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Sombor Index of k-Uniform Chemical Hypergraphs

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Abstract

Based on the Sombor index of graphs defined by Gutman in 2021, Shetty and Bhat defined the Sombor index of hypergraphs recently. Inspired by the work of Deng et al. [Int. J. Quantum Chem. 121 (2021) e26622] and Vukićević [Math. Montisnigri. 50 (2021) 5-14], we characterize the extremal hypergraph with the upper and lower bounds of Sombor index for k-uniform chemical hypergraphs with n vertices and give the corresponding value of Sombor index. Furthermore, we characterize the extremal hypergraph with the upper bound of Sombor index for k-uniform chemical hypertrees with n vertices and give the corresponding value of Sombor index.

1 Introduction

A hypergraph H denoted by $H = \big(V; E = (e_i)_{i\in I}\big)$ on a finite set V is a family $(e_i)_{i\in I}$, (I is a finite set of indexes) of subsets of V called

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hyperedges. The order of the hypergraph $H = (V;E)$ is the cardinality of V, i.e. $|V| = n$; its size is the cardinality of E, i.e. $|E| = m$. Two vertices in a hypergraph are *adjacent* if there is a hyperedge which contains both vertices. Two hyperedges in a hypergraph are *incident* if their intersection is not empty. The *degree* of a vertex $u \in V$ in a hypergraph, denoted by d_u, is the number of hyperedges that contain u. If each vertex has the same degree, we say that the hypergraph is *d-regular* if for every $u \in V, d_u = d$. A hypergraph H is said to be a *k-uniform hypergraph* if all the hyperedges of H have the same cardinality k. A *simple hypergraph* is a hypergraph $H = (V;E)$ such that: $e_i \subseteq e_j \Rightarrow i = j$. A simple hypergraph has no repeated hyperedge. A hypergraph is *linear* if it is simple and its any two hyperedges have at most one vertex in common. A *walk* in a hypergraph is a sequence of alternating vertices and hyperedges $v_0, e_1, v_1, e_2, v_2, \cdots, e_t, v_t$ such that for each i $(1 \leq i \leq t)$, the vertex v_{i-1} and v_i are both contained in the hyperedge e_i. A *hyperpath* in a hypergraph is a walk with no repeated vertices and no repeated hyperedges. Let P_n^k denote a k-uniform hyperpath with n vertices. A hypergraph is said to be *connected* if for any pair of vertices, there is a hyperpath which connects these vertices. A hypergraph $H = \left(V;E = (e_i)_{i\in I}\right)$ is *isomorphic* to a hypergraph $H' = \left(V', E' = \left(e'_j\right)_{j\in J}\right)$, written $H \cong H'$, if it exists a bijection: $f : V \to V'$ and a bijection $\pi : I \to J$ which induces a bijection: $g : E \to E'$ such that: $g(e_i) = e'_{\pi(i)}$, for all $e_i \in E$.

One research direction in topological indices is to explore their mathematical and computational properties, with the aim of finding optimal bounds and establishing relationships between existing topological indices. In recent years, due to the broad application prospects and development potential of topological indices and chemical graph theory, Gutman [4] proposed a class of geometry-based invariants in 2021, termed the Sombor index, denoted by $SO(G)$, i.e.

$$SO(G) = \sum_{uv\in E(G)} \sqrt{(d_u)^2 + (d_v)^2},$$

where d_u is the degree of the vertex u of G.

The study of Sombor index is of significant importance for understanding and addressing graph theory problems in chemistry and quantum chemistry. Gutman [4] determined that among all n-vertex trees, the graphs with the minimum and maximum Sombor indices are the path graph P_n and the star graph S_n, respectively. Cruz et al. [1] characterized the extremal graphs with respect to the Sombor index chemical graphs and chemical trees. Liu et al. [8] determined the minimum (resp. maximum) Sombor index of caterpillar trees with given degree sequence. Liu et al. [9] gave the classification of non-pendent tetracyclic (chemical) graphs with respect to the Sombor index, and determined the minimum Sombor indices of tetracyclic (chemical) graphs. Du et al. [3] studied the Sombor indices of some chemical graphs such as polyamidoamine, phthalocyanine, graphene, coronoid systems, carbon nanocones and four random chains. Vukićević [6] gave sharp bounds on the Sombor index of chemical trees. Deng et al. [2] determined the maximum Sombor index in chemical trees. Liu et al. [10] ordered the chemical trees, chemical unicyclic graphs, chemical bicyclic graphs and chemical tricyclic graphs with respect to Sombor index.

Based on the definition of the chemical graphs, we present the definition of *chemical hypergraphs* as follows.

Definition 1. *A hypergraph H is said to be chemical hypergraph if $d_u \leq 4$ for all $u \in V(H)$.*

Hu, Qi and Shao [5] give the definition of the power hypergraph as follows.

Definition 2. [5] *Let $G = (V, E)$ be a 2-uniform graph. For any $k \geq 3$, the kth power of G, $G^k = (V^k, E^k)$ is defined as the power hypergraph with the set of edges $E^k = \{e \bigcup \{i_{e,1}, \cdots, i_{e,k-2}\} \mid e \in E\}$, and the set of vertices $V^k = V \cup \{i_{e,1}, \cdots, i_{e,k-2}, e \in E\}$.*

From above definition we can obtain the definition of hypertrees as follows.

Definition 3. *Let $G = (V, E)$ be a 2-uniform tree. For any $k \geq 3$, the kth power of G, $G^k = (V^k, E^k)$ is defined as the hypertree with the set of edges $E^k = \{e \bigcup \{i_{e,1}, \cdots, i_{e,k-2}\} \mid e \in E\}$, and the set of vertices $V^k = V \cup \{i_{e,1}, \cdots, i_{e,k-2}, e \in E\}$.*

Based on the above definition, we observe the fact that hypertrees must be linear hypergraphs.

The *star* $H(x)$ centered in x is the family of hyperedges $(e_j)_{j\in J}$ containing x. A k-uniform chemical hypertree is said to be *hyperstar* S_n^k with n vertices if it has exactly one vertex of degree greater than two. For the linear k-uniform chemical hyperpath P_n^k with n vertices, the number of hyperedges is $m = \frac{n-1}{k-1}$.

In 2024, Shetty and Bhat [11] considered to generalize the idea of vertex degree-based topological indices from graphs to hypergraphs, and defined the Sombor index $SO(H)$ of a hypergraph H as

$$SO(H) = \sum_{e_i \in E} \sqrt{\sum_{u \in e_i} d_u^2},$$

where d_u is the degree of the vertex u of H. They gave the bounds for the Sombor index of hypergraphs and bipartite hypergraphs and obtained the extremal hypergraphs among the class of uniform, linear and general hypertrees. Wang et al. [12] obtained several upper and lower bounds of the Sombor index of uniform hypergraphs. Li et al. [7] obtained the extremal hypergraph with minimum Sombor index among uniform hypertrees and the corresponding value of minimum Sombor index. Furthermore, they also obtained the extremal hypergraph with maximum(minimum) Sombor index for uniform unicyclic hypergraphs and the corresponding values for maximum(minimum) Sombor index. Along this direction, we continue to focus on the Sombor index for k-uniform chemical hypergraphs. Unless otherwise specified, the hypergraphs studied in this paper are all simple and linear.

This paper is organized as follows. In Section 1, some necessary notations and concepts are presented. Then in the Section 2, we characterize the extremal hypergraph with the upper and lower bounds of Sombor index for k-uniform chemical hypergraphs with n vertices and give the corresponding value of Sombor index. Finally, in the Section 3, we characterize the extremal hypergraph with the upper bound of Sombor index for k-uniform chemical hypertrees with n vertices and give the corresponding value of Sombor index.

2 Upper and lower bounds for the Sombor index of k-uniform chemical hypergraphs

Let $\mathcal{CH}_n^k$ be the set of k-uniform chemical hypergraphs with n vertices and $H_n^k \in \mathcal{CH}_n^k$, $n_x(H_n^k)$ the number of vertices of degree x, denoted by n_x and $m_{x_1,x_2,\cdots,x_k}(H_n^k)$ the number of hyperedges of H_n^k containing k vertices of degrees $x_1, x_2, \cdots, x_k$ respectively, denoted by $m_{x_1,x_2,\cdots,x_k}$.

Clearly

$$n = n_1 + n_2 + n_3 + n_4, \tag{1}$$

and it is also well-known that the following relations hold

$$\begin{cases} n_1 = km_{1,1,\ldots,1,1} + (k-1)m_{1,1,\ldots,1,2} + (k-1)\, m_{1,1,\cdots,1,3} + \cdots \\ \qquad + m_{1,4,\ldots,4,4}, \\ 2n_2 = m_{1,\ldots,1,1,2} + 2m_{1,\ldots,1,2,2} + \cdots + m_{2,4,\ldots,4,4}, \\ 3n_3 = m_{1,\ldots,1,1,3} + 2m_{1,\ldots,1,3,3} + \cdots + m_{3,4,\ldots,4,4}, \\ 4n_4 = m_{1,\ldots,1,1,4} + m_{1,\ldots,1,2,4} + \cdots + km_{4,\ldots,4,4,4}. \end{cases} \tag{2}$$

Let

$$A = \left\{(x_1, x_2, \cdots x_k) \in N^k : 1 \le x_1 \le x_2 \le \cdots \le x_k \le 4\right\}.$$

It follows easily from (1) and (2) that

$$n = \sum_{(x_1,x_2,\cdots,x_k)\in A} \left(\sum_{i=1}^{k} \frac{1}{x_i}\right) m_{x_1,x_2,\cdots,x_k}. \tag{3}$$

Note that the expression SO is equivalent to

$$SO\left(H_n^k\right) = \sum_{(x_1,x_2,\cdots,x_k)\in A} m_{x_1,x_2,\cdots,x_k} \sqrt{\sum_{i=1}^{k} x_i^2}. \tag{4}$$

The next result gives the extremal chemical hypergraph with the maximum Sombor index of k-uniform chemical hypergraphs with n vertices, and give the corresponding value of Sombor index.

Theorem 4. *Let H_n^k be a k-uniform chemical hypergraph with n vertices. Then*

$$SO\left(H_n^k\right) \leq \frac{16\sqrt{k}}{k} n.$$

Equality occurs if and only if H is a 4-regular k-uniform hypergraph.

Proof. Let $B = \{(x_1, x_2, \cdots, x_k) \in A : (x_1, x_2, \cdots, x_k) \neq (4, 4, \cdots, 4)\}$. It is easy to check that

$$\sqrt{\sum_{i=1}^{k} x_i^2} - \frac{16\sqrt{k}}{k} \left(\sum_{i=1}^{k} \frac{1}{x_i}\right) < 0, \tag{5}$$

for all $(x_1, x_2, \cdots, x_k) \in B$. By (3), (4) and (5) we deduce that

$$\begin{aligned}
SO(H_n^k) &= 4m_{4,4,\ldots,4}\sqrt{k} + \sum_{(x_1,x_2,\ldots,x_k)\in B} m_{x_1,x_2,\ldots,x_k} \sqrt{\sum_{i=1}^{k} x_i^2} \\
&= \frac{16\sqrt{k}}{k} \left(n - \sum_{(x_1,x_2,\ldots,x_k)\in B} \left(\sum_{i=1}^{k} \frac{1}{x_i}\right) m_{x_1,x_2,\ldots,x_k}\right) \\
&\quad + \sum_{(x_1,x_2,\ldots,x_k)\in B} m_{x_1,x_2,\ldots,x_k} \sqrt{\sum_{i=1}^{k} x_i^2} \\
&= \sum_{(x_1,x_2,\ldots,x_k)\in B} \left(\sqrt{\sum_{i=1}^{k} x_i^2} - \frac{16\sqrt{k}}{k} \left(\sum_{i=1}^{k} \frac{1}{x_i}\right)\right) m_{x_1,x_2,\ldots,x_k} \\
&\quad + \frac{16\sqrt{k}}{k} n \\
&\leq \frac{16\sqrt{k}}{k} n.
\end{aligned} \tag{6}$$

If $SO\left(H_n^k\right) = \frac{16\sqrt{k}}{k} n$, then by (6),

$$\frac{16\sqrt{k}}{k} n + \sum_{(x_1,\cdots,x_k)\in B} \left(\sqrt{\sum_{i=1}^{k} x_i^2} - \frac{16\sqrt{k}}{k} \left(\sum_{i=1}^{k} \frac{1}{x_i}\right)\right) m_{x_1,\cdots,x_k} = \frac{16\sqrt{k}}{k} n,$$

and by (5), we conclude that $m_{x_1,x_2,\cdots,x_k} = 0$ for all $(x_1, x_2, \cdots, x_k) \in B$.

In other words, H_n^k is a 4-regular k-uniform hypergraph. Conversely, if H_n^k is a 4-regular k-uniform hypergraph, then $SO\left(H_n^k\right)=4\sqrt{k}m_{4,4,\cdots,4}=4\sqrt{k}\cdot\frac{4n}{k}=\frac{16\sqrt{k}}{k}n$. ■

We obtain the lower bounds for 3-uniform hypergraphs and completely characterized the extremal hypergraphs by classifying the vertex number n into three cases.

Theorem 5. *Let H_n^3 be a 3-uniform chemical hypergraphs with n vertices.*

1. *When $n\equiv 0\,(mod\ 3)$, then $SO\left(H_n^3\right)\geq\frac{\sqrt{3}}{3}n$, with equality holding if and only if $H_n^3\cong\frac{n}{3}P_3^3$.*
2. *When $n\equiv 1\,(mod\ 3)$, then $SO\left(H_n^3\right)\geq\frac{\sqrt{3}}{3}n+3\sqrt{11}-\frac{7\sqrt{3}}{3}$, with equality holding if and only if $H_n^3\cong\frac{n-7}{3}P_3^3\cup S_5^3$.*
3. *When $n\equiv 2\,(mod\ 3)$, then $SO\left(H_n^3\right)\geq\frac{n-5}{3}\sqrt{3}+2\sqrt{6}$, with equality holding if and only if $H_n^3\cong\frac{n-5}{3}P_3^3\cup P_5^3$.*

Proof. 1. When $n\equiv 0\,(mod\ 3)$ and let

$$C=\left\{(x_1,x_2,x_3)\in A:(x_1,x_2,x_3)\neq(1,1,1)\right\}.$$

Clearly

$$\sqrt{\sum_{i=1}^{3}x_i^2}-\frac{\sqrt{3}}{3}\left(\sum_{i=1}^{3}\frac{1}{x_i}\right)>0, \tag{7}$$

for all $(x_1,x_2,\cdots,x_k)\in C$. By (3), (4) and (7) we deduce that

$$\begin{aligned}SO\left(H_n^3\right)&=m_{1,1,1}\sqrt{3}+\sum_{(x_1,x_2,x_3)\in C}m_{x_1,x_2,x_3}\sqrt{\sum_{i=1}^{3}x_i^2}\\&=\frac{\sqrt{3}}{3}\left(n-\sum_{(x_1,x_2,x_k)\in C}\left(\sum_{i=1}^{3}\frac{1}{x_i}\right)m_{x_1,x_2,x_3}\right)\\&\quad+\sum_{(x_1,x_2,x_k)\in C}m_{x_1,x_2,x_3}\sqrt{\sum_{i=1}^{k}x_i^2}\end{aligned}$$

$$= \frac{\sqrt{3}}{3}n + \sum_{(x_1,x_2,x_3)\in C} \left(\sqrt{\sum_{i=1}^{3} x_i^2} - \frac{\sqrt{3}}{3} \left(\sum_{i=1}^{3} \frac{1}{x_i} \right) \right) m_{x_1,x_2,x_3} \tag{8}$$
$$\geq \frac{\sqrt{3}}{3}n.$$

If $SO\left(H_n^3\right) = \frac{\sqrt{3}}{3}n$, then by (8),

$$\frac{\sqrt{3}}{3}n + \sum_{(x_1,x_2,x_3)\in C} \left(\sqrt{\sum_{i=1}^{3} x_i^2} - \frac{\sqrt{3}}{3} \left(\sum_{i=1}^{3} \frac{1}{x_i} \right) \right) m_{x_1,x_2,x_3} = \frac{\sqrt{3}}{3}n,$$

and by (7), we conclude that $m_{x_1,x_2,x_3} = 0$ for all $(x_1, x_2, x_3) \in C$. Since n is divisible by 3, then clearly $H_n^3 \cong \frac{n}{3}P_3^3$. The converse is clear.
2. When $n \equiv 1\,(mod\ 3)$, we have $m_{1,1,1} \leq \frac{n-7}{3}$. Let $D_1 = \{(x_1, x_2, x_3) \in A : (x_1, x_2, x_3) \neq (1, 1, 1) \text{and} (x_1, x_2, x_3) \neq (1, 1, 3)\}$. It is easy to check that

$$\sum_{(x_1,x_2,x_3)\in D_1} \left[\sqrt{\sum_{i=1}^{3} x_i^2} - \frac{3\sqrt{11}}{7} \left(\sum_{i=1}^{3} \frac{1}{x_i} \right) \right] > 0 \tag{9}$$

for all $(x_1, x_2, x_3) \in D_1$. Now by (3), (4) and (9), it follows that

$$SO\left(H_n^3\right) = m_{1,1,1}\sqrt{3} + m_{1,1,3}\sqrt{11} + \sum_{(x_1,x_2,x_3)\in D_1} m_{x_1,x_2,x_3} \sqrt{\sum_{i=1}^{3} x_i^2}$$
$$= \left(\sqrt{3} - \frac{9\sqrt{11}}{7} \right) m_{1,1,1} + \frac{3\sqrt{11}}{7} n$$
$$+ \sum_{(x_1,x_2,x_3)\in D_1} \left(\sqrt{\sum_{i=1}^{3} x_i^2} - \frac{3\sqrt{11}}{7} \left(\sum_{i=1}^{3} \frac{1}{x_i} \right) \right) m_{x_1,x_2,x_3}$$
$$\geq \left(\sqrt{3} - \frac{9\sqrt{11}}{7} \right) m_{1,1,1} + \frac{3\sqrt{11}}{7} n$$
$$\geq \left(\sqrt{3} - \frac{9\sqrt{11}}{7} \right) \frac{n-7}{3} + \frac{3\sqrt{11}}{7} n \tag{10}$$
$$= \frac{\sqrt{3}}{3} n + 3\sqrt{11} - \frac{7\sqrt{3}}{3}.$$

If $\frac{\sqrt{3}}{3}n+3\sqrt{11}-\frac{7\sqrt{3}}{3}=SO\left(H_n^3\right)$, by (10), $m_{1,1,1}=\frac{n-7}{3}$ and $m_{x_1,x_2,x_3}=0$ for all $(x_1,x_2,x_3)\in D_1$. This clearly implies that $H_n^3\cong\frac{n-7}{3}P_3^3\cup S_5^3$. The converse is clear.

3. When $n\equiv 2\,(mod\ 3)$, we have $m_{1,1,1}\leq\frac{n-5}{3}$. Let $D_2=\{(x_1,x_2,x_3)\in A:(x_1,x_2,x_3)\neq(1,1,1)\text{and}(x_1,x_2,x_3)\neq(1,1,2)\}$.It is easy to check that

$$\sqrt{\sum_{i=1}^{3}x_i^2}-\frac{2\sqrt{6}}{5}\left(\sum_{i=1}^{3}\frac{1}{x_i}\right)>0, \tag{11}$$

for all $(x_1,x_2,x_3)\in D_2$. Now by (3), (4) and (11), it follows that

$$\begin{aligned}
SO\left(H_n^3\right) &= m_{1,1,1}\sqrt{3}+m_{1,1,2}\sqrt{5}+\sum_{(x_1,x_2,x_3)\in D_2}m_{x_1,x_2,x_3}\sqrt{\sum_{i=1}^{3}x_i^2}\\
&= \left(\sqrt{3}-\frac{6\sqrt{6}}{5}\right)m_{1,1,1}+\frac{2\sqrt{6}}{5}n\\
&\quad+\sum_{(x_1,x_2,x_3)\in D_2}\left(\sqrt{\sum_{i=1}^{3}x_i^2}-\frac{2\sqrt{6}}{5}\left(\sum_{i=1}^{3}\frac{1}{x_i}\right)\right)m_{x_1,x_2,x_3} \qquad (12)\\
&\geq \left(\sqrt{3}-\frac{6\sqrt{6}}{5}\right)m_{1,1,1}+\frac{2\sqrt{6}}{5}n\\
&\geq \left(\sqrt{3}-\frac{6\sqrt{6}}{5}\right)\frac{n-5}{3}+\frac{2\sqrt{6}}{5}n\\
&= \frac{n-5}{3}\sqrt{3}+2\sqrt{6}.
\end{aligned}$$

If $\frac{n-5}{3}\sqrt{3}+2\sqrt{6}=SO\left(H_n^3\right)$, by (12), $m_{1,1,1}=\frac{n-5}{3}$ and $m_{x_1,x_2,x_3}=0$ for all $(x_1,x_2,x_3)\in D_2$. This clearly implies that $H_n^3\cong\frac{n-5}{3}P_3^3\cup P_5^3$. The converse is clear. ■

Theorem 6. *Let H_n^k be a k-uniform chemical hypergraph with n vertices.*

1. *If n is divisible by k, then $SO\left(H_n^k\right)\geq\frac{\sqrt{k}}{k}n$. Equality occurs if and only if $H_n^k\cong\frac{n}{k}P_k^k$.*
2. *If n is not divisible by k. When $n\equiv k-1\,(mod\ k)$, $SO\left(H_n^k\right)\geq\frac{n-2k+1}{k}\sqrt{k}+2\sqrt{k+3}$. Equality occurs if and only $H_n^k\cong\frac{n-2k+1}{k}P_k^k\cup$*

P^k_{2k-1}.

Proof. 1. Assume that n is divisible by k and let

$$C_1 = \{(x_1, x_2, \cdots, x_k) \in A : (x_1, x_2, \cdots, x_k) \neq (1, 1, \cdots, 1)\}.$$

Clearly

$$\sqrt{\sum_{i=1}^{k} x_i^2} - \frac{\sqrt{k}}{k}\left(\sum_{i=1}^{k}\frac{1}{x_i}\right) > 0, \tag{13}$$

for all $(x_1, x_2, \cdots, x_k) \in C_1$. By (3), (4) and (13) we deduce that

$$\begin{aligned}
SO\left(H_n^k\right) &= m_{1,1,\cdots,1}\sqrt{k} + \sum_{(x_1,x_2,\cdots,x_k)\in C_1} m_{x_1,x_2,\cdots,x_k}\sqrt{\sum_{i=1}^{k} x_i^2} \\
&= \frac{\sqrt{k}}{k}\left(n - \sum_{(x_1,x_2,\cdots,x_k)\in C_1}\left(\sum_{i=1}^{k}\frac{1}{x_i}\right) m_{x_1,x_2,\cdots,x_k}\right) \\
&\quad + \sum_{(x_1,x_2,\cdots,x_k)\in C_1} m_{x_1,x_2,\cdots,x_k}\sqrt{\sum_{i=1}^{k} x_i^2} \\
&= \sum_{(x_1,x_2,\cdots,x_k)\in C_1}\left(\sqrt{\sum_{i=1}^{k} x_i^2} - \frac{\sqrt{k}}{k}\left(\sum_{i=1}^{k}\frac{1}{x_i}\right)\right) m_{x_1,x_2,\cdots,x_k} \\
&\quad + \frac{\sqrt{k}}{k} n \\
&\geq \frac{\sqrt{k}}{k} n.
\end{aligned} \tag{14}$$

If $SO\left(H_n^k\right) = \frac{\sqrt{k}}{k} n$, then by (14),

$$\frac{\sqrt{k}}{k} n + \sum_{(x_1,x_2,\cdots,x_k)\in C_1}\left(\sqrt{\sum_{i=1}^{k} x_i^2} - \frac{\sqrt{k}}{k}\left(\sum_{i=1}^{k}\frac{1}{x_i}\right)\right) m_{x_1,x_2,\cdots,x_k} = \frac{\sqrt{k}}{k} n,$$

and by (13), we conclude that $m_{x_1,x_2,\cdots,x_k} = 0$ for all $(x_1, x_2, \cdots, x_k) \in C_1$. Since n is divisible by k, then clearly $H_n^k \cong \frac{n}{k} P_k^k$. The converse is clear.

2. If n is not divisible by k. When $n \equiv k-1\,(mod\ k)$, Since H_n^k has no isolated vertices, $m_{1,1,\cdots,1} \leq \frac{n-2k+1}{k}$. Let

$$\begin{aligned} D_3 = \{&(x_1,x_2,\cdots,x_{k-1},x_k) \in A : (x_1,x_2,\cdots,x_{k-1},x_k) \neq (1,1,\cdots,1,1) \\ &\text{and}(x_1,x_2,\cdots,x_{k-1},x_k) \neq (1,1,\cdots,1,2)\}. \end{aligned}$$

It is easy to check that

$$\sqrt{\sum_{i=1}^{k} x_i^2} - \frac{2\sqrt{k+3}}{2k-1}\left(\sum_{i=1}^{k}\frac{1}{x_i}\right) > 0, \tag{15}$$

for all $(x_1,x_2,\cdots,x_{k-1},x_k) \in D_3$. Now by (3), (4) and (15), it follows that

$$\begin{aligned} SO\left(H_n^k\right) &= m_{1,1,\cdots,1,1}\sqrt{k} + m_{1,1,\cdots,1,2}\sqrt{k+3} \\ &\quad + \sum_{(x_1,x_2,\cdots,x_{k-1},x_k)\in D_3} m_{x_1,x_2,\cdots,x_{k-1},x_k}\sqrt{\sum_{i=1}^{k} x_i^2} \\ &= \left(\sqrt{k} - \frac{2k\sqrt{k+3}}{2k-1}\right) m_{1,1,\cdots,1,1} + \frac{2\sqrt{k+3}}{2k-1} n \\ &\quad + \sum_{(x_1,x_2,\cdots,x_k)\in D_3}\left(\sqrt{\sum_{i=1}^{k} x_i^2} - \frac{2\sqrt{k+3}}{2k-1}\left(\sum_{i=1}^{k}\frac{1}{x_i}\right)\right) m_{x_1,x_2,\cdots,x_k} \\ &\geq \left(\sqrt{k} - \frac{2k\sqrt{k+3}}{2k-1}\right) m_{1,1,\cdots,1,1} + \frac{2\sqrt{k+3}}{2k-1} n \\ &\geq \left(\sqrt{k} - \frac{2k\sqrt{k+3}}{2k-1}\right) \frac{n-2k+1}{k} + \frac{2\sqrt{k+3}}{2k-1} n \\ &= \frac{n-2k+1}{k}\sqrt{k} + 2\sqrt{k+3}. \end{aligned} \tag{16}$$

If $\frac{n-2k+1}{k}\sqrt{k} + 2\sqrt{k+3} = SO\left(H_n^k\right)$, by (16), $m_{1,1,\cdots,1,1} = \frac{n-2k+1}{k}$ and $m_{x_1,x_2,\cdots,x_{k-1},x_k} = 0$ for all $(x_1,x_2,\cdots,x_{k-1},x_k) \in D_3$. This clearly implies that $H_n^k \cong \frac{n-2k+1}{k} P_k^k \cup P_{2k-1}^k$. The converse is clear. ■

3 Upper bound for the Sombor index of k-uniform chemical hypertrees

S. Shetty et al. [11] established the upper and lower bounds for k-uniform chemical hypertrees with given number of hyperedges and characterized the corresponding extremal hypertrees.

Lemma 1. *[11] Let T_n^k be a k-uniform chemical hypertree with m hyperedges. Then $2\sqrt{k+3}+(m-2)\sqrt{k+6} \leq SO\left(T_n^k\right) \leq m\sqrt{km^2+1}$, with equality holds if and only if T_n^k is linear k-uniform hyperpath (lower bound) or T_n^k is isomorphic to the sunflower $S(m,k,k+1)$ (upper bound).*

Let $\mathcal{CT}_n^k$ be the set of k-uniform chemical hypertrees with n vertices. By Lemma 3.1, the k-uniform chemical hypertree with the lower bound of Sombor index in $\mathcal{CT}_n^k$ is k-uniform chemical hyperpath P_n^k. Now, we obtain the upper bound for the Sombor index of k-uniform chemical hypertrees in $\mathcal{CT}_n^k$. Note that if $T_n^k \in \mathcal{CT}_n^k$, $m_{1,1,\cdots,1} = m_{1,1,\cdots,1}\left(T_n^k\right) = 0$.

We have derived the formula for the Sombor index of k-uniform chemical hypertrees.

Lemma 2. *Let $T_n^k \in \mathcal{CT}_n^k$ with $n \geq 2k-1$, $P = \{(x,y) : (1,\cdots,1,x,y) \in N^k, 1 \leq x \leq y \leq 4\}$. Then*

$$SO\left(T_n^k\right) = \frac{2\sqrt{k+15}+\sqrt{k+30}}{3(k-1)}n + \frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3(k-1)} + \sum_{(x,y)\in P} f(x,y) m_{1,\cdots,1,x,y}, \tag{17}$$

where

$$f(x,y) = \sqrt{k-2+x^2+y^2} + \frac{4\sqrt{k+30}-4\sqrt{k+15}}{3}\frac{(k-2)xy+x+y}{xy} - \frac{(4k-3)\sqrt{k+30}-(4k-6)\sqrt{k+15}}{3}.$$

Proof. For any $T_n^k \in \mathcal{CT}_n^k$ with $n \geq 2k-1$, the following relation holds:

$$\sum_{(x,y)\in P} m_{1,1\cdots,1,x,y} = \frac{n-1}{k-1}. \tag{18}$$

By (3) and (18), we have:

$$(4k-3)m_{1,\ldots,1,1,4}+(4k-6)m_{1,\ldots,1,4,4} = 4n-\sum_{(x,y)\in P_1} 4\Big(\sum_{i=1}^{k}\frac{1}{x_i}\Big)m_{1,\ldots,1,x,y},$$

$$m_{1,\ldots,1,1,4}+m_{1,\ldots,1,4,4} = n-\sum_{(x,y)\in P_1} m_{1,\ldots,1,x,y},$$

where $P_1 = \{(x,y)\in P : (x,y)\neq(1,1)\,,(x,y)\neq(1,4)\,,(x,y)\neq(4,4)\}$.

From previous relations we obtain the following expressions for $m_{1,\cdots,1,1,4}$ and $m_{1,\cdots,1,4,4}$:

$$3m_{1,\cdots,1,1,4} = \frac{2n}{k-1}+\frac{4k-6}{k-1}-\sum_{(x,y)\in P_1}\left(4\left(\sum_{i=1}^{k}\frac{1}{x_i}\right)-4k-6\right)m_{1,\cdots,1,x,y},$$

$$3m_{1,\cdots,1,4,4} = \frac{n}{k-1}-\frac{4k-3}{k-1}-\sum_{(x,y)\in P_1}\left(4k-3-4\left(\sum_{i=1}^{k}\frac{1}{x_i}\right)\right)m_{1,\cdots,1,x,y}.$$

The Sombor index of T_n^k is

$$\begin{aligned}SO(T_n^k) &= m_{1,\cdots,1,1,4}\sqrt{k+15}+m_{1,\cdots,1,4,4}\sqrt{k+30}\\ &\quad+\sum_{(x,y)\in P_1} m_{1,\cdots,1,x,y}\sqrt{k-2+x^2+y^2}\\ &= \frac{2\sqrt{k+15}+\sqrt{k+30}}{3(k-1)}n \quad +\frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3(k-1)}\\ &\quad+\sum_{(x,y)\in P_1} f\,(x,y)\,m_{1,\cdots,1,x,y},\end{aligned}$$

where

$$\begin{aligned}f\,(x,y) &= \sqrt{k-2+x^2+y^2}+\frac{4\sqrt{k+30}-4\sqrt{k+15}}{3}\,\frac{(k-2)\,xy+x+y}{xy}\\ &\quad-\frac{(4k-3)\sqrt{k+30}-(4k-6)\sqrt{k+15}}{3}.\end{aligned}$$

Since $f(1,4) = f(4,4) = 0$ and $m_{1,1\cdots,1,1} = 0$, we obtain the result. ■

Remark. When $k = 2$, the hypergraph is a graph, and the inequality for $f(x,y)$ is given that

$$f(2,2) < f(1,2) < f(2,3) < f(2,4) < 0 = f(1,4) = f(4,4),$$
$$f(2,3) < f(3,3) < f(1,3) < f(3,4) < 0 = f(1,4) = f(4,4),$$
$$f(2,2) < 2f(2,4),$$
$$f(3,3) < 2f(3,4).$$

When $k \geq 3$, we obtain inequalities similar to those mentioned above, as follows:

$$f(2,2) < f(2,3) < f(1,2) < f(2,4) < 0 = f(1,4) = f(4,4), \quad (19)$$
$$f(2,3) < f(3,3) < f(1,3) < f(3,4) < 0 = f(1,4) = f(4,4), \quad (20)$$
$$f(2,2) < 2f(2,4), \quad (21)$$
$$f(3,3) < 2f(3,4). \quad (22)$$

The upper bound for k-uniform chemical hypertrees are given as follows.

Theorem 7. *Let $T_n^k \in \mathcal{CT}_n^k$ with $n \geq 2k-1$. Then*

$$SO\left(T_n^k\right) \leq \frac{2\sqrt{k+15}+\sqrt{k+30}}{3(k-1)} n + \frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3(k-1)}. \quad (23)$$

Equality occurs if and only if $n_2\left(T_n^k\right) = n_3\left(T_n^k\right) = 0$.

Proof. From (19) and (20), $f(x,y) \leq 0$ for all $(x,y) \in P$, then by (17) in Lemma 2, we obtain

$$SO\left(T_n^k\right) \leq \frac{2\sqrt{k+15}+\sqrt{k+30}}{3(k-1)} n + \frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3(k-1)}.$$

If $SO\left(T_n^k\right) = \frac{2\sqrt{k+15}+\sqrt{k+30}}{3(k-1)} n + \frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3(k-1)}$, we conclude that $m_{1,\cdots,1,x,y} = 0$ for all $(x,y) \in P_1$ and this occurs if and only if T_n^k has no vertices of degree 2 or 3. Conversely, if T_n^k has no vertices of degree 2 or 3, by (17) and the fact that $f(1,4) = f(4,4) = 0$ and $m_{1,1\cdots,1,1} = 0$, we obtain

$$SO\left(T_n^k\right) = \frac{2\sqrt{k+15}+\sqrt{k+30}}{3(k-1)}n + \frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3(k-1)} + \sum_{(x,y)\in P_1} f(x,y)\, m_{1,\cdots,1,x,y}$$
$$= \frac{2\sqrt{k+15}+\sqrt{k+30}}{3(k-1)}n + \frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3(k-1)}.$$

■

Let n be a positive integer and consider the following subsets of $\mathcal{CT}_n^k$:

$$C_{00}(n) = \left\{T_n^k \in \mathcal{CT}_n^k \ : \ n_2\left(T_n^k\right) = n_3\left(T_n^k\right) = 0\right\},$$
$$C_{10}(n) = \left\{T_n^k \in \mathcal{CT}_n^k \ : \ n_2\left(T_n^k\right) = 1, n_3\left(T_n^k\right) = 0\right\},$$
$$C_{01}(n) = \left\{T_n^k \in \mathcal{CT}_n^k \ : \ n_2\left(T_n^k\right) = 0, n_3\left(T_n^k\right) = 1\right\}.$$

In k-uniform chemical hypertrees with n vertices, we established the structural properties of k-uniform chemical hypertrees.

Lemma 3. *Let n be a positive integer. Then*

1. *For $n \geq 2k-1$, $\frac{1}{k-1}n + \frac{k-2}{k-1} \equiv 0\,(mod\ 3)$ if and only if $C_{10}(n) \neq \emptyset$;*
2. *For $n \geq 3k-2$, $\frac{1}{k-1}n + \frac{k-2}{k-1} \equiv 1\,(mod\ 3)$ if and only if $C_{01}(n) \neq \emptyset$;*
3. *For $n \geq 4k-3$, $\frac{1}{k-1}n + \frac{k-2}{k-1} \equiv 2\,(mod\ 3)$ if and only if $C_{00}(n) \neq \emptyset$.*

Proof. 1. We can define recursively the linear k-uniform chemical hypertrees with n vertices in Fig. 1.

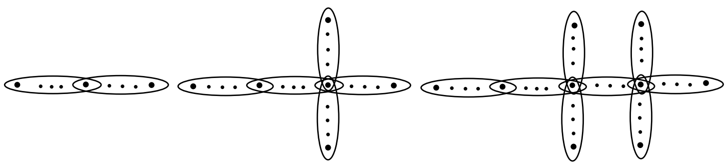

Figure 1. *k-uniform chemical hypertree in $C_{10}(n)$ when $\frac{1}{k-1}n + \frac{k-2}{k-1} \equiv 0\,(mod\ 3)$*

Hence we can construct a linear k-uniform chemical hypertree in $C_{10}(n)$ for each $\frac{1}{k-1}n + \frac{k-2}{k-1} \equiv 0\,(mod\ 3)$. Conversely, assume that $U \in C_{10}(n)$ has degree sequence $(n_1, 1, 0, n_4)$. The following relation is well known:

$$n_1 = n_3 + 2n_4 + \frac{(k-2)(n-1)}{k-1} + 2. \tag{24}$$

Then by (1) and (24), $n = n_1 + 1 + n_4$ and $n_1 = 2n_4 + \frac{(k-2)(n-1)}{k-1} + 2$, which implies $n = 3n_4 + \frac{(k-2)(n-1)}{k-1} + 3$. Hence, $\frac{1}{k-1}n + \frac{k-2}{k-1} \equiv 0\,(mod\ 3)$.
2. We can define recursively the linear k-uniform chemical hypertrees with n vertices in Fig. 2.

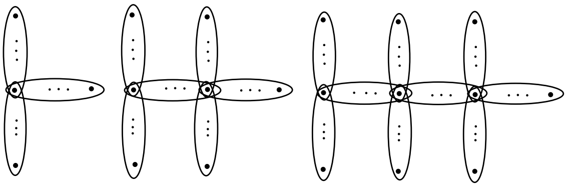

Figure 2. *k-uniform chemical hypertree in $C_{01}(n)$ when* $\frac{1}{k-1}n + \frac{k-2}{k-1} \equiv 1\,(mod\ 3)$

Consequently, there is a linear k-uniform chemical hypertree in $C_{01}(n)$ for each $\frac{1}{k-1}n + \frac{k-2}{k-1} \equiv 1\,(mod\ 3)$. Conversely, assume that $U \in C_{01}(n)$ has degree sequence $(n_1, 0, 1, n_4)$. Then by (1) and (24), $n = n_1 + 1 + n_4$ and $n_1 = 2n_4 + \frac{(k-2)(n-1)}{k-1} + 3$, which implies $n = 3n_4 + \frac{(k-2)(n-1)}{k-1} + 4$. Hence, $\frac{1}{k-1}n + \frac{k-2}{k-1} \equiv 1\,(mod\ 3)$.
3. We can define recursively the linear k-uniform chemical hypertrees with n vertices in Fig. 3.

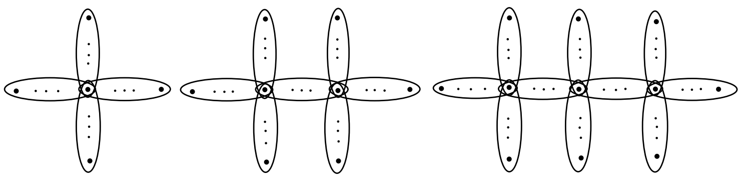

Figure 3. *k-uniform chemical hypertree in $C_{00}(n)$ when* $\frac{1}{k-1}n + \frac{k-2}{k-1} \equiv 2\,(mod\ 3)$

Note that there is a linear k-uniform chemical hypertree in $C_{00}(n)$ for each $\frac{1}{k-1}n+\frac{k-2}{k-1}\equiv 2\,(mod\ 3)$. Conversely, assume that $U\in C_{00}(n)$ has degree sequence $(n_1,0,0,n_4)$. Then by (1) and (24), $n=n_1+n_4$ and $n_1=2n_4+\frac{(k-2)(n-1)}{k-1}+2$, which implies $n=3n_4+\frac{(k-2)(n-1)}{k-1}+2$. Hence, $\frac{1}{k-1}n+\frac{k-2}{k-1}\equiv 2\,(mod\ 3)$. ■

We now characterize the extremal chemical hypertrees with the upper bound of Sombor index for k-uniform chemical hypertrees in $\mathcal{CT}_n^k$.

Theorem 8. *Let n be a positive integer. Then, among all hypertrees in $T_n^k\in\mathcal{CT}_n^k$, the maximal value of Sombor index is attained in:*

1. *$W\in C_{00}(n)$ if $\frac{1}{k-1}n+\frac{k-2}{k-1}\equiv 2\,(mod\ 3)$ and $n\geq 4k-3$;*
2. *$U\in C_{10}(n)$ such that $\frac{1}{k-1}n+\frac{k-2}{k-1}\equiv 0\,(mod\ 3)$ and $n\geq 8k-7$;*
3. *$V\in C_{01}(n)$ such that $m_{1,1\cdots,1,3}(V)=0$ if $\frac{1}{k-1}n+\frac{k-2}{k-1}\equiv 1\,(mod\ 3)$ and $n\geq 12k-11$.*

Proof. 1. Note that Sombor index is constant in $C_{00}(n)$ since for any $W\in C_{00}(n)$, $SO\left(T_n^k\right)=\frac{2\sqrt{k+15}+\sqrt{k+30}}{3(k-1)}n+\frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3(k-1)}$. By Theorem 7 we are done. The hypergraphs in $C_{00}(n)$ are depicted in Fig. 4.

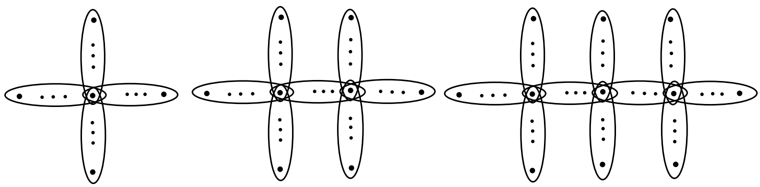

Figure 4. *k-uniform chemical hypertrees in C_{00}*

2. If $\frac{1}{k-1}n+\frac{k-2}{k-1}\equiv 0\,(mod\ 3)$, then $C_{00}(n)=\varnothing$ and $C_{01}(n)=\varnothing$. By (2) (17), (19), (20), and (21) we have

$$SO\left(T_n^k\right) \le \frac{2\sqrt{k+15}+\sqrt{k+30}}{3\left(k-1\right)}n + \frac{\left(4k-6\right)\sqrt{k+15}-\left(4k-3\right)\sqrt{k+30}}{3\left(k-1\right)}$$
$$+ f\left(1,2\right) m_{1,\cdots,1,1,2} + f\left(2,2\right) m_{1,\cdots,1,2,2} + f\left(2,3\right) m_{1,\cdots,1,2,3}$$
$$+ f\left(2,4\right) m_{1,\cdots,1,2,4}$$
$$\le \frac{2\sqrt{k+15}+\sqrt{k+30}}{3\left(k-1\right)}n + \frac{\left(4k-6\right)\sqrt{k+15}-\left(4k-3\right)\sqrt{k+30}}{3\left(k-1\right)}$$
$$+ f\left(2,4\right)\left(m_{1,\cdots,1,1,2} + 2m_{1,\cdots,1,2,2} + m_{1,\cdots,1,2,3} + m_{1,\cdots,1,2,4}\right)$$
$$= \frac{2\sqrt{k+15}+\sqrt{k+30}}{3\left(k-1\right)}n + \frac{\left(4k-6\right)\sqrt{k+15}-\left(4k-3\right)\sqrt{k+30}}{3\left(k-1\right)}$$
$$+ 2n_2\left(T\right) f\left(2,4\right).$$

If $n_2\left(T_n^k\right) = 0$, then

$$SO\left(T_n^k\right) < \frac{2\sqrt{k+15}+\sqrt{k+30}}{3\left(k-1\right)}n + \frac{\left(4k-6\right)\sqrt{k+15}-\left(4k-3\right)\sqrt{k+30}}{3\left(k-1\right)},$$

since the equality only occurs if $T_n^k \in C_{00}\left(n\right)$ and $C_{00}\left(n\right) = \varnothing$.
If $n_2\left(T_n^k\right) \ge 1$, then

$$SO\left(T_n^k\right) \le \frac{2\sqrt{k+15}+\sqrt{k+30}}{3\left(k-1\right)}n + \frac{\left(4k-6\right)\sqrt{k+15}-\left(4k-3\right)\sqrt{k+30}}{3\left(k-1\right)}$$
$$+ 2n_2\left(T\right) f\left(2,4\right)$$
$$\le \frac{2\sqrt{k+15}+\sqrt{k+30}}{3\left(k-1\right)}n + \frac{\left(4k-6\right)\sqrt{k+15}-\left(4k-3\right)\sqrt{k+30}}{3\left(k-1\right)}$$
$$+ 2f\left(2,4\right).$$

The equality in the previous relation occurs if and only if $m_{1,\cdots,1,2,4} = 2$ and $m_{1,\cdots,1,1,2} = m_{1,\cdots,1,1,3} = m_{1,\cdots,1,2,2} = m_{1,\cdots,1,2,3} = m_{1,\cdots,1,3,3} = m_{1,\cdots,1,3,4} = 0$. This implies $n_2\left(T_n^k\right) = 1$ and $n_3\left(T_n^k\right) = 0$. Then, if $\frac{1}{k-1}n + \frac{k-2}{k-1} \equiv 0\,(mod\ 3)$ and $n \ge 8k-7$, then the maximal value of Sombor index over $\mathcal{CT}_n^k$ is attained at $U \in C_{10}\left(n\right)$ such that $m_{1,\cdots,1,1,2}\left(U\right) = 0$. The hypergraphs in C_{10} with $m_{1,\cdots,1,1,2} = 0$ are depicted in Fig. 5.

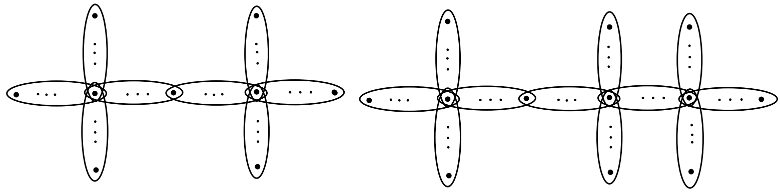

Figure 5. *k-uniform chemical hypertree in* C_{10} *with* $m_{1,\cdots,1,1,2}=0$

3. If $\frac{1}{k-1}n+\frac{k-2}{k-1}\equiv 1\,(mod\ 3)$, then $C_{00}\,(n)=\varnothing$ and $C_{10}\,(n)=\varnothing$. By (2), (17), (19), (20) and (21) we have

$$\begin{aligned}SO\left(T_n^k\right) \leq\ & \frac{2\sqrt{k+15}+\sqrt{k+30}}{3\,(k-1)}n+\frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3\,(k-1)}\\ &+f\,(1,3)\,m_{1,\cdots,1,1,3}+f\,(2,3)\,m_{1,\cdots,1,2,3}+f\,(3,3)\,m_{1,\cdots,1,3,3}\\ &+f\,(3,4)\,m_{1,\cdots,1,3,4}\end{aligned}$$

$$\begin{aligned}&\leq \frac{2\sqrt{k+15}+\sqrt{k+30}}{3\,(k-1)}n+\frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3\,(k-1)}\\ &\quad+f\,(3,4)\left(m_{1,\cdots,1,1,3}+m_{1,\cdots,1,2,3}+2m_{1,\cdots,1,3,3}+m_{1,\cdots,1,3,4}\right)\\ &= \frac{2\sqrt{k+15}+\sqrt{k+30}}{3\,(k-1)}n+\frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3\,(k-1)}\\ &\quad+3n_3\,(T)\,f\,(3,4)\,.\end{aligned}$$

If $n_3\left(T_n^k\right)=0$, then

$$SO\left(T_n^k\right)<\frac{2\sqrt{k+15}+\sqrt{k+30}}{3\,(k-1)}n+\frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3\,(k-1)},$$

since the equality only occurs if $T_n^k\in C_{00}\,(n)$ and $C_{00}\,(n)=\varnothing$.
If $n_3\left(T_n^k\right)\geq 1$, then

$$\begin{aligned}SO\left(T_n^k\right) \leq\ & \frac{2\sqrt{k+15}+\sqrt{k+30}}{3\,(k-1)}n+\frac{(4k-6)\sqrt{k+15}-(4k-3)\sqrt{k+30}}{3\,(k-1)}\\ &+3n_3\left(T_n^k\right)f\,(3,4)\end{aligned}$$

$$\leq \frac{2\sqrt{k+15}+\sqrt{k+30}}{3\,(k-1)}n+\frac{(4k-6)\,\sqrt{k+15}-(4k-3)\,\sqrt{k+30}}{3\,(k-1)} + 3f\,(3,4)\,.$$

The equality in the previous relation occurs if and only if $m_{1,\cdots,1,3,4}=3$ and $m_{1,\cdots,1,1,2}=m_{1,\cdots,1,1,3}=m_{1,\cdots,1,2,2}=m_{1,\cdots,1,2,3}=m_{1,\cdots,1,2,4}=m_{1,\cdots,1,3,3}=0$. This implies $n_2\left(T_n^k\right)=0$ and $n_3\left(T_n^k\right)=1$. Then, if $\frac{1}{k-1}n+\frac{k-2}{k-1}\equiv 1\,(mod\ 3)$ and $n\geq 12k-11$, then the maximal value of Sombor index over $\mathcal{CT}_n^k$ is attained at $V\in C_{01}\,(n)$ such that $m_{1,\cdots,1,1,3}=0$. The hypergraphs in C_{01} with $m_{1,\cdots,1,1,3}=0$ are depicted in Fig. 6. ■

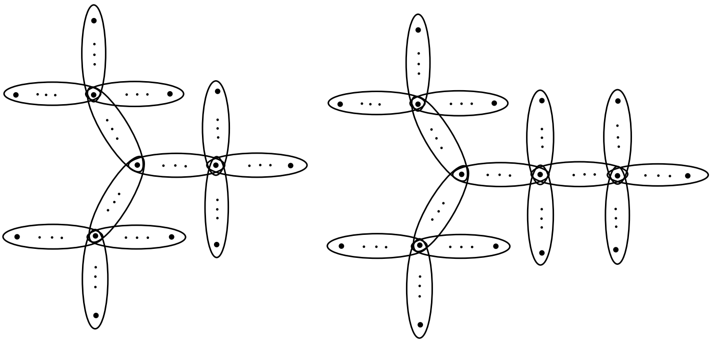

Figure 6. *k-uniform chemical hypertrees in C_{01} with $m_{1,\cdots,1,1,3}=0$*

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