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The Chemical Trees with Minimum Inverse Symmetric Division Deg Index

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Abstract Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The inverse symmetric division deg index of G is defined as $ISDD(G)=\sum_{uv\in E(G)}\frac{d_ud_v}{d_u^2+d_v^2}$, where d_u and d_v are the degrees of u and v, respectively. A tree T is a chemical tree if $d_u\le 4$ for each vertex $u\in V(T)$. In this paper, we characterize the structure of chemical trees with minimum inverse symmetric division deg index among all chemical trees of order n.

Keywords graph; inverse symmetric division deg index; chemical tree

MR(2020) Subject Classification 05C05

1. Introduction

Let $G=(V(G),E(G))$ be a simple connected graph with vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$ and edge set $E(G)$. For $u\in V(G)$, d_u and $N(u)$ are the degree and the set of neighbors of u, respectively. The inverse symmetric division deg index (*ISDD* index, for short) of G is defined as [1]

$$ISDD(G)=\sum_{uv\in E(G)}\frac{d_ud_v}{d_u^2+d_v^2}.$$

Chemical tree is a kind of tree whose maximum degree is no more than 4, which has extensive applications. In recent years, the problem of finding the upper and lower bounds for different molecular topological indices in all chemical trees has attracted considerable attention in mathematical-chemistry literature.

Liu et al. [2] obtained the minimum and maximum values of the harmonic index for the molecular tree with given pendent vertices. Ali et al. [3] gave the best possible upper bound, and established a lower bound on the symmetric division deg index of any molecular (n,m)-graph. Vujoašević et al. [4] characterized the chemical tree with the largest arithtic-geometric index by deleting and adding edges from graph G. Chen et al. [5] studied the chemical tree with the maximum Sombor index and obtained the corresponding value. Jiang et al. [6] used breadth first search to characterize the chemical tree with the maximum inverse sum indeg index. Gutman et

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al. [7] described the structure of chemical trees with the first maximum, the second maximum and the third maximum Randić indices. Vassilev et al. [8] explored the n-order ($n \le 12$) chemical tree with the smallest atom-bond connectivity index.

In 2021, Pattabiramanć [9] presented bounds on the symmetric division deg coindex of edge corona product of two graphs and Mycielskian of a graph by classifying graghs. In this paper, a similar method is used to classify the adjacency of vertices and characterize the structure of chemical trees with minimum inverse symmetric division deg index.

2. Lemmas

For a chemical tree T of order n, let n_i be the number of vertices with degree i, and m_{ij} be the number of edges joining a vertex of degree i and a vertex of degree j. Then it is clear that

$$n_1 + n_2 + n_3 + n_4 = n, \tag{2.1}$$

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1), \tag{2.2}$$

$$m_{12} + m_{13} + m_{14} = n_1, \tag{2.3}$$

$$m_{21} + 2m_{22} + m_{23} + m_{24} = 2n_2, \tag{2.4}$$

$$m_{31} + m_{32} + 2m_{33} + m_{34} = 3n_3, \tag{2.5}$$

$$m_{41} + m_{42} + m_{43} + 2m_{44} = 4n_4. \tag{2.6}$$

Lemma 2.1 *Let T be a chemical tree of order n. Then*

$$\begin{aligned} ISDD(T) =& \frac{11n}{34} - \frac{23}{34} + \frac{209}{510}m_{12} + \frac{8}{85}m_{13} + \frac{3}{17}m_{22} + \\ & \frac{523}{3978}m_{23} - \frac{1}{85}m_{24} + \frac{1}{17}m_{33} + \frac{4}{425}m_{34}. \end{aligned} \tag{2.7}$$

Proof Let T be a chemical tree of order n. Then

$$\begin{aligned} ISDD(T) =& \sum_{1\le i\le j\le 4} \frac{ij}{i^2+j^2} m_{ij} \\ =& \frac{2}{5}m_{12} + \frac{3}{10}m_{13} + \frac{4}{17}m_{14} + \frac{1}{2}m_{22} + \frac{6}{13}m_{23} + \\ & \frac{2}{5}m_{24} + \frac{1}{2}m_{33} + \frac{12}{25}m_{34} + \frac{1}{2}m_{44}. \end{aligned} \tag{2.8}$$

Moreover, Gutman et al. in [10] established the following relations:

$$m_{14} = \frac{2n+2}{3} - \frac{4}{3}m_{12} - \frac{10}{9}m_{13} - \frac{2}{3}m_{22} - \frac{4}{9}m_{23} - \frac{1}{3}m_{24} - \frac{2}{9}m_{33} - \frac{1}{9}m_{34}, \tag{2.9}$$

$$m_{44} = \frac{n-5}{3} + \frac{1}{3}m_{12} + \frac{1}{9}m_{13} - \frac{1}{3}m_{22} - \frac{5}{9}m_{23} - \frac{2}{3}m_{24} - \frac{7}{9}m_{33} - \frac{8}{9}m_{34}. \tag{2.10}$$

Substituting (2.9) and (2.10) into (2.8), then (2.7) holds. □

Lemma 2.2 *Let T be a chemical tree with the minimum ISDD index. Then any two vertices with degree 2 are not adjacent.*

Proof Suppose to the contrary that there are vertices $u, v \in V(T)$ with $d_u = d_v = 2$, and

$uv \in E(T)$. We will prove that T is not chemical tree with the minimum ISDD index.

Denote $N(u) = \{x, v\}$, and $N(v) = \{y, u\}$. Let T' be the chemical tree obtained from T by the operation as shown in Figure 1. Then

$$ISDD(T') - ISDD(T) = \frac{3d_x}{3^2 + d_x^2} + \frac{3d_y}{3^2 + d_y^2} + \frac{3}{10} - \frac{2d_x}{2^2 + d_x^2} - \frac{2d_y}{2^2 + d_y^2} - \frac{1}{2}.$$

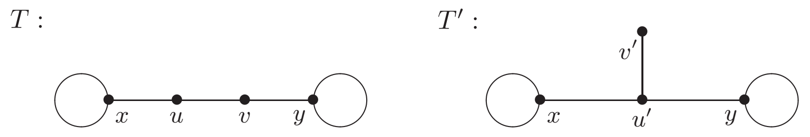


Figure 1 Chemical tree T and T' for Lemma 2.2

Note that $1 \le d_x, d_y \le 4$. Without loss of generality, assume that $d_x \le d_y$. Then (d_x, d_y) will be one element of the set $\{(1,1), (1,2), (1,3), (1,4), (2,2), (2,3), (2,4), (3,3), (3,4), (4,4)\}$. It is not difficult to check $ISDD(T') < ISDD(T)$. □

Lemma 2.3 *Let T be a chemical tree with the minimum ISDD index. Then any vertex with degree 2 is not adjacent to the vertex with degree 3 in T.*

Proof Suppose to the contrary that there are vertices $u, v \in V(T)$ with $d_u = 3$, $d_v = 2$ and $uv \in E(T)$. We will prove that T is not the minimum chemical tree with ISDD index.

Denote $N(u) = \{x, y, v\}$, and $N(v) = \{z, u\}$. Let T' be the chemical tree obtained from T by the operation as shown in Figure 2. Then

$$\begin{aligned} ISDD(T') - ISDD(T) = & \frac{4d_x}{4^2 + d_x^2} + \frac{4d_y}{4^2 + d_y^2} + \frac{4d_z}{4^2 + d_z^2} + \frac{4}{17} - \frac{3d_x}{3^2 + d_x^2} - \\ & \frac{3d_y}{3^2 + d_y^2} - \frac{2d_z}{2^2 + d_z^2} - \frac{6}{13}. \end{aligned}$$

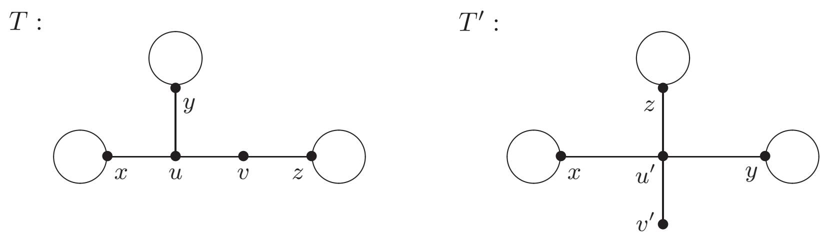


Figure 2 Chemical trees T and T' for Lemma 2.3

Note that $1 \le d_x, d_y, d_z \le 4$, and $d_z \ne 2$ by Lemma 2.2. It is not difficult to check $ISDD(T') < ISDD(T)$. □

Lemma 2.4 *Let T be a chemical tree with the minimum ISDD index. Then any two vertices with degree 3 are not adjacent in T.*

Proof Suppose to the contrary that there are vertices $u, v \in V(T)$ with $d_u = d_v = 3$ and $uv \in E(T)$. We will prove that T is not the minimum chemical tree with ISDD index.

Denote $N(u) = \{x, y, v\}$, and $N(v) = \{z, u, w\}$. Let $d_z = \max\{d_x, d_y, d_w, d_z\}$ and T' be the chemical tree obtained from T by the operation as shown in Figure 3. Then

$$\begin{aligned} ISDD(T') - ISDD(T) =& \frac{4d_x}{4^2+d_x^2} + \frac{4d_y}{4^2+d_y^2} + \frac{4d_w}{4^2+d_w^2} + \frac{2d_z}{2^2+d_z^2} + \frac{2}{5} - \\ & \frac{3d_x}{3^2+d_x^2} - \frac{3d_y}{3^2+d_y^2} - \frac{3d_w}{3^2+d_w^2} - \frac{3d_z}{3^2+d_z^2} - \frac{1}{2}. \end{aligned}$$

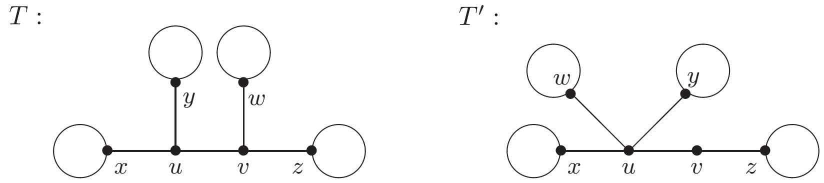


Figure 3 Chemical trees T and T' for Lemma 2.4

Note that d_x, d_y, d_w, d_z are the elements of $\{1, 3, 4\}$ by Lemma 2.3. It is not difficult to check $ISDD(T') < ISDD(T)$. □

Lemma 2.5 *Let T be a chemical tree with the minimum ISDD index. Then it is impossible for T to have vertices with degrees 2 and 3 at the same time.*

Proof Suppose to the contrary that there are vertices $u, v \in V(T)$ with $d_u = 3$ and $d_v = 2$. We will prove that T is not the minimum chemical tree with ISDD index.

Denote $N(u) = \{x, y, w\}$, and $N(v) = \{z, q\}$. By Lemma 2.3, we know that $uv \notin E(T)$. Therefore, there is a unique path from u to v through, without loss of generality, w, z. By previous lemmas, $d_x, d_y, d_w, d_q, d_z \in \{1, 4\}$. Thus $d_w = d_z = 4$, and (d_x, d_y, d_q) will be one element of the set $\{(1,1,1), (4,4,4), (1,4,1), (4,1,1), (1,1,4), (4,1,4), (4,4,1), (1,4,4)\}$. Let T' be the chemical tree obtained from T by the operation as shown in Figure 4. Then

$$\begin{aligned} ISDD(T') - ISDD(T) =& \frac{4d_x}{4^2+d_x^2} + \frac{4d_y}{4^2+d_y^2} + \frac{4d_q}{4^2+d_q^2} + \frac{4}{17} + \frac{1}{2} - \\ & \frac{3d_x}{3^2+d_x^2} - \frac{3d_y}{3^2+d_y^2} - \frac{2d_q}{2^2+d_q^2} - \frac{12}{25} - \frac{2}{5} < 0, \end{aligned}$$

that is, $ISDD(T') < ISDD(T)$. □

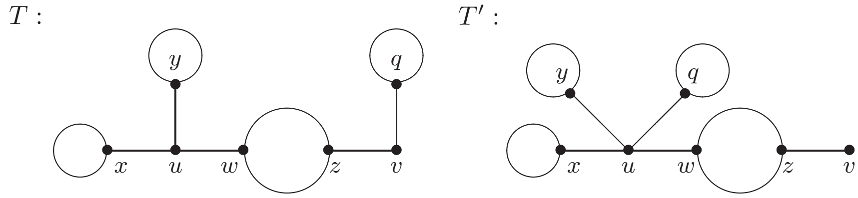


Figure 4 Chemical trees T and T' for Lemma 2.5

Lemma 2.6 *Let T be a chemical tree with the minimum ISDD index. Then there is at most one vertex of degree 3 in T.*

Proof Suppose to the contrary that there are vertices $u, v \in V(T)$ with $d_u = d_v = 3$. We will prove that T is not the minimum chemical tree with ISDD index.

Denote $N(u) = \{x, y, w\}$, $N(v) = \{z, q, t\}$, and $d_z = \max\{d_x, d_w, d_q, d_z\}$. By Lemma 2.4, we know that $uv \notin E(T)$. Thus, there is a unique path from u to v through, without loss of generality, y, t. By previous lemmas, the degrees of vertices x, y, w, q, t, z are from the set $\{1, 4\}$. Therefore, $d_y = d_t = 4$. Note that and (d_x, d_w, d_q, d_z) will be one element of the set $\{(1,1,1,1), (1,1,1,4), (1,1,4,4), (1,4,1,4), (4,1,1,4), (4,1,4,4), (4,4,4,4), (4,4,1,4), (1,4,4,4)\}$. Let T' be the chemical tree obtained from T by the operation as shown in Figure 5. Then

$$\begin{aligned} ISDD(T') - ISDD(T) =& \frac{4d_x}{4^2+d_x^2} + \frac{4d_w}{4^2+d_w^2} + \frac{4d_q}{4^2+d_q^2} + \frac{2d_z}{2^2+d_z^2} + \frac{2}{5} + \frac{1}{2} - \\ & \frac{3d_x}{3^2+d_x^2} - \frac{3d_w}{3^2+d_w^2} - \frac{3d_q}{3^2+d_q^2} - \frac{3d_z}{3^2+d_z^2} - \frac{24}{25} < 0, \end{aligned}$$

that is, $ISDD(T') < ISDD(T)$. □

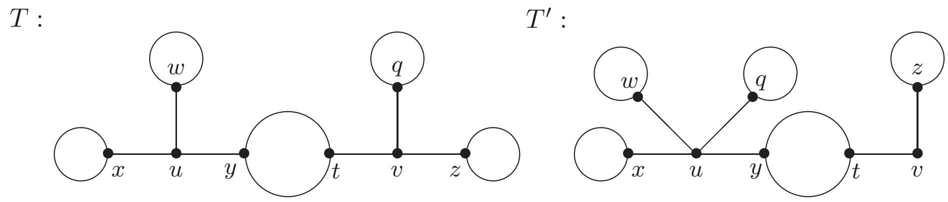


Figure 5 Chemical trees T and T' for Lemma 2.6

Lemma 2.7 *Let $n \geq 13$, and T be a chemical tree of order n with the minimum ISDD index. If u is the vertex of degree 3 in T, then u is only adjacent to vertices of degree 4.*

Proof Let u be a vertex of degree 3 in T. By Lemmas 2.5 and 2.6, $n_2 = 0$, and $d_v \in \{1, 4\}$ for each $v \in N(u)$. Then by Lemma 2.1,

$$ISDD(T) = \frac{11n}{34} - \frac{23}{34} + \frac{8}{85}m_{13} + \frac{4}{425}m_{34}.$$

Case 1. Among $N(u)$, there are two vertices of degree 1, and one vertex of degree 4.

Then $m_{13} = 2$, and $m_{34} = 1$. So

$$ISDD(T) = \frac{11n}{34} - \frac{23}{34} + \frac{16}{85} + \frac{4}{425} = \frac{11n}{34} - \frac{407}{850}.$$

Case 2. Among $N(u)$, there are two vertices of degree 4, and one vertex of degree 1.

Then $m_{13} = 1$, and $m_{34} = 2$. So

$$ISDD(T) = \frac{11n}{34} - \frac{23}{34} + \frac{8}{85} + \frac{8}{425} = \frac{11n}{34} - \frac{479}{850}.$$

Case 3. Among $N(u)$, there are three vertices of degree 4.

Then $m_{13} = 0$, and $m_{34} = 3$. So

$$ISDD(T) = \frac{11n}{34} - \frac{23}{34} + \frac{12}{425} = \frac{11n}{34} - \frac{551}{850}.$$

Since $\frac{11n}{34} - \frac{407}{850} > \frac{11n}{34} - \frac{479}{850} > \frac{11n}{34} - \frac{551}{850}$, the conclusion is obvious. $\square$

Lemma 2.8 *Let $n \geq 9$, and T be a chemical tree of order n with the minimum ISDD index. If y is a vertex of degree 2 in T, then y is only adjacent to the vertices of degree 4.*

Proof Let y be a vertex of degree two in T. Let $N(y) = \{x, u\}$. By Lemmas 2.2 and 2.5, $d_x, d_u \in \{1, 4\}$. Without loss of generality, suppose to the contrary that $d_x = 1$ and $d_u = 4$. We will prove that T is not the minimum chemical tree with ISDD index.

Denote $N(u) = \{y, z, q, w\}$, and $d_q = \max\{d_q, d_w, d_z\}$. Note that $n \geq 9$. By Lemma 2.5, we know that $d_q = 2$ or $d_q = 4$. Let T' be the chemical tree obtained from T by the operation as shown in Figure 6. Then

$$ISDD(T') - ISDD(T) = \frac{2d_q}{2^2 + d_q^2} + \frac{2}{5} + \frac{4}{17} - (\frac{4d_q}{4^2 + d_q^2} + \frac{2}{5} + \frac{2}{5}) < 0,$$

that is, $ISDD(T') < ISDD(T)$, a contradiction. $\square$

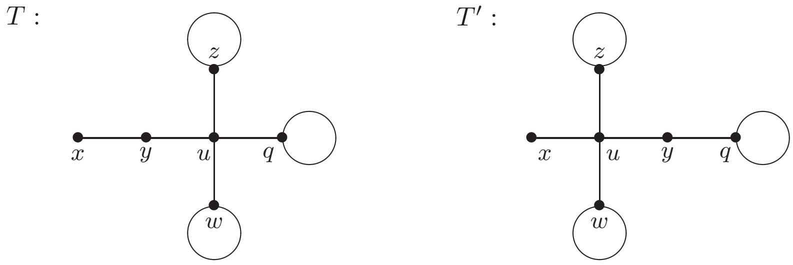


Figure 6 Chemical trees T and T' for Lemma 2.8

Theorem 2.9 *Let $n \geq 13$, and T be a chemical tree of order n with the minimum ISDD index. Then T satisfies the following conditions.*

(1) It is impossible for T to have vertices with degrees 2 and 3 at the same time;

(2) $n_3 \leq 1$, $m_{12} = 0$, $m_{13} = 0$, $m_{22} = 0$, $m_{23} = 0$, and $m_{33} = 0$.

3. Main results

For a tree T of order n, we use $\pi(T)$ to denote the degrees sequence of T.

Theorem 3.1 *Let $n \geq 13$, and T be a chemical tree of order n with the minimum ISDD index.*

- *If $n \equiv 0 \pmod 4$, then $\pi(T) = (\underbrace{4, 4, \ldots, 4}_{\frac{n}{4}}, \underbrace{2, 2, \ldots, 2}_{\frac{n}{4}-2}, \underbrace{1, 1, \ldots, 1}_{\frac{n}{2}+2})$, and $ISDD(T) = \frac{27n}{85} - \frac{107}{170}$;*
- *If $n \equiv 1 \pmod 4$, then $\pi(T) = (\underbrace{4, 4, \ldots, 4}_{\frac{n-1}{4}}, \underbrace{2, 2, \ldots, 2}_{\frac{n-5}{4}}, \underbrace{1, 1, \ldots, 1}_{\frac{n+3}{2}})$, and $ISDD(T) = \frac{27n}{85} - \frac{11}{17}$;*
- *If $n \equiv 2 \pmod 4$, then $\pi(T) = (\underbrace{4, 4, \ldots, 4}_{\frac{n+2}{4}}, \underbrace{2, 2, \ldots, 2}_{\frac{n-14}{4}}, \underbrace{1, 1, \ldots, 1}_{\frac{n}{2}+3})$, and $ISDD(T) = \frac{27n}{85} - \frac{101}{170}$;*

- *If* $n \equiv 3 \pmod 4$, *then* $\pi(T) = (\underbrace{4, 4, \ldots, 4}_{\frac{n+1}{4}}, \underbrace{2, 2, \ldots, 2}_{\frac{n-11}{4}}, \underbrace{1, 1, \ldots, 1}_{\frac{n+5}{2}})$, *and* $ISDD(T) = \frac{27n}{85} - \frac{52}{85}$.

Proof By Theorem 2.9, $m_{12} = 0$, $m_{13} = 0$, $m_{22} = 0$, $m_{23} = 0$, and $m_{33} = 0$. Then by Lemma 2.1,

$$ISDD(T) = \frac{11n}{34} - \frac{23}{34} - \frac{1}{85}m_{24} + \frac{4}{425}m_{34}. \tag{3.1}$$

Since T is a chemical tree of order n with the minimum ISDD index, so $m_{34} = 0$ and $m_{24} > 0$. That is

$$ISDD(T) = \frac{11}{34}n - \frac{23}{34} - \frac{1}{85}m_{24}. \tag{3.2}$$

By Lemma 2.8, the vertices of degree 2 can only be connected to the vertices of degree 4, it implies that $n_2 \le n_4 - 1$.

If $n_2 = n_4 - 1$, then from (2.1) and (2.2), $n_4 = \frac{n-1}{4}$, $n_2 = \frac{n-5}{4}$, and $m_{24} = 2n_2 = \frac{n-5}{2}$. So $n \equiv 1 \pmod 4$, and by (3.2),

$$ISDD(T) = \frac{27n}{85} - \frac{11}{17}.$$

Now, the minimum chemical trees are as shown in Figure 7.

T :

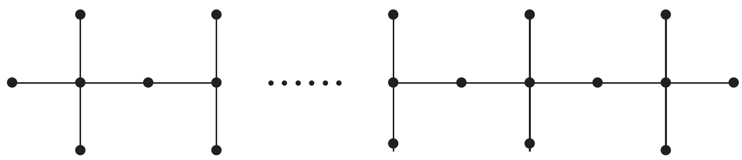


Figure 7 Chemical trees T for $n \equiv 1 \pmod 4$

If $n_2 = n_4 - 2$, then from (2.1) and (2.2), $n_4 = \frac{n}{4}$, $n_2 = \frac{n}{4} - 2$, and $m_{24} = 2n_2 = \frac{n}{2} - 4$. So $n \equiv 0 \pmod 4$, and by (3.2),

$$ISDD(T) = \frac{27n}{85} - \frac{107}{170}.$$

Now, the minimum chemical trees are as shown in Figure 8.

T :

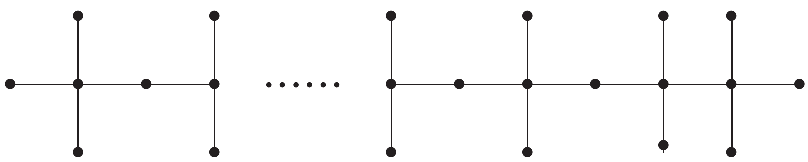


Figure 8 Chemical trees T for $n \equiv 0 \pmod 4$

If $n_2 = n_4 - 3$, then from (2.1) and (2.2), $n_4 = \frac{n+1}{4}$, $n_2 = \frac{n-11}{4}$, and $m_{24} = 2n_2 = \frac{n-11}{2}$. So $n \equiv 3 \pmod 4$, and by (3.2),

$$ISDD(T) = \frac{27n}{85} - \frac{52}{85}.$$

Now, the minimum chemical trees are as shown in Figure 9.

T :

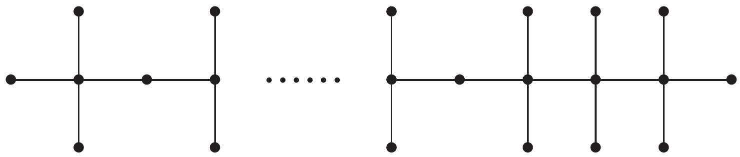


Figure 9 Chemical trees T for $n \equiv 3 \pmod 4$

If $n_2 = n_4 - 4$, then from (2.1) and (2.2), $n_4 = \frac{n+2}{4}$, $n_2 = \frac{n-14}{4}$, and $m_{24} = 2n_2 = \frac{n-14}{2}$. So $n \equiv 2 \pmod 4$, and by (3.2),

$$ISDD(T) = \frac{27n}{85} - \frac{101}{170}.$$

Now, the minimum chemical trees are as shown in Figure 10.

T :

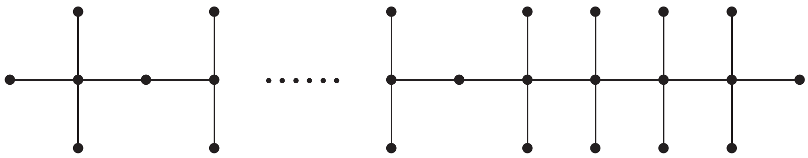


Figure 10 Chemical trees T for $n \equiv 2 \pmod 4$

Case 1. $n \equiv 0 \pmod 4$.

In this case, $n_2 = n_4 - 2$, or $n_2 \le n_4 - 5$.

If $n_2 = n_4 - 2$, then $ISDD(T) = \frac{27n}{85} - \frac{107}{170}$. If $n_2 \le n_4 - 5$, then $m_{24} = 2n_2 < 2(n_4 - 2) = \frac{n}{2} - 4$, and $ISDD(T) = \frac{11}{34}n - \frac{23}{34} - \frac{1}{85}m_{24} > \frac{27n}{85} - \frac{107}{170}$.

Since T is a chemical tree of order n with the minimum ISDD index, so $n_2 = n_4 - 2$. From (2.1) and (2.2), $n_4 = \frac{n}{4}$, $n_2 = \frac{n}{4} - 2$, $n_1 = \frac{n}{2} + 2$, that is,

$$\pi(T) = (\underbrace{4, 4, \ldots, 4}_{\frac{n}{4}}, \underbrace{2, 2, \ldots, 2}_{\frac{n}{4}-2}, \underbrace{1, 1, \ldots, 1}_{\frac{n}{2}+2}), \quad \text{and} \quad ISDD(T) = \frac{27n}{85} - \frac{107}{170}.$$

Case 2. $n \equiv 1 \pmod 4$.

In this case, $n_2 = n_4 - 1$, or $n_2 \le n_4 - 5$.

If $n_2 = n_4 - 1$, then $ISDD(T) = \frac{27n}{85} - \frac{11}{17}$. If $n_2 \le n_4 - 5$, then $m_{24} = 2n_2 < 2(n_4 - 1) = \frac{n-5}{2}$, and $ISDD(T) = \frac{11}{34}n - \frac{23}{34} - \frac{1}{85}m_{24} > \frac{27n}{85} - \frac{11}{17}$.

Since T is a chemical tree of order n with the minimum ISDD index, so $n_2 = n_4 - 1$. From (2.1) and (2.2), $n_4 = \frac{n-1}{4}$, $n_2 = \frac{n-5}{4}$, $n_1 = \frac{n+3}{2}$, that is,

$$\pi(T) = (\underbrace{4, 4, \ldots, 4}_{\frac{n-1}{4}}, \underbrace{2, 2, \ldots, 2}_{\frac{n-5}{4}}, \underbrace{1, 1, \ldots, 1}_{\frac{n+3}{2}}), \quad \text{and} \quad ISDD(T) = \frac{27n}{85} - \frac{11}{17}.$$

Case 3. $n \equiv 2 \pmod 4$.

In this case, $n_2 = n_4 - 4$, or $n_2 \leq n_4 - 5$.

If $n_2 = n_4 - 4$, then $ISDD(T) = \frac{27n}{85} - \frac{101}{170}$. If $n_2 \leq n_4 - 5$, then $m_{24} = 2n_2 < 2(n_4 - 4) = \frac{n-14}{2}$, and $ISDD(T) = \frac{11}{34}n - \frac{23}{34} - \frac{1}{85}m_{24} > \frac{27n}{85} - \frac{101}{170}$.

Since T is a chemical tree of order n with the minimum ISDD index, so $n_2 = n_4 - 4$. From (2.1) and (2.2), $n_4 = \frac{n+2}{4}$, $n_2 = \frac{n-14}{4}$, $n_1 = \frac{n}{2} + 3$, that is,

$$\pi(T) = (\underbrace{4, 4, \ldots, 4}_{\frac{n+2}{4}}, \underbrace{2, 2, \ldots, 2}_{\frac{n-14}{4}}, \underbrace{1, 1, \ldots, 1}_{\frac{n}{2}+3}), \quad \text{and} \quad ISDD(T) = \frac{27n}{85} - \frac{101}{170}.$$

Case 4. $n \equiv 3 \pmod 4$.

In this case, $n_2 = n_4 - 3$, or $n_2 \leq n_4 - 5$.

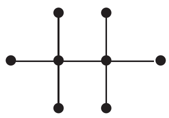
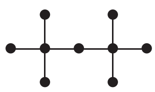
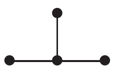
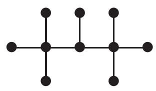
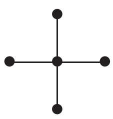
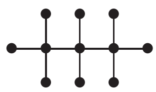
If $n_2 = n_4 - 3$, then $ISDD(T) = \frac{27n}{85} - \frac{52}{85}$. If $n_2 \leq n_4 - 5$, then $m_{24} = 2n_2 < 2(n_4 - 3) = \frac{n-11}{2}$, and $ISDD(T) = \frac{11}{34}n - \frac{23}{34} - \frac{1}{85}m_{24} > \frac{27n}{85} - \frac{52}{85}$.

Since T is a chemical tree of order n with the minimum ISDD index, so $n_2 = n_4 - 3$. From (2.1) and (2.2), $n_4 = \frac{n+1}{4}$, $n_2 = \frac{n-11}{4}$, $n_1 = \frac{n+5}{2}$, that is,

$$\pi(T) = (\underbrace{4, 4, \ldots, 4}_{\frac{n+1}{4}}, \underbrace{2, 2, \ldots, 2}_{\frac{n-11}{4}}, \underbrace{1, 1, \ldots, 1}_{\frac{n+5}{2}}), \quad \text{and} \quad ISDD(T) = \frac{27n}{85} - \frac{52}{85}.$$

The theorem now follows. □

The following table gives the chemical trees of order n with minimum ISDD indices and their corresponding minimum ISDD indices for $2 \leq n \leq 12$.

n	Chemical tree T	$ISDD(T)$	n	Chemical tree T	$ISDD(T)$
2		$\frac{1}{2}$	8		$\frac{65}{34}$
3		$\frac{4}{5}$	9		$\frac{188}{85}$
4		$\frac{9}{10}$	10		$\frac{2271}{850}$
5		$\frac{16}{17}$	11		$\frac{49}{17}$

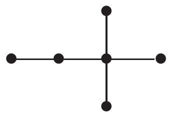
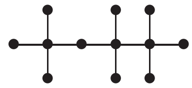
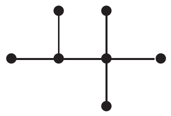
6		$\frac{128}{85}$	12		$\frac{541}{170}$
7		$\frac{759}{425}$			

Table 1 The minimum chemical trees of order n with $n = 2, 3, \ldots, 12$

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