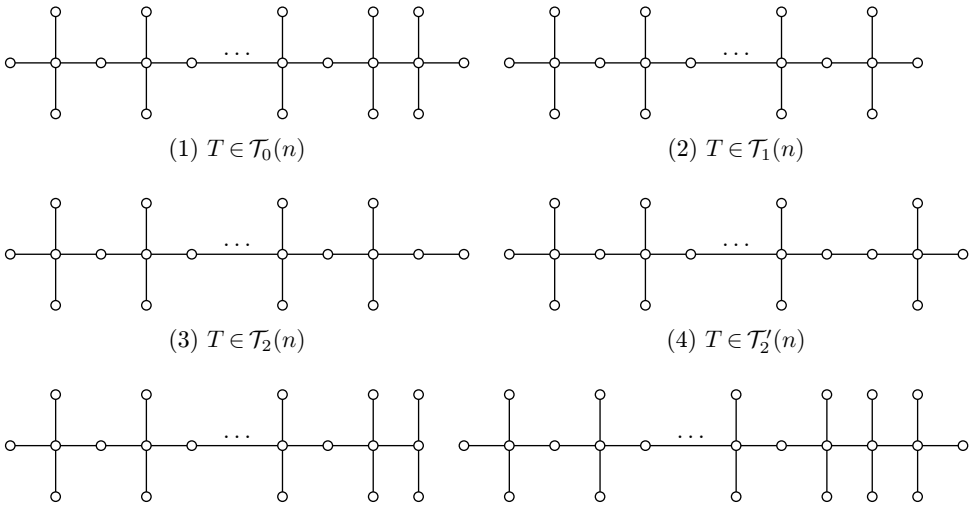


Figure 1. Some examples of molecular trees.

Theorem 3.2. *Let $T \in \mathcal{CT}_n$ with $n \geqslant 8$. Then*

(3.5)

$$\mathcal{SO}_5(T) \leqslant \begin{cases} \Big(\dfrac{12(n-8)}{\sqrt{2}+4\sqrt{5}} + \dfrac{15(n+4)}{\sqrt{2}+2\sqrt{17}}\Big)\pi & \text{if } n \equiv 0 \pmod 4, \\ \Big(\dfrac{12(n-5)}{\sqrt{2}+4\sqrt{5}} + \dfrac{15(n+3)}{\sqrt{2}+2\sqrt{17}}\Big)\pi & \text{if } n \equiv 1 \pmod 4, \\ \Big(\dfrac{12(n-4)}{\sqrt{2}+4\sqrt{5}} + \dfrac{15n}{\sqrt{2}+2\sqrt{17}} + \dfrac{6}{\sqrt{2}+2\sqrt{5}}\Big)\pi & \text{if } n \equiv 2 \pmod 4, \\ \Big(\dfrac{12(n-7)}{\sqrt{2}+4\sqrt{5}} + \dfrac{15(n-1)}{\sqrt{2}+2\sqrt{17}} + \dfrac{14}{10+\sqrt{2}} + \dfrac{16\sqrt{2}}{1+2\sqrt{5}}\Big)\pi & \text{if } n \equiv 3 \pmod 4, \end{cases}$$

(3.6)
$$\mathcal{SO}_6(T)$$
$$\leqslant \begin{cases} \dfrac{(227251-7744\sqrt{10}-8450\sqrt{34})n-4(10877-15488\sqrt{10}+8450\sqrt{34})}{81796}\pi \\ \qquad\qquad \text{if } n\equiv 0 \pmod 4, \\ \dfrac{(227251-7744\sqrt{10}-8450\sqrt{34})n+5(9349+7744\sqrt{10}-5070\sqrt{34})}{81796}\pi \\ \qquad\qquad \text{if } n\equiv 1 \pmod 4, \\ \dfrac{(227251-7744\sqrt{10}-8450\sqrt{34})n-2(90253-23232\sqrt{10}+8450\sqrt{34})}{81796}\pi \\ \qquad\qquad \text{if } n\equiv 2 \pmod 4, \\ \dfrac{(227251-7744\sqrt{10}-8450\sqrt{34})n-(133761-85184\sqrt{10}+42250\sqrt{34})}{81796}\pi \\ \qquad\qquad \text{if } n\equiv 3 \pmod 4. \end{cases}$$

The equality in (3.5) *holds if and only if* $T\in\mathcal{T}_i(n)$ *for* $n\equiv i \pmod 4$ $(i=0,1,2,3)$, *and the equality in* (3.6) *holds if and only if* $T\in\mathcal{T}_i(n)$ *for* $n\equiv i \pmod 4$ $(i=0,1)$ *and* $T\in\mathcal{T}_i'(n)$ *for* $n\equiv i \pmod 4$ $(i=2,3)$.

P r o o f. Let $T\in\mathcal{CT}_n$ with $n\geqslant 8$. After a direct calculation, by (2.1) and (2.2), we have that

$$\begin{aligned} (3.7)\quad \mathcal{SO}_5(T) &= 2\pi\sum_{1\leqslant i<j\leqslant 4} m_{ij}\omega_{ij}^5 \\ &= 2\pi\Big(\frac{3m_{12}}{\sqrt{2}+2\sqrt{5}}+\frac{8m_{13}}{\sqrt{2}+2\sqrt{10}}+\frac{15m_{14}}{\sqrt{2}+2\sqrt{17}}+\frac{5m_{23}}{\sqrt{2}+2\sqrt{13}} \\ &\quad +\frac{12m_{24}}{\sqrt{2}+4\sqrt{5}}+\frac{7m_{34}}{10+\sqrt{2}}\Big), \\ (3.8)\quad \mathcal{SO}_6(T) &= \pi\sum_{1\leqslant i<j\leqslant 4} m_{ij}\omega_{ij}^6 \\ &= \pi\Big(\frac{(11-2\sqrt{10})m_{12}}{18}+\frac{(672-128\sqrt{5})m_{13}}{361}+\frac{(875-50\sqrt{34})m_{14}}{242} \\ &\quad +\frac{(27-2\sqrt{26})m_{23}}{50}+\frac{(328-32\sqrt{10})m_{24}}{169}+\frac{(51-10\sqrt{2})m_{34}}{98}\Big). \end{aligned}$$

Replacing m_{14} and m_{24} in (3.7) and (3.8) by (3.4), we have

$$\begin{aligned} (3.9)\quad \mathcal{SO}_k(T) &= \pi(M_0^{(k)}-M_{12}^{(k)}m_{12}-M_{13}^{(k)}m_{13}-M_{22}^{(k)}m_{22} \\ &\quad -M_{23}^{(k)}m_{23}-M_{33}^{(k)}m_{33}-M_{34}^{(k)}m_{34}-M_{44}^{(k)}m_{44}), \quad k=5,6, \end{aligned}$$

where

$$M_0^{(5)} = \frac{15(n+3)}{\sqrt{2}+2\sqrt{17}} + \frac{12(n-5)}{\sqrt{2}+4\sqrt{5}},$$
$$M_{12}^{(5)} = \frac{45}{\sqrt{2}+2\sqrt{17}} - \frac{12}{\sqrt{2}+4\sqrt{5}} - \frac{6}{\sqrt{2}+2\sqrt{5}} \doteq 2.4804,$$
$$M_{13}^{(5)} = \frac{35}{\sqrt{2}+2\sqrt{17}} - \frac{4}{\sqrt{2}+4\sqrt{5}} - \frac{8\sqrt{2}}{1+2\sqrt{5}} \doteq 1.16936,$$
$$M_{22}^{(5)} = \frac{15}{\sqrt{2}+2\sqrt{17}} + \frac{12}{\sqrt{2}+4\sqrt{5}} \doteq 2.7112,$$
$$M_{23}^{(5)} = \frac{5}{\sqrt{2}+2\sqrt{17}} + \frac{20}{\sqrt{2}+4\sqrt{5}} - \frac{10}{\sqrt{2}+2\sqrt{13}} \doteq 1.28898,$$
$$M_{33}^{(5)} = \frac{28}{\sqrt{2}+4\sqrt{5}} - \frac{5}{\sqrt{2}+2\sqrt{17}} \doteq 2.18552,$$
$$M_{34}^{(5)} = \frac{32}{\sqrt{2}+4\sqrt{5}} - \frac{10}{\sqrt{2}+2\sqrt{17}} - \frac{14}{10+\sqrt{2}} \doteq 0.827563,$$
$$M_{44}^{(5)} = \frac{36}{\sqrt{2}+4\sqrt{5}} - \frac{15}{\sqrt{2}+2\sqrt{17}} \doteq 1.92268$$

and

$$M_0^{(6)} = \frac{(227251 - 7744\sqrt{10} - 8450\sqrt{34})n + 5(9349 + 7744\sqrt{10} - 5070\sqrt{34})}{81796},$$
$$M_{12}^{(6)} = \frac{2828363 + 151492\sqrt{10} - 228150\sqrt{34}}{736164} \doteq 2.68567,$$
$$M_{13}^{(6)} = \frac{180124653 + 31409664\sqrt{5} + 2795584\sqrt{10} - 21353150\sqrt{34}}{88585068} \doteq 1.52046,$$
$$M_{22}^{(6)} = \frac{227251 - 7744\sqrt{10} - 8450\sqrt{34}}{81796} \doteq 1.87651,$$
$$M_{23}^{(6)} = \frac{10306137 - 968000\sqrt{10} + 245388\sqrt{26} - 211250\sqrt{34}}{6134700} \doteq 1.18417,$$
$$M_{33}^{(6)} = \frac{407757 - 54208\sqrt{10} + 8450\sqrt{34}}{245388} \doteq 1.1639,$$
$$M_{34}^{(6)} = \frac{5183124 + 613470\sqrt{2} - 1517824\sqrt{10} + 414050\sqrt{34}}{6012006} \doteq 0.609651,$$
$$M_{44}^{(6)} = \frac{90253 + 23232\sqrt{10} + 8450\sqrt{34}}{81796} \doteq 0.807601.$$

Since all $M_{12}^{(k)}$, $M_{13}^{(k)}$, $M_{22}^{(k)}$, $M_{23}^{(k)}$, $M_{33}^{(k)}$, $M_{34}^{(k)}$, $M_{44}^{(k)}$ $(k = 5, 6)$ are positive, we have

$$\mathcal{SO}_k(T) \leqslant \pi M_0^{(k)}, \quad k = 5, 6. \tag{3.10}$$

If the condition

$$m_{12} = m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = m_{44} = 0 \tag{3.11}$$

holds, then by (3.4), $n_2 = \frac{1}{4}(n-5)$. So $n \equiv 1 \pmod 4$ and $T \in \mathcal{T}_1(n)$. It implies that the equality in (3.10) holds if and only if $T \in \mathcal{T}_1(n)$.

We now assume that $n \not\equiv 1 \pmod 4$. Then the condition (3.11) cannot be satisfied, and so $\mathcal{SO}_k(T) < \pi M_0^{(k)}$ for $k = 5, 6$. In order to find the maximal $\mathcal{SO}_k$ $(k = 5, 6)$ molecular trees, we have to make the values of the parameters m_{12}, m_{13}, m_{22}, m_{23}, m_{33}, m_{34}, m_{44} as close to zero as possible compatible to the existence of a molecular tree. Note that

$$\begin{aligned} &M_{22}^{(5)} > M_{12}^{(5)} > M_{44}^{(5)}, \quad M_{23}^{(5)} > M_{13}^{(5)} > M_{34}^{(5)}, \\ &M_{12}^{(6)} > M_{22}^{(6)} > M_{44}^{(6)}, \quad M_{13}^{(6)} > M_{23}^{(6)} > M_{34}^{(6)}. \end{aligned} \tag{3.12}$$

We consider the following two cases.

Case 1. $n_3 = 0$. Then $m_{13} = m_{23} = m_{33} = m_{34} = 0$, and so $m_{12} + m_{22} + m_{44} \geqslant 1$. By (3.9), we have

$$\mathcal{SO}_k(T) = \pi(M_0^{(k)} - M_{12}^{(k)} m_{12} - M_{22}^{(k)} m_{22} - M_{44}^{(k)} m_{44}), \quad k = 5, 6. \tag{3.13}$$

Since n_4 is an integer, by the last equation in (3.4), $n - (m_{12} + m_{22} - m_{44} + 1)$ has to be a multiple of 4.

If $n \equiv 0 \pmod 4$, then $m_{12} + m_{22} - m_{44} + 1 \equiv 0 \pmod 4$. By (3.12) and (3.13), we have

$$\begin{aligned} \mathcal{SO}_k(T) &\leqslant \pi(M_0^{(k)} - M_{12}^{(k)} m_{12} - M_{22}^{(k)} m_{22} - M_{44}^{(k)} m_{44})\big|_{(m_{12}, m_{22}, m_{44}) = (0,0,1)} \\ &= \pi(M_0^{(k)} - M_{44}^{(k)}), \quad k = 5, 6, \end{aligned} \tag{3.14}$$

and the equality holds if and only if $m_{12} = m_{22} = 0$ and $m_{44} = 1$, that is, $T \in \mathcal{T}_0(n)$.

If $n \equiv 2 \pmod 4$, then $m_{12} + m_{22} - m_{44} - 1 \equiv 0 \pmod 4$. The possible values of (m_{12}, m_{22}, m_{44}) that may achieve the minimum of $M_{12}^{(k)} m_{12} + M_{22}^{(k)} m_{22} + M_{44}^{(k)} m_{44}$ are $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 3)$.

Note that $3M_{44}^{(5)} > M_{12}^{(5)}$ and $3M_{44}^{(6)} > M_{22}^{(6)}$. By (3.12) and (3.13), it is not difficult to find that

$$\begin{aligned} \mathcal{SO}_5(T) &\leqslant \pi(M_0^{(5)} - M_{12}^{(5)} m_{12} - M_{22}^{(5)} m_{22} - M_{44}^{(5)} m_{44})\big|_{(m_{12}, m_{22}, m_{44}) = (1,0,0)} \\ &= \pi(M_0^{(5)} - M_{12}^{(5)}), \end{aligned} \tag{3.15}$$

$$\begin{aligned} \mathcal{SO}_6(T) &\leqslant \pi(M_0^{(6)} - M_{12}^{(6)} m_{12} - M_{22}^{(6)} m_{22} - M_{44}^{(6)} m_{44})\big|_{(m_{12}, m_{22}, m_{44}) = (0,1,0)} \\ &= \pi(M_0^{(6)} - M_{22}^{(6)}). \end{aligned} \tag{3.16}$$

The equality in (3.15) holds if and only if $m_{12} = 1$ and $m_{22} = m_{44} = 0$, that is, $T \in \mathcal{T}_2(n)$; and the equality in (3.16) holds if and only if $m_{22} = 1$ and $m_{12} = m_{44} = 0$, that is, $T \in \mathcal{T}_2'(n)$.

If $n \equiv 3 \pmod 4$, then $m_{12} + m_{22} - m_{44} - 2 \equiv 0 \pmod 4$. By (3.12) and (3.13), we have

$$\begin{aligned}(3.17)\quad \mathcal{SO}_k(T) &\leqslant \pi(M_0^{(k)} - M_{12}^{(k)} m_{12} - M_{22}^{(k)} m_{22} - M_{44}^{(k)} m_{44})\big|_{(m_{12},m_{22},m_{44})=(0,0,2)} \\ &= \pi(M_0^{(k)} - 2M_{44}^{(k)}), \quad k = 5, 6,\end{aligned}$$

and the equality holds if and only if $m_{12} = m_{22} = 0$ and $m_{44} = 2$, that is, $T \in \mathcal{T}_3'(n)$.

Case 2. $n_3 \geqslant 1$. Since T is a tree, we have $m_{33} \leqslant n_3 - 1$, and so by the fifth equation in (3.4), $3n_3 = m_{13} + m_{23} + 2m_{33} + m_{34} \leqslant m_{13} + m_{23} + 2(n_3 - 1) + m_{34}$. Thus,

$$(3.18)\qquad m_{13} + m_{23} + m_{34} \geqslant n_3 + 2.$$

We consider three subcases.

Subcase 2.1. $n_3 \geqslant 2$. By (3.18), $m_{13} + m_{23} + m_{34} \geqslant 4$. Then by (3.9) and (3.12), we have

$$\begin{aligned}(3.19)\qquad \mathcal{SO}_k(T) &\leqslant \pi(M_0^{(k)} - M_{13}^{(k)} m_{13} - M_{23}^{(k)} m_{23} - M_{34}^{(k)} m_{34}) \\ &\leqslant \pi(M_0^{(k)} - (m_{13} + m_{23} + m_{34}) M_{34}^{(k)}) \\ &\leqslant \pi(M_0^{(k)} - 4M_{34}^{(k)}), \quad k = 5, 6.\end{aligned}$$

Subcase 2.2. $n_3 = 1$ and $m_{12} + m_{22} + m_{44} \geqslant 1$. By (3.9), (3.12), and (3.18),

$$\begin{aligned}(3.20)\quad \mathcal{SO}_k(T) &\leqslant \pi(M_0^{(k)} - (m_{13} + m_{23} + m_{34}) M_{34}^{(k)} - (m_{12} + m_{22} + m_{44}) M_{44}^{(k)}) \\ &\leqslant \pi(M_0^{(k)} - 3M_{34}^{(k)} - M_{44}^{(k)}), \quad k = 5, 6.\end{aligned}$$

Subcase 2.3. $n_3 = 1$ and $m_{12} = m_{22} = m_{44} = 0$. Then $m_{33} = 0$ and $m_{13} + m_{23} + m_{34} = 3$, and so (3.4) becomes

$$\begin{aligned} m_{14} &= \frac{n+3}{2} - \frac{7m_{13}}{6} - \frac{m_{23}}{6} + \frac{m_{34}}{3}, \\ m_{24} &= \frac{n-5}{2} + \frac{m_{13}}{6} - \frac{5m_{23}}{6} - \frac{4m_{34}}{3} \\ n_1 &= \frac{n+3}{2} - \frac{m_{13}}{6} - \frac{m_{23}}{6} + \frac{m_{34}}{3}, \\ n_2 &= \frac{n-5}{4} + \frac{7m_{13}}{12} + \frac{m_{23}}{12} - \frac{2m_{34}}{3}, \\ n_4 &= \frac{n-1}{4} - \frac{m_{13}}{4} - \frac{m_{23}}{4}. \end{aligned}$$

The following table shows the values of m_{14}, m_{24}, n_1, n_2 and n_4 for all possible choices of (m_{13}, m_{23}, m_{34}). Note that all m_{14}, m_{24}, n_1, n_2 and n_4 are integers. The last column of Table 1 indicates the requirements for the order n for all possible choices of (m_{13}, m_{23}, m_{34}).

m_{13}	m_{23}	m_{34}	m_{14}	m_{24}	n_1	n_2	n_4	Note
0	3	0	$\frac{n}{2}+1$	$\frac{n}{2}-5$	$\frac{n}{2}+1$	$\frac{n}{4}-1$	$\frac{n}{4}-1$	$n \equiv 0 \pmod 4$
0	0	3	$\frac{n+1}{2}+2$	$\frac{n+1}{2}-7$	$\frac{n+1}{2}+2$	$\frac{n-1}{4}-3$	$\frac{n-1}{4}$	$n \equiv 1 \pmod 4$
2	1	0	$\frac{n}{2}-1$	$\frac{n}{2}-3$	$\frac{n}{2}+1$	$\frac{n}{4}$	$\frac{n}{4}-1$	$n \equiv 0 \pmod 4$
2	0	1	$\frac{n-1}{2}$	$\frac{n-1}{2}-3$	$\frac{n+1}{2}+1$	$\frac{n-3}{4}$	$\frac{n-3}{4}$	$n \equiv 3 \pmod 4$
1	2	0	$\frac{n}{2}$	$\frac{n}{2}-4$	$\frac{n}{2}+1$	$\frac{n-2}{4}$	$\frac{n}{4}-1$	No such case
0	2	1	$\frac{n+1}{2}+1$	$\frac{n+1}{2}-6$	$\frac{n+1}{2}+1$	$\frac{n-3}{4}-1$	$\frac{n-3}{4}$	$n \equiv 3 \pmod 4$
1	0	2	$\frac{n}{2}+1$	$\frac{n}{2}-5$	$\frac{n}{2}+2$	$\frac{n}{4}-2$	$\frac{n-2}{4}$	No such case
0	1	2	$\frac{n}{2}+2$	$\frac{n}{2}-6$	$\frac{n}{2}+2$	$\frac{n-2}{4}-2$	$\frac{n-2}{4}$	$n \equiv 2 \pmod 4$
1	1	1	$\frac{n+1}{2}$	$\frac{n+1}{2}-5$	$\frac{n+1}{2}+1$	$\frac{n-1}{4}-1$	$\frac{n-3}{4}$	No such case

Table 1. The values of m_{14}, m_{24}, n_1, n_2 and n_4 for all possible choices of (m_{13}, m_{23}, m_{34}).

If $n \equiv 0 \pmod 4$, then $(m_{13}, m_{23}, m_{34}) = (0, 3, 0)$ or $(2, 1, 0)$. So by (3.9) and (3.12),

$$\mathcal{SO}_5(T) \leqslant \pi(M_0^{(5)} - 2M_{13}^{(5)} - M_{23}^{(5)}), \tag{3.21}$$

$$\mathcal{SO}_6(T) \leqslant \pi(M_0^{(6)} - 3M_{23}^{(6)}). \tag{3.22}$$

If $n \equiv 2 \pmod 4$, then $(m_{13}, m_{23}, m_{34}) = (0, 1, 2)$. So by (3.9),

$$\mathcal{SO}_k(T) \leqslant \pi(M_0^{(k)} - M_{23}^{(k)} - 2M_{34}^{(k)}), \quad k = 5, 6. \tag{3.23}$$

If $n \equiv 3 \pmod 4$, then $(m_{13}, m_{23}, m_{34}) = (2, 0, 1)$ or $(0, 2, 1)$. By (3.9) and (3.12),

$$\mathcal{SO}_5(T) \leqslant \pi(M_0^{(5)} - 2M_{13}^{(5)} - M_{34}^{(5)}), \tag{3.24}$$

$$\mathcal{SO}_6(T) \leqslant \pi(M_0^{(6)} - 2M_{23}^{(6)} - M_{34}^{(6)}). \tag{3.25}$$

The equality in (3.24) holds if and only if $m_{13} = 2$, $m_{23} = 0$ and $m_{34} = 1$, that is, $T \in \mathcal{T}_3(n)$.

Combining the discussions of Cases 1 and 2, we now arrive at the next conclusions.

(1) For $\mathcal{SO}_5$, noting that

$$\begin{aligned}
M_0^{(5)} - M_{44}^{(5)} &> M_0^{(5)} - 4M_{34}^{(5)},\\
M_0^{(5)} - M_{44}^{(5)} &> M_0^{(5)} - 3M_{34}^{(5)} - M_{44}^{(k)},\\
M_0^{(5)} - M_{44}^{(5)} &> M_0^{(5)} - 2M_{13}^{(5)} - M_{23}^{(5)},\\
M_0^{(5)} - M_{12}^{(5)} &> M_0^{(5)} - 4M_{34}^{(5)},\\
M_0^{(5)} - M_{12}^{(5)} &> M_0^{(5)} - 3M_{34}^{(5)} - M_{44}^{(k)},\\
M_0^{(5)} - M_{12}^{(5)} &> M_0^{(k)} - M_{23}^{(k)} - 2M_{34}^{(k)},\\
M_0^{(5)} - 2M_{13}^{(5)} - M_{34}^{(5)} &> M_0^{(5)} - 2M_{44}^{(5)},\\
M_0^{(5)} - 2M_{13}^{(5)} - M_{34}^{(5)} &> M_0^{(5)} - 4M_{34}^{(5)},\\
M_0^{(5)} - 2M_{13}^{(5)} - M_{34}^{(5)} &> M_0^{(5)} - 3M_{34}^{(5)} - M_{44}^{(5)},
\end{aligned}$$

we get that

- ▷ if $n \equiv 0 \pmod 4$, then by (3.14), (3.19), (3.20) and (3.21), T is a maximal $\mathcal{SO}_5$ molecular tree if and only if $T \in \mathcal{T}_0(n)$, and the maximum value of $\mathcal{SO}_5$ is given in (3.14);
- ▷ if $n \equiv 2 \pmod 4$, then by (3.15), (3.19), (3.20) and (3.23), T is a maximal $\mathcal{SO}_5$ molecular tree if and only if $T \in \mathcal{T}_2(n)$, and the maximum value of $\mathcal{SO}_5$ is given in (3.15); and
- ▷ if $n \equiv 3 \pmod 4$, then by (3.17), (3.19), (3.20) and (3.24), T is a maximal $\mathcal{SO}_5$ molecular tree if and only if $T \in \mathcal{T}_3(n)$, and the maximum value of $\mathcal{SO}_5$ is given in (3.24).

(2) For $\mathcal{SO}_6$, noting that

$$\begin{aligned}
M_0^{(6)} - M_{44}^{(6)} &> M_0^{(6)} - 4M_{34}^{(6)},\\
M_0^{(6)} - M_{44}^{(6)} &> M_0^{(6)} - 3M_{34}^{(6)} - M_{44}^{(k)},\\
M_0^{(6)} - M_{44}^{(6)} &> M_0^{(6)} - 3M_{23}^{(6)},\\
M_0^{(6)} - M_{22}^{(6)} &> M_0^{(6)} - 4M_{34}^{(6)},\\
M_0^{(6)} - M_{22}^{(6)} &> M_0^{(6)} - 3M_{34}^{(6)} - M_{44}^{(k)},\\
M_0^{(6)} - M_{22}^{(6)} &> M_0^{(k)} - M_{23}^{(k)} - 2M_{34}^{(k)},\\
M_0^{(6)} - 2M_{44}^{(6)} &> M_0^{(6)} - 4M_{34}^{(6)},\\
M_0^{(6)} - 2M_{44}^{(6)} &> M_0^{(6)} - 3M_{34}^{(6)} - M_{44}^{(6)},\\
M_0^{(6)} - 2M_{44}^{(6)} &> M_0^{(6)} - 2M_{23}^{(6)} - M_{34}^{(6)},
\end{aligned}$$

we get that

- ▷ if $n \equiv 0 \pmod 4$, then by (3.14), (3.19), (3.20) and (3.22), T is a maximal $\mathcal{SO}_6$ molecular tree if and only if $T \in \mathcal{T}_0(n)$, and the maximum value of $\mathcal{SO}_6$ is given in (3.14);
- ▷ if $n \equiv 2 \pmod 4$, then by (3.16), (3.19), (3.20) and (3.23), T is a maximal $\mathcal{SO}_6$ molecular tree if and only if $T \in \mathcal{T}_2'(n)$, and the maximum value of $\mathcal{SO}_6$ is given in (3.16); and
- ▷ if $n \equiv 3 \pmod 4$, then by (3.17), (3.19), (3.20) and (3.25), T is a maximal $\mathcal{SO}_6$ molecular tree if and only if $T \in \mathcal{T}_3'(n)$, and the maximum value of $\mathcal{SO}_6$ is given in (3.17).

This proof is complete. □

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Author's address: Wei Gao, Department of Mathematics, Pennsylvania State University at Abington, 1600 Woodland Rd, Abington, PA, 19001, USA, e-mail: `wvg5121@psu.edu`.