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ORIGINAL PAPER

On a novel connectivity index

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Abstract We present a novel connectivity index for (molecular) graphs, called sum-connectivity index and give several basic properties for this index, especially lower and upper bounds in terms of graph (structural) invariants. It appears that this and the original Randić connectivity index that we call product-connectivity index are highly intercorrelated molecular descriptors, the value of the correlation coefficient being 0.991 for trees representing lower alkanes. We determine the unique tree with fixed numbers of vertices and pendant vertices with the minimum value of the sum-connectivity index, and trees with the minimum, second minimum and third minimum, and the maximum, second maximum and third maximum values of this index. Additionally, we discuss the properties of this novel connectivity index for a class of trees representing acyclic hydrocarbons.

Keywords Randić connectivity index · Sum-connectivity index · Product-connectivity index · Zagreb indices · Molecular graphs · Lower and upper bounds

1 Introduction

In 1975, Randić proposed a structural descriptor called branching index [1] that later became well-known Randić connectivity index, which is the most used molecular descriptor in QSPR and QSAR [e.g., 2–6]. The name connectivity index that replaced

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the original Randić term branching index has been suggested by Kier as stated by Randić [7]. The first paper in which the Randić connectivity index was used in QSAR appeared soon after the original publication, also in [8]. Mathematicians too exhibited considerable interest in the properties of the Randić connectivity index [e.g., 9–16].

The Randić connectivity index has also evolved into several variants [5–7,17], including the concept of overall connectivity by Bonchev [18], and even the semi-empirical formulation [5]. After Estrada introduced the edge-connectivity index [19], the Randić connectivity index was occasionally called the vertex-connectivity index [20,21]. Several people in view of the successful applications of the Randić connectivity index in QSPR and QSAR gave a physicochemical interpretation of this molecular descriptor [e.g., 4–6,22–25].

The Randić connectivity index has been extended as the general Randić connectivity index and general zeroth-order Randić connectivity index, and then the Zagreb indices appear to be the special cases of them [13,26]. The Zagreb indices have been introduced in 1972 in the report of Gutman and Trinajstić on the topological basis of the π-electron energy [27]—two terms appeared in the topological formula for the total π-energy of alternant hydrocarbons, which were in 1975 used by Gutman et al. [28] as branching indices, denoted by M_1 and M_2, and later employed as molecular descriptors in QSPR and QSAR [e.g., 29,30]. The name Zagreb indices instead of the term branching indices was first used by Balaban et al. [31]. Mathematical and computational properties of Zagreb indices have also been considered [e.g., 32–37]. In due course also emerged variants of the Zagreb indices [e.g., 38–40].

In this report, we give some basic properties, especially lower and upper bounds in terms of other graph invariants, of a novel variant of the connectivity index that we call the sum-connectivity index. We determine the unique tree with fixed numbers of vertices and pendant vertices with the minimum value of the sum-connectivity index, and trees with the minimum, second minimum and third minimum, and the maximum, second maximum and third maximum values of this index. We discuss the properties of the sum-connectivity index for molecular graphs representing hydrocarbons with emphasis on molecular trees. In our exposition we will use the terminology and apparatus of (chemical) graph theory [e.g., 41–43].

2 Definitions

For a simple graph G with vertex-set $V(G)$ and $v \in V(G)$, $\Gamma(v)$ denotes the set of its (first) neighbors in G and the degree of v is $d_v = |\Gamma(v)|$. The Randić connectivity index [1] $R = R(G)$ of G is defined as

$$R = R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-1/2}$$

where $E(G)$ is the edge-set of G.

A novel connectivity index $\chi = \chi(G)$, that we call the sum-connectivity index, is defined as

$$\chi = \chi(G) = \sum_{uv \in E(G)} (d_u + d_v)^{-1/2}.$$

Recall that the first Zagreb index $M_1 = M_1(G)$ and the second Zagreb index $M_2 = M_2(G)$ [27,28,32,33,38] of the graph G are given by

$$M_1 = M_1(G) = \sum_{u \in V(G)} d_u^2,$$

$$M_2 = M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

Note that the first Zagreb index may also be given as

$$M_1 = M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

because

$$\sum_{uv \in E(G)} (d_u + d_v) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in \Gamma(u)} d_u + \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in \Gamma(v)} d_v = \sum_{u \in V(G)} d_u^2.$$

We call $R(G)$ and $\chi(G)$ the product-connectivity index and the sum-connectivity index of G, respectively. These two molecular descriptors are highly intercorrelated quantities; for example, the value of the correlation coefficient is 0.99088 for 136 trees representing the lower alkanes taken from Ivanciuc et al. [44].

Let P_n and S_n be respectively the path and the star with n vertices. Let K_n be the complete graph with n vertices. Note that a path is a tree with two vertices of degree one and all the other vertices of degree two, a star is a tree with one vertex being adjacent to all the other vertices and a complete graph is a simple graph in which every pair of distinct vertices is adjacent. A bipartite graph G is a graph whose vertex-set V can be partitioned into two subsets V_1 and V_2 such that every edge of G connects a vertex in V_1 and a vertex in V_2. The graph $G \cup H$ denotes the vertex-disjoint union of graphs G and H. Let $\overline{G}$ be the complement of the graph G. The complement $\overline{G}$ of G is a simple graph which has $V(G)$ as its vertex-set and in which two vertices are adjacent if and only if they are not adjacent in G. A pendant vertex is a vertex of degree one.

3 Bounds for the sum-connectivity indices of general graphs

Proposition 1 *Let G be a graph without pendant vertices. Then $\chi(G) \geq R(G)$ with equality if and only if all non-isolated vertices have degree two.*

Proof For any edge uv of G, $d_u d_v \geq 2(d_u + d_v) - 4 \geq d_u + d_v$ and thus $\chi(G) \geq R(G)$ with equality if and only if $d_u d_v = d_u + d_v$ for every edge uv of G, i.e., $d_u = d_v = 2$ for every edge uv of G. □

Note that Proposition 1 is not true for graphs with pendant vertices. For the path P_n with $n \geq 3$, $\chi(P_n) = \frac{2}{\sqrt{3}} + \frac{n-3}{2} < R(P_n) = \frac{2}{\sqrt{2}} + \frac{n-3}{2}$.

Proposition 2 *Let G be a graph with $m \geq 1$ edges. Then*

$$\chi(G) \geq \frac{m\sqrt{m}}{\sqrt{M_1(G)}}$$

with equality if and only if $d_u + d_v$ is a constant for every edge uv of G.

Proof Since $x^{-1/2}$ is a strictly convex function for $x > 0$, we have

$$\sum_{uv \in E(G)} \frac{(d_u + d_v)^{-1/2}}{m} \geq \left(\sum_{uv \in E(G)} \frac{d_u + d_v}{m} \right)^{-1/2}$$

and then

$$\chi(G) \geq m \left(\sum_{uv \in E(G)} \frac{d_u + d_v}{m} \right)^{-1/2} = \frac{m\sqrt{m}}{\sqrt{\sum\limits_{uv \in E(G)} (d_u + d_v)}} = \frac{m\sqrt{m}}{\sqrt{M_1(G)}}$$

with equality if and only if $d_u + d_v$ is a constant for every edge uv of G. □

There are lots of upper bounds for the first Zagreb index [45–48], from which we may deduce lower bounds for χ by Proposition 2. We give such examples in (a)–(d).

(a) Let G be a graph with m edges. For any edge uv of G, $d_u + d_v \leq m + 1$ with equality if and only if every other edge of G is adjacent to the edge uv. Then

$$M_1(G) \leq \sum_{uv \in E(G)} (m + 1) = m(m + 1),$$

and thus

$$\chi(G) \geq \frac{m}{\sqrt{m + 1}}$$

with equality when G has no isolated vertices if and only if G has no two independent edges, i.e., $G = S_{m+1}$ or K_3. (This also follows directly from the definition of χ.)

(b) Let G be a graph with n vertices and $m \geq 1$ edges. Then [45,46]

$$M_1(G) \leq m\left(\frac{2m}{n-1} + n - 2\right)$$

with equality if and only if $G = K_n$, S_n or $K_1 \cup K_{n-1}$, and thus

$$\chi(G) \geq \frac{\sqrt{n-1}m}{\sqrt{2m + (n-1)(n-2)}}$$

with equality if and only if $G = K_n$, S_n or $K_1 \cup K_{n-1}$.

(c) Let G be a graph with n vertices, m edges, maximum degree Δ and minimum degree δ. Then [47]

$$M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta$$

with equality if and only if G has only two types of degrees Δ and δ, and thus

$$\chi(G) \geq \frac{m\sqrt{m}}{\sqrt{2m(\Delta + \delta) - n\Delta\delta}}$$

with equality if and only if one vertex has degree Δ and the other vertex has degree δ for every edge.

(d) Let G be a triangle- and a quadrangle-free graph. Then [48]

$$M_1(G) \leq n(n-1)$$

with equality if and only if G is S_n or a Moore graph of diameter 2, and thus

$$\chi(G) \geq \frac{m\sqrt{m}}{\sqrt{n(n-1)}}$$

with equality if and only if G is S_n or a Moore graph of diameter 2.

Bollobás and Erdös [9] showed that if G is a graph with n vertices containing no isolated vertices, then $R(G) \geq \sqrt{n-1}$ with equality if and only if $G = S_n$. For the index χ, we note $\chi(P_2 \cup P_2) = \sqrt{2} < \chi(S_4) = \frac{3}{2}$. As the following proposition shows, this is the only exception.

Proposition 3 *Let G be a graph with $n \geq 5$ vertices containing no isolated vertices. Then*

$$\chi(G) \geq \frac{n-1}{\sqrt{n}}$$

with equality if and only if $G = S_n$.

Proof First suppose that G is a connected graph. Let m be the number of edges of G. Then $m \geq n-1$. Obviously, $\frac{m}{\sqrt{m+1}}$ is increasing for $m \geq 1$. From item (a) above, $\chi(G) \geq \frac{m}{\sqrt{m+1}} \geq \frac{n-1}{\sqrt{n}}$ with equality if and only if $G = S_{m+1}$ and $m = n-1$, i.e., $G = S_n$.

Now suppose that G is disconnected with components G_i, $i = 1, 2, \ldots, k$ where $k \geq 2$. Let n_i be the number of vertices of G_i. Then $n_i \geq 2$, and $\sum_{i=1}^{k} n_i = n$ and

$$\chi(G) = \sum_{i=1}^{k} \chi(G_i) \geq \sum_{i=1}^{k} \frac{n_i - 1}{\sqrt{n_i}}.$$

If every n_i is equal to 2 for $i = 1, 2, \ldots, k$, then $\chi(G) \geq \sum_{i=1}^{k} \frac{n_i-1}{\sqrt{n_i}} = \frac{n}{2\sqrt{2}} > \frac{n-1}{\sqrt{n}}$ for $n \geq 6$. Suppose that at least one of n_i for $i = 1, 2, \ldots, k$ is at least 3, say $n_1 \geq 3$. For $l(x) = \frac{x-1}{\sqrt{x}}$ with $x \geq 1$, $l''(x) < 0$, and then $l(x) - l(x-2)$ is decreasing when $x \geq 3$, which implies that $\frac{n_1+n_2-1}{\sqrt{n_1+n_2}} - \frac{n_1+n_2-3}{\sqrt{n_1+n_2-2}} \leq \frac{4}{\sqrt{5}} - \frac{2}{\sqrt{3}} < \frac{1}{\sqrt{2}}$, and thus

$$\begin{aligned}
\frac{n_1-1}{\sqrt{n_1}} + \frac{n_2-1}{\sqrt{n_2}} &= \left(\sqrt{n_1} + \sqrt{n_2}\right)\left(1 - \frac{1}{\sqrt{n_1 n_2}}\right) \\
&\geq \left(\sqrt{n_1+n_2-2} + \sqrt{2}\right)\left(1 - \frac{1}{\sqrt{2(n_1+n_2-2)}}\right) \\
&= \frac{n_1+n_2-3}{\sqrt{n_1+n_2-2}} + \frac{1}{\sqrt{2}} > \frac{n_1+n_2-1}{\sqrt{n_1+n_2}}.
\end{aligned}$$

It follows that $\chi(G) > \frac{n_1+n_2+n_3-1}{\sqrt{n_1+n_2+n_3}} + \sum_{i=4}^{k} \frac{n_i-1}{\sqrt{n_i}} > \cdots > \frac{n_1+\cdots+n_k-1}{\sqrt{n_1+\cdots+n_k}} = \frac{n-1}{\sqrt{n}}$. The result follows. □

Proposition 4 *Let G be a triangle-free graph with n vertices and $m \geq 1$ edges. Then*

$$\chi(G) \geq \frac{m}{\sqrt{n}}$$

with equality if and only if G is a complete bipartite graph.

Proof For any edge uv of G, $d_u + d_v \leq n$ and thus

$$\chi(G) \geq \sum_{uv \in E(G)} \frac{1}{\sqrt{n}} = \frac{m}{\sqrt{n}}$$

with equality if and only if $d_u + d_v = n$ for every edge uv of G, i.e., G is a complete bipartite graph. □

Proposition 5 *Let G be a graph with n vertices. Then*

$$\chi(G) + \chi(\overline{G}) \geq \frac{n\sqrt{n-1}}{2\sqrt{2}}$$

with equality if and only if $G = K_n$ *or* $\overline{G} = K_n$.

Proof Let m and $\overline{m}$ be respectively the numbers of edges of G and $\overline{G}$. Then

$$\begin{aligned}\chi(G) + \chi(\overline{G}) &= \sum_{uv \in E(G)} (d_u + d_v)^{-1/2} + \sum_{uv \in E(\overline{G})} (n - 1 - d_u + n - 1 - d_v)^{-1/2} \\ &\geq m\,(2n-2)^{-1/2} + \overline{m}\,(2n-2)^{-1/2} \\ &= (m + \overline{m})\,\frac{1}{\sqrt{2(n-1)}} = \frac{n\sqrt{n-1}}{2\sqrt{2}}\end{aligned}$$

with equality if and only if either $d_u = d_v = n - 1$ for every edge $uv \in E(G)$ or $E(G) = \emptyset$, i.e., $G = K_n$ or $\overline{G} = K_n$. □

Let G be a graph with m edges. A trivial upper bound for $\chi(G)$ is $\chi(G) \leq \frac{m}{\sqrt{2}}$ with equality if and only if G consists of m copies of K_2 and arbitrary number of isolated vertices.

Proposition 6 *Let* G *be a graph with* n *vertices and* $m \geq 1$ *edges. Then* $\chi(G) < \sqrt{\frac{nm}{2}}$.

Proof By the Cauchy-Schwarz inequality, $\sum_{u \in V(G)} \sqrt{d_u} \leq \sqrt{n \sum_{u \in V(G)} d_u}$ and then it is easily seen that

$$\begin{aligned}\chi(G) &= \frac{1}{2} \sum_{\substack{u \in V(G) \\ d_u > 0}} \sum_{v \in \Gamma(u)} \frac{1}{\sqrt{d_u + d_v}} < \frac{1}{2} \sum_{\substack{u \in V(G) \\ d_u > 0}} \sum_{v \in \Gamma(u)} \frac{1}{\sqrt{d_u}} \\ &= \frac{1}{2} \sum_{\substack{u \in V(G) \\ d_u > 0}} \frac{1}{\sqrt{d_u}} \sum_{v \in \Gamma(u)} 1 = \frac{1}{2} \sum_{\substack{u \in V(G) \\ d_u > 0}} \frac{d_u}{\sqrt{d_u}} \\ &= \frac{1}{2} \sum_{u \in V(G)} \sqrt{d_u} \leq \frac{1}{2} \sqrt{n \sum_{u \in V(G)} d_u} = \sqrt{\frac{nm}{2}}.\end{aligned}$$

This proves the result. □

Recall that [49] if G is a graph with $n \geq 2$ vertices, then $R(G) \leq \frac{n}{2}$ with equality if and only if every component is a regular graph with at least two vertices. However, the range of the sum-connectivity indices are much wider than the product-connectivity index, as we can see from the following proposition.

Proposition 7 *Let* G *be a graph with* n *vertices and maximum degree* Δ. *Then*

$$\chi(G) \leq \frac{n\sqrt{\Delta}}{2\sqrt{2}}$$

with equality if and only if G is regular of degree Δ. *Furthermore,*

$$\chi(G) \leq \frac{n\sqrt{n-1}}{2\sqrt{2}}$$

with equality if and only if $G = K_n$.

Proof It is trivial for $\Delta = 0, 1$. Suppose that $\Delta \geq 2$. We may also assume that G has no isolated vertices. Denote by x_{ij} the number of edges of G that connect vertices of degree i and j, where $1 \leq i \leq j \leq \Delta$. Note that $x_{ij} = x_{ji}$. Then $\chi(G) = \sum_{1\leq i\leq j\leq\Delta} \frac{x_{ij}}{\sqrt{i+j}}$. Denote by n_i the number of vertices of G with degree i. Then $\sum_{i=1}^{\Delta} n_i = n$ and $\sum_{j=1}^{\Delta} x_{ij} + x_{ii} = in_i$ for $i = 1, 2, \ldots, \Delta$. From these relations, we have $n_\Delta = n - \sum_{i=1}^{\Delta-1} n_i = n - \sum_{i=1}^{\Delta-1} \frac{1}{i} \left(\sum_{j=1}^{\Delta} x_{ij} + x_{ii}\right)$, $x_{\Delta\Delta} = \frac{1}{2}\left(\Delta n_\Delta - \sum_{j=1}^{\Delta-1} x_{\Delta j}\right)$, and $x_{\Delta\Delta} = \frac{\Delta}{2}\left(n - \sum_{i=1}^{\Delta-1}\sum_{j=1}^{\Delta} \frac{x_{ij}}{i} - \sum_{i=1}^{\Delta-1} \frac{x_{ii}}{i}\right) - \frac{1}{2}\sum_{j=1}^{\Delta-1} x_{\Delta j}$. It follows that

$$\begin{aligned}
\chi(G) &= \sum_{\substack{1\leq i\leq j\leq\Delta \\ (i,j)\neq(\Delta,\Delta)}} \frac{x_{ij}}{\sqrt{i+j}} + \frac{x_{\Delta\Delta}}{\sqrt{2\Delta}} \\
&= \sum_{\substack{1\leq i\leq j\leq\Delta \\ (i,j)\neq(\Delta,\Delta)}} \frac{x_{ij}}{\sqrt{i+j}} + \frac{1}{\sqrt{2\Delta}}\left[\frac{\Delta}{2}\left(n - \sum_{i=1}^{\Delta-1}\sum_{j=1}^{\Delta}\frac{x_{ij}}{i} - \sum_{i=1}^{\Delta-1}\frac{x_{ii}}{i}\right) - \frac{1}{2}\sum_{j=1}^{\Delta-1} x_{\Delta j}\right] \\
&= \frac{n\sqrt{\Delta}}{2\sqrt{2}} + \sum_{\substack{1\leq i\leq j\leq\Delta \\ (i,j)\neq(\Delta,\Delta)}} \frac{x_{ij}}{\sqrt{i+j}} - \frac{\sqrt{\Delta}}{2\sqrt{2}}\left(\sum_{i=1}^{\Delta-1}\sum_{j=1}^{\Delta}\frac{x_{ij}}{i} + \sum_{j=1}^{\Delta-1}\frac{x_{\Delta j}}{\Delta} + \sum_{i=1}^{\Delta-1}\frac{x_{ii}}{i}\right) \\
&= \frac{n\sqrt{\Delta}}{2\sqrt{2}} + \sum_{\substack{1\leq i\leq j\leq\Delta \\ (i,j)\neq(\Delta,\Delta)}} \frac{x_{ij}}{\sqrt{i+j}} - \frac{\sqrt{\Delta}}{2\sqrt{2}} \sum_{\substack{1\leq i\leq j\leq\Delta \\ (i,j)\neq(\Delta,\Delta)}} \left(\frac{1}{i}+\frac{1}{j}\right)x_{ij} \\
&= \frac{n\sqrt{\Delta}}{2\sqrt{2}} + \sum_{\substack{1\leq i\leq j\leq\Delta \\ (i,j)\neq(\Delta,\Delta)}} \left[\frac{1}{\sqrt{i+j}} - \frac{\sqrt{\Delta}}{2\sqrt{2}}\left(\frac{1}{i}+\frac{1}{j}\right)\right]x_{ij}.
\end{aligned}$$

For $1 \leq i \leq j \leq \Delta$ and $(i, j) \neq (\Delta, \Delta)$, it is easily seen that

$$\frac{\sqrt{\Delta}}{2\sqrt{2}}\sqrt{i+j}\left(\frac{1}{i}+\frac{1}{j}\right) \geq \frac{\sqrt{\Delta}}{2\sqrt{2}}\sqrt{i+j}\frac{2}{\sqrt{ij}} = \frac{\sqrt{\Delta}}{\sqrt{2}}\sqrt{\frac{1}{i}+\frac{1}{j}} > \frac{\sqrt{\Delta}}{\sqrt{2}}\sqrt{\frac{2}{\Delta}} = 1$$

which implies that $\frac{1}{\sqrt{i+j}} - \frac{\sqrt{\Delta}}{2\sqrt{2}}\left(\frac{1}{i}+\frac{1}{j}\right) < 0$. Therefore, $\chi(G) \leq \frac{n\sqrt{\Delta}}{2\sqrt{2}}$ with equality if and only if $x_{ij} = 0$ for $1 \leq i \leq j \leq \Delta$ and $(i, j) \neq (\Delta, \Delta)$, i.e., all vertices are of degree Δ. This proves the first part of the proposition. The second part of the proposition follows from the first part. □

Let G be a graph with $n \geq 2$ vertices. From Proposition 7, we have $\chi(G)+\chi(\overline{G}) < \frac{n\sqrt{n-1}}{\sqrt{2}}$.

4 The sum-connectivity indices of trees

By Proposition 3, the star is the unique n-vertex tree with the minimum sum-connectivity index. In the following we go further. We need two lemmas.

Lemma 1 *Let x be a positive real number.*

(i) The function $f(x) = \frac{1}{\sqrt{x+2}} + \frac{x-2}{\sqrt{x+1}} - \frac{x-2}{\sqrt{x}}$ is decreasing for $x > 0$.
(ii) The function $g(x) = \frac{1}{\sqrt{x+2}} + \frac{x-1}{\sqrt{x+1}} + \frac{1}{\sqrt{3}} + \frac{n-x-2}{2}$ is decreasing for $2 \leq x \leq n-2$.
(iii) The function $h(x) = \frac{x}{\sqrt{x+2}} + \frac{n-x-2}{\sqrt{n-x}} + \frac{1}{\sqrt{n}}$ is decreasing for $\frac{n-2}{2} \leq x \leq n-3$.

Proof (i) Let $f_1(x) = \frac{1}{\sqrt{x+1}} + \frac{x-2}{\sqrt{x}}$. Then $f(x) = f_1(x+1) - f_1(x)$. Since $f_1{}''(x) = \frac{3}{4}(x+1)^{-5/2} - \frac{1}{4}x^{-3/2} - \frac{3}{2}x^{-5/2} < 0$, $f_1{}'(x)$ is decreasing with x, and then $f'(x) = f_1'(x+1) - f_1'(x) < 0$, implying that $f(x)$ is decreasing with x.
(ii) It is easily seen that $g(x+1)-g(x) = \left(\frac{1}{\sqrt{x+3}} - \frac{1}{2}\right) + (x-1)\left(\frac{1}{\sqrt{x+2}} - \frac{1}{\sqrt{x+1}}\right) < 0$, which implies that $g(x)$ is decreasing with x.
(iii) Note that $h(x) = \sqrt{x+2} + \sqrt{n-x} - \frac{2}{\sqrt{x+2}} - \frac{2}{\sqrt{n-x}} + \frac{1}{\sqrt{n}}$. Let $a = \sqrt{x+2}$ and $b = \sqrt{n-x}$. Then $a^2 + b^2 = n+2$. Thus $h(x) = a + b - \frac{2}{a} - \frac{2}{b} + \frac{1}{\sqrt{n}} = (a+b)\left(1 - \frac{2}{ab}\right) + \frac{1}{\sqrt{n}}$. Let $a_1 = \sqrt{x+3}$ and $b_1 = \sqrt{n-x-1}$. Then $a_1 b_1 < ab$, $a_1 + b_1 < a + b$, and thus $h(x+1) - h(x) = (a_1+b_1)\left(1 - \frac{2}{a_1 b_1}\right) - (a+b)\left(1 - \frac{2}{ab}\right) < 0$, implying that $h(x)$ is decreasing with x for $\frac{n-2}{2} \leq x \leq n-3$. □

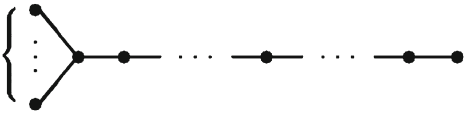
For integers n, p with $2 \leq p \leq n-1$, let $S_{n,p}$ be the tree formed by attaching $p-1$ pendant vertices to an end vertex of the path P_{n-p+1}, see Fig. 1. Evidently, $S_{n,2} = P_n$ and $S_{n,n-1} = S_n$.

Lemma 2 *Let T be a tree with n vertices and p pendant vertices, where $2 \leq p \leq n-2$. If u is a pendant vertex being adjacent to the vertex v, then*

$$\chi(T) - \chi(T-u) \geq \frac{p-2}{\sqrt{p+1}} + \frac{1}{\sqrt{p+2}} - \frac{p-2}{\sqrt{p}}$$

with equality if and only if $T = S_{n,p}$ and $d_v = p$.

Fig. 1 The tree $S_{n,p}$



Proof Note that $p \le n-2$. Then $\Gamma(v)\backslash\{u\}$ contains some vertex of degree at least two. It is easily seen that

$$\begin{aligned}\chi(T)-\chi(T-u) &= \frac{1}{\sqrt{d_v+1}} - \sum_{w\in\Gamma(v)\backslash\{u\}}\left(\frac{1}{\sqrt{d_v-1+d_w}}-\frac{1}{\sqrt{d_v+d_w}}\right)\\ &\ge \frac{1}{\sqrt{d_v+1}} - \left(\frac{1}{\sqrt{d_v-1+2}}-\frac{1}{\sqrt{d_v+2}}\right)\\ &\quad -(d_v-2)\left(\frac{1}{\sqrt{d_v-1+1}}-\frac{1}{\sqrt{d_v+1}}\right)\\ &= \frac{1}{\sqrt{d_v+2}}+\frac{d_v-2}{\sqrt{d_v+1}}-\frac{d_v-2}{\sqrt{d_v}}\end{aligned}$$

with equality if and only if of the d_v neighbors of v, one has degree two, and others are pendant vertices. Since $d_v \le p$, we have by Lemma 1 (i) that

$$\chi(T)-\chi(T-u) \ge \frac{1}{\sqrt{p+2}}+\frac{p-2}{\sqrt{p+1}}-\frac{p-2}{\sqrt{p}}$$

with equality if and only if of the $d_v = p$ neighbors of v, one has degree two, and others are pendant vertices, i.e., $T = S_{n,p}$ and $d_v = p$. □

The product-connectivity index for trees with given numbers of vertices and pendant vertices has been studied in [50].

Proposition 8 *Let T be a tree with n vertices and p pendant vertices, where $3 \le p \le n-2$. Then*

$$\chi(T) \ge \frac{1}{\sqrt{p+2}}+\frac{p-1}{\sqrt{p+1}}+\frac{1}{\sqrt{3}}+\frac{n-p-2}{2}$$

with equality if and only if $T = S_{n,p}$.

Proof We argue by induction on n. It is trivial for $n = 5$. Suppose that $n \ge 6$. Let u be a pendant vertex being adjacent to the vertex v. First suppose that $d_v = 2$. If $p = 3$, then such u and v always exist. Then the unique vertex w in $\Gamma(v)\backslash\{u\}$ has degree at least two, and thus

$$\chi(T)-\chi(T-u) = \frac{1}{\sqrt{d_w+2}}+\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{d_w+1}} \ge \frac{1}{\sqrt{2+2}}+\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{2+1}} = \frac{1}{2}$$

with equality if and only if $d_w = 2$. In this case $T-u$ possesses p pendant vertices. If $p = n-2$, then $T-u$ is a star, and thus $T = S_{n,n-2}$. If $p \le (n-1)-2$, then by

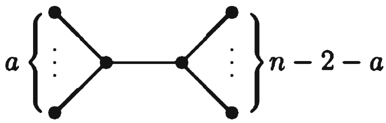


Fig. 2 The tree $T_{n,a}$

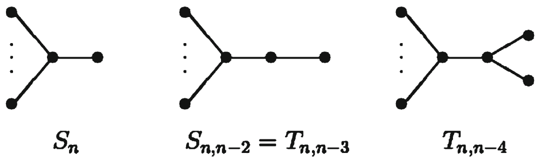


Fig. 3 The trees in Proposition 9

the induction hypothesis to $T-u$,

$$\chi(T) \geq \chi(T-u) + \frac{1}{2} \geq \frac{1}{\sqrt{p+2}} + \frac{p-1}{\sqrt{p+1}} + \frac{1}{\sqrt{3}} + \frac{n-p-2}{2}$$

with equality if and only if $T-u = S_{n-1,p}$ and $d_w = 2$, i.e., $T = S_{n,p}$.

Now suppose that $d_v \geq 3$ and $p > 3$. Then $T-u$ possesses $p-1$ pendant vertices. By Lemma 2 and the induction hypothesis to $T-u$,

$$\begin{aligned}\chi(T) &\geq \chi(T-u) + \frac{1}{\sqrt{p+2}} + \frac{p-2}{\sqrt{p+1}} - \frac{p-2}{\sqrt{p}} \\ &\geq \left(\frac{1}{\sqrt{p+1}} + \frac{p-2}{\sqrt{p}} + \frac{1}{\sqrt{3}} + \frac{n-p-2}{2}\right) + \frac{1}{\sqrt{p+2}} + \frac{p-2}{\sqrt{p+1}} - \frac{p-2}{\sqrt{p}} \\ &= \frac{1}{\sqrt{p+2}} + \frac{p-1}{\sqrt{p+1}} + \frac{1}{\sqrt{3}} + \frac{n-p-2}{2}\end{aligned}$$

with equality if and only if $T-u = S_{n-1,p-1}$ and $d_v = p$, i.e., $T = S_{n,p}$. □

Any n-vertex tree T with $n-2$ pendant vertices may be formed by attaching a and $n-2-a$ pendant vertices to the two vertices of the path P_2, respectively, for $\frac{n-2}{2} \leq a \leq n-3$, for which we denote by $T_{n,a}$, see Fig. 2. Evidently, $T_{n,n-3} = S_{n,n-2}$.

Proposition 9 $S_{n,n-1} = S_n$, $S_{n,n-2} = T_{n,n-3}$ *are respectively the unique n-vertex trees with the minimum and second minimum sum-connectivity indices* $\frac{n-1}{\sqrt{n}}$ *and* $\frac{n-3}{\sqrt{n-1}} + \frac{1}{\sqrt{n}} + \frac{1}{\sqrt{3}}$ *for* $n \geq 4$, *while* $T_{n,n-4}$ *is the unique n-vertex tree with the third minimum sum-connectivity index* $\frac{n-4}{\sqrt{n-2}} + \frac{1}{\sqrt{n}} + 1$ *for* $n \geq 6$ (Fig. 3).

Proof The first part follows from Propositions 3, 8 and Lemma 1 (ii). Let T be a tree with n vertices and p pendant vertices, where $2 \leq p \leq n-2$ and $n \geq 6$. If $p = n-2$, then T is of the form $T_{n,a}$ for some a with $\frac{n-2}{2} \leq a \leq n-3$, for which we have by Lemma 1 (iii) that

$$\chi(T_{n,a}) = h(a) = \frac{a}{\sqrt{a+2}} + \frac{n-a-2}{\sqrt{n-a}} + \frac{1}{\sqrt{n}}$$

is decreasing for $\frac{n-2}{2} \leq a \leq n-3$, and thus the sum-connectivity indices of n-vertex trees with $n-2$ pendant vertices may be ordered as

$$\chi\left(T_{n,n-3}\right) < \cdots < \chi\left(T_{n,\lceil (n-2)/2\rceil}\right).$$

On the other hand, if $p \leq n-3$, then by Proposition 8 and Lemma 1 (ii),

$$\chi(T) \geq g(n-3) = \frac{1}{\sqrt{n-1}} + \frac{n-4}{\sqrt{n-2}} + \frac{1}{\sqrt{3}} + \frac{1}{2} > \frac{n-4}{\sqrt{n-2}} + \frac{1}{\sqrt{n}} + 1 = \chi(T_{n,n-4}).$$

Thus, $T_{n,n-4}$ is the unique tree with the third minimum sum-connectivity index. □

We note that by Proposition 8 and Lemma 1 (ii), $S_{n,n-d+1}$ is the unique n-vertex tree of diameter d where $3 \leq d \leq n-2$ with the minimum sum-connectivity index.

In [49], the n-vertex trees with the maximum and second maximum product-connectivity indices have already been determined. Now we determine the n-vertex trees with the maximum, second maximum and third maximum sum-connectivity indices.

Proposition 10 *For $n \geq 4$, P_n is the unique n-vertex tree with the maximum sum-connectivity index $\frac{n-3}{2} + \frac{2}{\sqrt{3}}$, and for $n \geq 7$, the trees with a single vertex of degree three, adjacent to three vertices of degree two and without vertices of degree at least four are the unique n-vertex trees with the second maximum sum-connectivity index $\frac{n-7}{2} + \frac{3}{\sqrt{3}} + \frac{3}{\sqrt{5}}$, the trees with a single vertex of degree three, adjacent to two vertices of degree two and one vertex of degree one, and without vertices of degree at least four are the unique n-vertex trees with the third maximum sum-connectivity index $\frac{n-5}{2} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{5}}$.*

Proof Suppose that Q is a connected graph with at least two vertices. For $a \geq b \geq 1$, let G_1 be the graph obtained from Q by attaching two paths P_a and P_b to $u \in V(Q)$, and G_2 the graph obtained from Q by attaching a path P_{a+b} to u. Let d_1 be the degree of u in G_1, and d_x the degree of x in Q. If $a = 1$ and $b = 1$, then

$$\begin{aligned}\chi(G_2) - \chi(G_1) &= \left(\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{d_1+1}} + \sum_{xu \in E(Q)} \frac{1}{\sqrt{d_1 - 1 + d_x}}\right) - \left(\frac{2}{\sqrt{d_1+1}} + \sum_{xu \in E(Q)} \frac{1}{\sqrt{d_1 + d_x}}\right)\\ &= \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{d_1+1}}\right) + \sum_{xu \in E(Q)} \left(\frac{1}{\sqrt{d_1 - 1 + d_x}} - \frac{1}{\sqrt{d_1 + d_x}}\right) > 0.\end{aligned}$$

If $a \geq 2$ and $b = 1$, then

$$\chi(G_2) - \chi(G_1) = \left(\frac{1}{2} - \frac{1}{\sqrt{d_1+2}}\right) + \sum_{xu \in E(Q)} \left(\frac{1}{\sqrt{d_1 - 1 + d_x}} - \frac{1}{\sqrt{d_1 + d_x}}\right) > 0.$$

If $a \geq 2$ and $b \geq 2$, then as it is may be checked that $\frac{1}{\sqrt{d_1+1}} - \frac{2}{\sqrt{d_1+2}}$ is increasing for $\left(1 + \frac{1}{d_1+1}\right)^3 \leq 4$, and this is obvious for $d_1 \geq 3$, we have

$$\chi(G_2) - \chi(G_1) = \left(1 - \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{d_1+1}} - \frac{2}{\sqrt{d_1+2}}\right) + \sum_{xu \in E(Q)} \left(\frac{1}{\sqrt{d_1 - 1 + d_x}} - \frac{1}{\sqrt{d_1 + d_x}}\right)$$
$$\geq 1 - \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{d_1+1}} - \frac{2}{\sqrt{d_1+2}} \geq 1 - \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{3+1}} - \frac{2}{\sqrt{3+2}} > 0.$$

It follows that $\chi(G_1) < \chi(G_2)$.

Let T be an n-vertex tree with $n \geq 4$. If $T \neq P_n$, then by applying the above transformation to the tree T, we have $\chi(T) < \chi(P_n)$. Thus, P_n is the unique n-vertex tree with the maximum sum-connectivity index $\frac{n-3}{2} + \frac{2}{\sqrt{3}}$.

If the maximum degree of T is at least four, or the maximum degree is three and there are at least two vertices of degree three, then by applying the above transformation to the tree T, we find that there is an n-vertex tree T^* with exactly one vertex, say v of maximum degree three such that $\chi(T) < \chi(T^*)$. If the degrees of the neighbors of v are 1, 1 and 2, then $n \geq 5$, $\chi(T^*) = \frac{n-3}{2} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{5}}$. If the degrees of the neighbors of v are 1, 2 and 2, then $n \geq 6$, $\chi(T^*) = \frac{n-5}{2} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{5}}$. If the degrees of the neighbors of v are 2, 2 and 2, then $n \geq 7$, $\chi(T^*) = \frac{n-7}{2} + \frac{3}{\sqrt{3}} + \frac{3}{\sqrt{5}}$. For $n \geq 7$, $\frac{n-7}{2} + \frac{3}{\sqrt{3}} + \frac{3}{\sqrt{5}} > \frac{n-5}{2} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{5}} > \frac{n-3}{2} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{5}}$, and thus the trees with a single vertex of degree three, adjacent to three vertices of degree two and without vertices of degree at least four are the unique n-vertex trees with the second maximum sum-connectivity index $\frac{n-7}{2} + \frac{3}{\sqrt{3}} + \frac{3}{\sqrt{5}}$.

If there are at least two vertices of degree three in T, then by applying the above transformation to the tree T, we have either an n-vertex tree T^* with exactly one vertex of maximum degree three such that $\chi(T) < \chi(T^*) \leq \frac{n-5}{2} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{5}}$ or otherwise, an n-vertex tree T^* with exactly two vertices of maximum degree three, each is adjacent to two vertices of degree two and then $\chi(T) \leq \chi(T^*) = \frac{n-10}{2} + \frac{4}{\sqrt{3}} + \frac{4}{\sqrt{5}} + \frac{1}{\sqrt{6}}$ for $n \geq 10$ if they are adjacent, and each is adjacent to three vertices of degree two and then $\chi(T) \leq \chi(T^*) = \frac{n-11}{2} + \frac{4}{\sqrt{3}} + \frac{6}{\sqrt{5}}$ for $n \geq 11$ if they are not adjacent, and thus $\chi(T) < \frac{n-5}{2} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{5}}$. If the maximum degree of T is at least four, then by applying the above transformation to the tree T, we have either an n-vertex tree T^* with exactly one vertex of maximum degree three such that $\chi(T) < \chi(T^*) \leq \frac{n-5}{2} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{5}}$ or otherwise, an n-vertex tree T^* for $n \geq 9$ with exactly one vertex of maximum degree four, adjacent to four vertices of degree two, and without vertices of degree three such that $\chi(T) \leq \chi(T^*) = \frac{n-9}{2} + \frac{4}{\sqrt{6}} + \frac{4}{\sqrt{3}} < \frac{n-5}{2} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{5}}$. It follows that for $n \geq 7$, the trees with a single vertex of degree three, adjacent to two vertices of degree two and one vertex of degree one, and without vertices of degree at least four are the unique n-vertex trees with the third maximum sum-connectivity index $\frac{n-5}{2} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{5}}$. □

5 The sum-connectivity indices of molecular trees

In this section we deal with molecular graphs representing hydrocarbons [43,51] with emphasis on molecular trees [43]. Molecular graphs in this case are connected graphs with maximum degree at most four. We have already determined n-vertex trees with the maximum, second maximum and third maximum values of the sum-connectivity index for $n \geq 7$. All such trees are molecular trees (actually trees with degree at most three). This leads us to think about what happens for n-vertex molecular trees with small sum-connectivity indices.

Gutman et al. [52] determined molecular trees with the minimum, second minimum and third minimum, and the maximum, second maximum and third maximum product-connectivity indices. This was extended to general molecular graphs with $n \geq 5$ vertices and m edges, $n-1 \leq m \leq 2n$, in [53,54]. Denote by x_{ij} the number of edges of G that connect vertices of degree i and j, where $1 \leq i \leq j \leq 4$. Gutman [53] deduced the following relations:

$$x_{14} = \frac{4n-2m}{3} - \frac{4}{3}x_{12} - \frac{10}{9}x_{13} - \frac{2}{3}x_{22} - \frac{4}{9}x_{23} - \frac{1}{3}x_{24} - \frac{2}{9}x_{33} - \frac{1}{9}x_{34},$$
$$x_{44} = \frac{5m-4n}{3} + \frac{1}{3}x_{12} + \frac{1}{9}x_{13} - \frac{1}{3}x_{22} - \frac{5}{9}x_{23} - \frac{2}{3}x_{24} - \frac{7}{9}x_{33} - \frac{8}{9}x_{34}.$$

Substituting these into $\chi(G) = \frac{x_{12}}{\sqrt{3}} + \frac{x_{13}}{2} + \frac{x_{14}}{\sqrt{5}} + \frac{x_{22}}{2} + \frac{x_{23}}{\sqrt{5}} + \frac{x_{24}}{\sqrt{6}} + \frac{x_{33}}{\sqrt{6}} + \frac{x_{34}}{\sqrt{7}} + \frac{x_{44}}{\sqrt{8}}$ to get

$$\begin{aligned}\chi(G) = {} & \frac{4n-2m}{3\sqrt{5}} + \frac{5m-4n}{3\sqrt{8}} + \left(\frac{1}{\sqrt{3}} - \frac{4}{3\sqrt{5}} + \frac{1}{3\sqrt{8}}\right)x_{12} \\ & + \left(\frac{1}{2} - \frac{10}{9\sqrt{5}} + \frac{1}{9\sqrt{8}}\right)x_{13} + \left(\frac{1}{2} - \frac{2}{3\sqrt{5}} - \frac{1}{3\sqrt{8}}\right)x_{22} \\ & + \left(\frac{1}{\sqrt{5}} - \frac{4}{9\sqrt{5}} - \frac{5}{9\sqrt{8}}\right)x_{23} + \left(\frac{1}{\sqrt{6}} - \frac{1}{3\sqrt{5}} - \frac{2}{3\sqrt{8}}\right)x_{24} \\ & + \left(\frac{1}{\sqrt{6}} - \frac{2}{9\sqrt{5}} - \frac{7}{9\sqrt{8}}\right)x_{33} + \left(\frac{1}{\sqrt{7}} - \frac{1}{9\sqrt{5}} - \frac{8}{9\sqrt{8}}\right)x_{34}\end{aligned}$$

with positive coefficients for $x_{12}, x_{13}, x_{22}, x_{23}, x_{24}, x_{33}, x_{34}$. Similarly, from [53]

$$x_{12} = 2(n-m) - \frac{2}{3}x_{13} - \frac{1}{2}x_{14} + \frac{1}{3}x_{23} + \frac{1}{2}x_{24} + \frac{2}{3}x_{33} + \frac{5}{6}x_{34} + x_{44},$$
$$x_{22} = 3m - 2n - \frac{1}{3}x_{13} - \frac{1}{2}x_{14} - \frac{4}{3}x_{23} - \frac{3}{2}x_{24} - \frac{5}{3}x_{33} - \frac{11}{6}x_{34} - 2x_{44},$$

we have

$$
\begin{aligned}
\chi(G) = {} & \frac{2(n-m)}{\sqrt{3}} + \frac{3m-2n}{2} - \left(\frac{2}{3\sqrt{3}} + \frac{1}{6} - \frac{1}{2}\right) x_{13} \\
& - \left(\frac{1}{2\sqrt{3}} + \frac{1}{4} - \frac{1}{\sqrt{5}}\right) x_{14} - \left(\frac{2}{3} - \frac{1}{3\sqrt{3}} - \frac{1}{\sqrt{5}}\right) x_{23} \\
& - \left(\frac{3}{4} - \frac{1}{2\sqrt{3}} - \frac{1}{\sqrt{6}}\right) x_{24} - \left(\frac{5}{6} - \frac{2}{3\sqrt{3}} - \frac{1}{\sqrt{6}}\right) x_{33} \\
& - \left(\frac{11}{12} - \frac{5}{6\sqrt{3}} - \frac{1}{\sqrt{7}}\right) x_{34} - \left(1 - \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{8}}\right) x_{44}
\end{aligned}
$$

with negative coefficients for $x_{13}, x_{14}, x_{23}, x_{24}, x_{33}, x_{34}, x_{44}$. Thus we have:

Proposition 11 *Let G be a molecular graph with $n \geq 5$ vertices and m edges with $n-1 \leq m \leq 2n$. Then*

$$
\frac{4}{3}\left(\frac{1}{\sqrt{5}} - \frac{1}{\sqrt{8}}\right) n + \frac{1}{3}\left(\frac{5}{\sqrt{8}} - \frac{2}{\sqrt{5}}\right) m \leq \chi(G) \leq \left(\frac{2}{\sqrt{3}} - 1\right) n + \left(\frac{3}{2} - \frac{2}{\sqrt{3}}\right) m
$$

with left equality if and only if G has only vertices of degree one and four, and with right equality if and only if G is either a path or a cycle.

Now suppose that G is a tree, i.e., $m = n-1$. Let $F = \chi(G) - \left(\frac{2n+2}{3\sqrt{5}} + \frac{n-5}{3\sqrt{8}}\right)$. Then

$$
\begin{aligned}
F = {} & 0.098916605 x_{12} + 0.042379715 x_{13} + 0.084006473 x_{22} + 0.052033447 x_{23} \\
& + 0.023474832 x_{24} + 0.033881521 x_{33} + 0.014004393 x_{34}.
\end{aligned}
$$

Let n_i be the number of vertices of degree i, $i = 1, 2, 3, 4$. Then $2n_2 = x_{12} + 2x_{22} + x_{23} + x_{24}$, $3n_3 = x_{13} + x_{23} + 2x_{33} + x_{34}$. If $n_2 = 3$ and $n_3 = 0$, then

$$
\begin{aligned}
F &= 0.098916605 x_{12} + 0.084006473 x_{22} + 0.023474832 x_{24} \\
&\geq 0.023474832 \times 6 > 0.12.
\end{aligned}
$$

If $n_2 = 2$ and $n_3 = 1$, then

$$
F \geq 0.023474832 \times 4 + 0.014004393 \times 3 > 0.12.
$$

If $n_2 = 1$ and $n_3 = 2$, then

$$
F \geq 0.023474832 \times 2 + 0.014004393 \times 6 > 0.12.
$$

If $n_2 = 0$ and $n_3 = 3$, then

$$
F \geq 0.014004393 \times 9 > 0.12.
$$

In summary, if $n_2 + n_3 = 3$, then $F > 0.12$. If $n_2 + n_3 = s \geq 4$, the by similar argument it is easily checked that $F > 0.12$.

For $n_2 + n_3 = 0, 1, 2$, the graphical feasible combinations of $x_{12}, x_{13}, x_{22}, x_{23}, x_{24}, x_{33}, x_{34}$, for which $F < 0.12$ are listed below, where $n \equiv k(\text{mod}3)$:

n_2	n_3	Non-zero x_{ij}	F	k	n
0	0		0	2	$n \geq 5$
1	1	$x_{24} = 2, x_{34} = 3$	0.088963	2	$n \geq 17$
1	1	$x_{24} = 1, x_{34} = 2, x_{23} = 1$	0.103517	2	$n \geq 14$
0	1	$x_{34} = 3$	0.042013	1	$n \geq 13$
0	1	$x_{34} = 2,, x_{13} = 1$	0.070389	1	$n \geq 10$
2	0	$x_{24} = 4$	0.093899	1	$n \geq 13$
0	1	$x_{34} = 1, x_{13} = 2$	0.098764	1	$n \geq 7$
1	0	$x_{24} = 2$	0.046950	0	$n \geq 9$
0	2	$x_{34} = 6$	0.084026	0	$n \geq 21$
0	2	$x_{34} = 4, x_{33} = 1$	0.089899	0	$n \geq 18$
0	2	$x_{34} = 5, x_{13} = 1$	0.112402	0	$n \geq 18$

Let $MT(n)$ be the set of molecular trees with n vertices. From the results above (the smaller F, the smaller χ-value), we have:

Proposition 12 (i) *If* $n \equiv 2(\text{mod}3)$, *then among trees in* $MT(n)$,

(a) *for* $n \geq 5$ *the ones with only degrees one and four are the unique trees with the minimum sum-connectivity index* $\frac{2n+2}{3\sqrt{5}} + \frac{n-5}{3\sqrt{8}}$;

(b) *for* $n \geq 17$ *the ones with a single vertex of degree two adjacent to two vertices of degree four, and a single vertex of degree three adjacent to three vertices of degree four are the unique trees with the second minimum sum-connectivity index* $\frac{2n-1}{3\sqrt{5}} + \frac{n-17}{3\sqrt{8}} + \frac{2}{\sqrt{6}} + \frac{3}{\sqrt{7}}$;

(c) *for* $n \geq 17$ *the ones with a single vertex of degree two adjacent to a vertex of degree three and a vertex of degree four, and with a single vertex of degree three adjacent to one vertex of degree two and two vertices of degree four are the unique trees with the third minimum sum-connectivity index* $\frac{2n-1}{3\sqrt{5}} + \frac{n-14}{3\sqrt{8}} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{7}}$ (*when* $n = 14$, *there is only one such graph which achieves the second minimum sum-connectivity index*).

(ii) *If* $n \equiv 1(\text{mod}3)$, *then among trees in* $MT(n)$ *for* $n \geq 13$,

(a) *the ones with a single vertex of degree three adjacent to three vertices of degree four, and without vertices of degree two are the unique trees with the minimum sum-connectivity index* $\frac{2n+1}{3\sqrt{5}} + \frac{n-13}{3\sqrt{8}} + \frac{3}{\sqrt{7}}$;

(b) *the ones with a single vertex of degree three adjacent to one vertex of degree one and two vertices of degree four, and without vertices of degree two are the unique trees with the second minimum sum-connectivity index* $\frac{2n-2}{3\sqrt{5}} + \frac{n-10}{3\sqrt{8}} + \frac{1}{2} + \frac{2}{\sqrt{7}}$ (*when* $n = 10$, *there is only one such graph which achieves the minimum sum-connectivity index*);

(c) *the ones with two vertices of degree two adjacent to four vertices of degree four, and without vertices of degree three are the unique trees with the third minimum sum-connectivity index* $\frac{2n-2}{3\sqrt{5}} + \frac{n-13}{3\sqrt{8}} + \frac{4}{\sqrt{6}}$.

(iii) *If* $n \equiv 0(\mathrm{mod}\,3)$, *then among trees in* $MT(n)$,

(a) *for* $n \geq 9$ *the ones with a single vertex of degree two adjacent to two vertices of degree four, and without vertices of degree three are the unique trees with the minimum sum-connectivity index* $\frac{2n}{3\sqrt{5}} + \frac{n-9}{3\sqrt{8}} + \frac{2}{\sqrt{6}}$;

(b) *for* $n \geq 21$ *the ones with two vertices of degree three, each adjacent to three vertices of degree four, and without vertices of degree two are the unique trees with the second minimum sum-connectivity index* $\frac{2n}{3\sqrt{5}} + \frac{n-21}{3\sqrt{8}} + \frac{6}{\sqrt{7}}$;

(c) *for* $n \geq 21$ *the ones with two adjacent vertices of degree three adjacent to four vertices of degree four together, and without vertices of degree two are the unique trees with the third minimum sum-connectivity index* $\frac{2n}{3\sqrt{5}} + \frac{n-18}{3\sqrt{8}} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{7}}$ (*when* $n = 18$, *there is only one such graph which achieves the second minimum sum-connectivity index*).

From the discussion previous to the proposition, we also know that if $n \equiv 1$ (mod 3), then the trees with $n_2 = 0, n_3 = 1, x_{34} = 1, x_{13} = 2$ are the unique trees with the minimum sum-connectivity index when $n = 7$, the second minimum sum-connectivity index when $n = 10$, and the fourth minimum sum-connectivity index when $n \geq 13$; if $n \equiv 0$(mod 3), then when $n = 18$, the trees with $n_2 = 0, n_3 = 2, x_{34} = 5, x_{13} = 1$ are the unique trees with the third minimum sum-connectivity index. Therefore, we have determined the n-vertex molecular trees with the minimum sum-connectivity indices for $n = 5$ and $n \geq 7$, with the second minimum sum-connectivity indices for $n = 10$, 13, 14 and $n \geq 16$, with the third minimum sum-connectivity indices for $n = 13$, and $n \geq 16$.

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