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The σ-Irregularity of Chemical Trees

Žana Kovijanić Vukićević[a], Goran Popivoda[a,*], Saša Vujošević[b], Riste Škrekovski[c], Darko Dimitrov[d]

[a] *University of Montenegro, Faculty of Science and Mathematics, 81000 Podgorica, Montenegro*
[b] *University of Montenegro, Faculty of Economics, 81000 Podgorica, Montenegro*
[c] *University of Ljubljana, FMF, 1000 Ljubljana, Slovenia*
[d] *Faculty of Information Studies, 8000 Novo Mesto, Slovenia*

zanak@ucg.ac.me, goranp@ucg.ac.me, vsasa@ucg.ac.me, darko.dimitrov11@gmail.com

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Abstract

The σ-irregularity index is a variant of the well-established Albertson irregularity index. For a graph $G = (V, E)$ it is defined as $\sigma(G) = \sum_{uv \in E}(d(u) - d(v))^2$, where $d(u)$ and $d(v)$ denote the degrees of vertices u and v, respectively. In this note, we characterize chemical trees of a given order with maximal σ-irregularity index.

1 Introduction

The graphs considered here are simple and finite. The vertex and the edge sets of a graph G are denoted by $V(G)$ and $E(G)$. For a vertex $v \in V(G)$, we denote the degree of v in G by $d_G(v)$. The subscript G will be omitted if from the context it is clear which graph is considered.

A graph G is *regular* if all its vertices have the same degree, otherwise, it is *irregular*. A topological invariant $\mathrm{I}(G)$ of a graph G is called an

*Corresponding author.

irregularity measure or irregularity index, if $\mathrm{I}(G) \geq 0$ and $\mathrm{I}(G) = 0$ if and only if graph G is a regular graph.

Irregularity measures of graphs play a significant role in many scientific areas including chemistry and network theory [6–9, 13, 14]. One of the best-known and most thoroughly investigated irregularity measures is the *Albertson irregularity index* [4]:

$$\mathrm{irr}(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|.$$

For results on the Albertson irregularity index, we refer the readers to [1,2,4,9,11]. Trying to avoid the absolute value calculation in the Albertson irregularity index, one naturally arrived to the $\sigma(G)$-irregularity index:

$$\sigma(G) \quad = \quad \sum_{uv \in E(G)} (d_G(u) - d_G(v))^2.$$

The first results on σ-irregularity were obtained by Gutman et al. in [10]. In this seminal work, some fundamental properties of the σ-irregularity were presented including the relation

$$\sigma(G) = F(G) - 2M_2(G),$$

where

$$F(G) = \sum_{u \in V(G)} d(u)^3 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

are the *forgotten index* and the *second Zagreb index*, respectively.

The general graphs with maximal σ-irregularity were characterized in [3], where also some lower bounds on σ-irregularity were presented. The so-called inverse problem, which in this context means proving or disproving the existence of a graph whose σ-irregularity is equal to a given non-negative integer, was resolved in [3, 10].

For some classes of graphs, Réti [12] compared the σ-irregularity with a couple of well-known irregularity measures.

A connected k-cyclic graph is a connected graph of order n and size

$n + k - 1$. Recently, in [5], connected k-cyclic graphs with maximal σ-irregularity were determined.

A connected graph with the maximum degree at most 4 is called *a chemical graph*. A non-cyclic chemical graph is *a chemical tree*. Among the (chemical) trees in [3] it was shown that the path graph has the smallest σ-irregularity. Here we characterize the chemical trees with maximal σ-irregularity. Before we proceed with the characterization, we present in the next section the necessary additional notation and preliminaries.

1.1 Additional notation and preliminaries

Let T be a chemical tree. If $d(v) = k$, we name a vertex $v \in V(T)$ as k-vertex. Let us denote by n_i the number of vertices in T of degree i, $i = 1, 2, 3, 4$, and by m_{ij}, $1 \leq i \leq j \leq 4$, the number of edges in T with end-vertices of degrees i and j. If T is a chemical tree with maximal σ-irregularity, then T will be called extremal.

Let denote by $\mathcal{H}(n)$ the family of chemical trees of order n with all vertices of degree either 1 or 4. Note, this family is nonempty if and only if $n \equiv 2 \pmod 3$. For the trees of this family, we have: $n_1 = 2(n+1)/3$, $n_4 = (n-2)/3$, $m_{44} = (n-5)/3$.

An edge subdivision of an edge uv is a deletion of uv and an addition of two edges uw and wv along with the new vertex w. For any $T \in \mathcal{H}(n)$, integer $k \leq (n-5)/3$, and any k edges $e_1, \ldots, e_k$ of T whose both end-vertices are 4-vertices, we denote by $T^*(e_1, \ldots, e_k)$ the chemical tree obtained from T by subdividing the edges $e_1, \ldots, e_k$. We designate the family of all trees as T^* obtained this way with $\mathcal{H}(n, k)$.

The main result, which we prove in the next section is as follows.

Theorem 1. *Let T be a chemical tree of order $n \in [8, \infty) \setminus \{10\}$, and let $s = \max\{k \in \mathbb{N}_0 \,|\, 4k \leq n - 5$ and $n - 2 - k \equiv 0 \pmod 3\}$. Then,*

$$\sigma(T) \leq 6n + 2s + 6.$$

The equality holds if and only if $T \in \mathcal{H}(n - s, s)$.

As an immediate corollary of Theorem 1, a characterization of chemical trees with maximal σ-irregularity follows.

Corollary 1. *Let T be a chemical tree with maximal σ-irregularity of order $n \in [8, \infty) \setminus \{10\}$. Then, $T \in \mathcal{H}(n - n_2, n_2)$, where the number of vertices of T with degree 2 is uniquely determined by $n_2 = \max\{k \in \mathbb{N}_0 \,|\, 4k \leq n-5$ and $n-2-k \equiv 0 \pmod{3}\}$. The numbers of the remaining vertices of T, which are of degree 1 and 4, are $n_1 = 2(n - n_2 + 1)/3$ and $n_4 = (n - n_2 - 2)/3$, respectively.*

An illustration of chemical trees with maximal σ-irregularity that satisfy Corollary 1 and are of order $8, 9, 11, 12$, and 13 is given in Figure 1, while chemical trees with maximal σ-irregularity that satisfy Corollary 1 and are of order $14, \dots, 26$ are depicted in Figure 2. Observe that for a given $n \geq 14$, the chemical trees with maximal σ-irregularity are not unique. An example in Figure 3 shows all three non-isomorphic chemical trees of order 15 with maximal σ-irregularity.

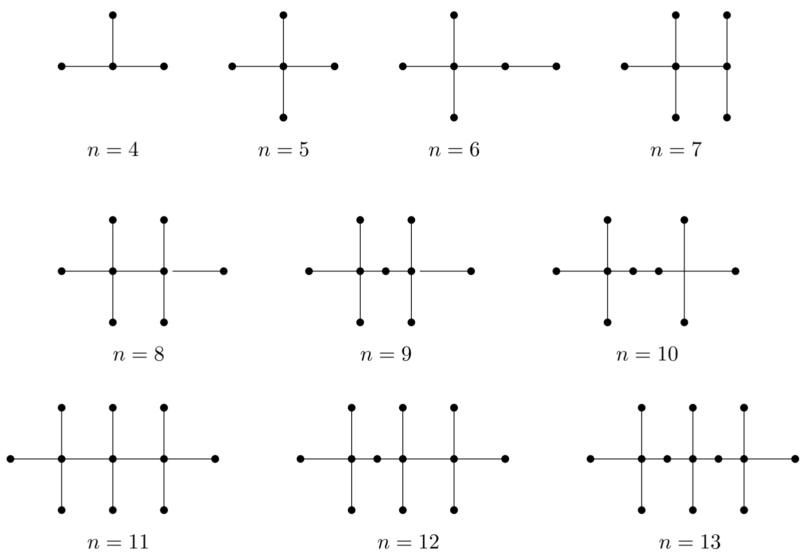

Figure 1. Extremal chemical trees of order $4 \leq n \leq 13$ obtained by a computer-based search.

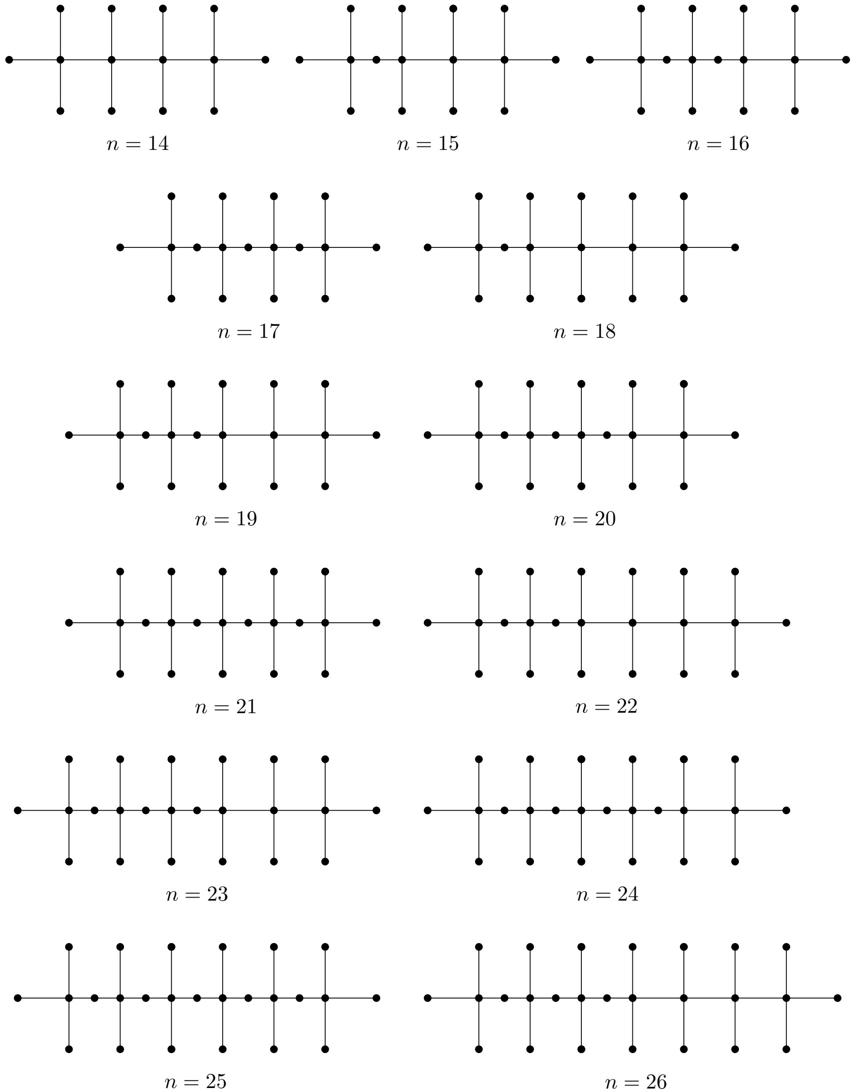

Figure 2. Extremal chemical trees of order $14 \leq n \leq 26$.

The following transformation will be frequently used in the rest of the paper. Let T be a chemical tree, $uv \in E(T)$ and $w \in V(T)$ such that $d(w) < 4$, $w \neq u, v$, and $uw \notin E(T)$. By T' we denote the chemical tree

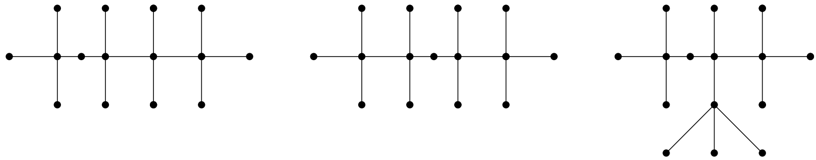

Figure 3. All non-isomorphic extremal chemical trees of order 15. They all satisfy Corollary 1, and therefore, have the same number of vertices of degree 1, 2, and 4.

obtained from T by deleting the edge uv and by adding the edge uw, i.e., $T' = T - uv + uw$. We denote this transformation by $[uv \xrightarrow{u} w]$.

2 Results

In this section, we first prove some auxiliary results needed for the proof of Theorem 1. The proofs of these results (Lemmas 1-3) will be derived for chemical trees of order $n \geq 14$. The extremal chemical trees with $4 \leq n \leq 13$ vertices can be easily computed by a computer-based search, and they are shown in Figure 1. The extremal trees with less than 4 vertices are self-evident and are omitted here.

Lemma 1. *Let T be an extremal chemical tree. Then $m_{12} = 0$.*

Proof. Firstly, we prove the following properties:

(i) there is no path uvw in T such that $d(u) = 1$, $d(v) = d(w) = 2$;

(ii) there is no path uvw in T such that $d(u) = 1$, $d(v) = 2$ and $d(w) = 3$;

(iii) if T has a path uvw such that $d(u) = 1$, $d(v) = 2$ and $d(w) = 4$, then v is the unique 2-vertex of T, i.e., $n_2 = 1$, and there is no 3-vertex in T, i.e., $n_3 = 0$.

We proceed by the assumption that $m_{12} \neq 0$ and obtain a contradiction to the extremality of T.

(i) Assume that there is a such path uvw in T with $d(u) = 1$, and $d(v) = d(w) = 2$. Let $x \in V(T)$ be a neighbor of w, different from v, and let T' be the chemical tree obtained by applying the transformation

$[uv \xrightarrow{u} w]$. Then,

$$\sigma(T') - \sigma(T) = 4 + 4 + (d(x) - 3)^2 - 1 - (d(x) - 2)^2 = 12 - 2d(x) > 0,$$

since $d(x) \leq 4$. It follows that T is not extremal, which contradicts the initial assumption.

(*ii*) Again, assume the opposite, that there is a path uvw in T such that $d(u) = 1$, $d(v) = 2$, and $d(w) = 3$. Let x, y be the neighbors of w, different from v. Denote by T' the chemical tree obtained by $[uv \xrightarrow{u} w]$ transformation of T. Then,

$$\begin{aligned}\sigma(T') - \sigma(T) &= 9 + 9 + (d(x) - 4)^2 + (d(y) - 4)^2 \\ &\quad - 2 - (d(x) - 3)^2 - (d(y) - 3)^2 \\ &= 30 - 2d(x) - 2d(y) > 0,\end{aligned}$$

since $d(x), d(y) \leq 4$. Thus, T is not extremal, which leads to a contradiction.

(*iii*) Let us prove the first part of the claim. Assume that there is a path uvw in T such that $d(u) = 1$, $d(v) = 2$ and $d(w) = 4$, and there exists a vertex $a \neq v$ of degree 2. Let x, y be the neighbors of a. Applying the transformation $[uv \xrightarrow{u} a]$ on T, we obtain the chemical tree T'. We have that

$$\begin{aligned}\sigma(T') - \sigma(T) &= 4 + 9 + (d(x) - 3)^2 + (d(y) - 3)^2 \\ &\quad - 1 - 4 - (d(x) - 2)^2 - (d(y) - 2)^2 \\ &= 18 - 2d(x) - 2d(y) > 0,\end{aligned}$$

since $d(x), d(y) \leq 4$, that is, T is not extremal.

To prove the second part of the claim, suppose that there exists a vertex a of degree 3 in T and let x, y, z be the neighbors of a. Let T' be the chemical tree obtained by $[uv \xrightarrow{u} a]$ transformation of T. Then,

$$\begin{aligned}\sigma(T') - \sigma(T) &= 9 + 9 + (d(x) - 4)^2 + (d(y) - 4)^2 + (d(z) - 4)^2 \\ &\quad - 1 - 4 - (d(x) - 3)^2 - (d(y) - 3)^2 - (d(z) - 3)^2\end{aligned}$$

$$= 34 - 2d(x) - 2d(y) - 2d(z) > 0,$$

since $d(x), d(y), d(z) \leq 4$, so T is not extremal.

From assertions (i), (ii), and (iii), we may conclude that if T is an extremal chemical tree with $m_{12} \neq 0$, then T has only one 2-vertex and all other vertices of T are of degree 1 or 4. Denote by u the pendant neighbor of this unique 2-vertex and by w its non-pendant neighbor. We have that $d(w) = 4$ and since $n \geq 14$, at least one neighbor of w is a 4-vertex. Denote it by a. Let $T' = T - \{vu, wa\} + \{wu, ua\}$. Then,

$$\sigma(T') - \sigma(T) = 9 + 4 + 4 - 1 - 4 = 12 > 0.$$

Thus, we obtain a contradiction, and we conclude that $m_{12} = 0$. ■

Lemma 2. *Let T be an extremal chemical tree. Then $m_{22} = 0$.*

Proof. We prove that if T is an extremal chemical tree, then T satisfies the following properties:

(i) there is no path $v_1v_2v_3$ in T with $d(v_i) = 2$, $i = 1, 2, 3$;

(ii) there is no path $v_1v_2 \ldots v_3v_4$ in T with $d(v_i) = 2$, $i = 1, 2, 3, 4$;

(iii) there is no path $v_1v_2 \ldots v_3v_4$ in T with $d(v_1) = d(v_2) = 2$, and $d(v_3), d(v_4) \geq 3$.

We prove all the above claims again by a contradiction.

(i) Assume that there is a path $xv_1v_2v_3y$ such that $d(v_i) = 2$, $i = 1, 2, 3$. We apply the transformation depicted in Figure 4, obtaining a chemical tree $T' = T - \{xv_1, v_1v_2\} + \{xv_3, v_3v_1\}$. It holds that

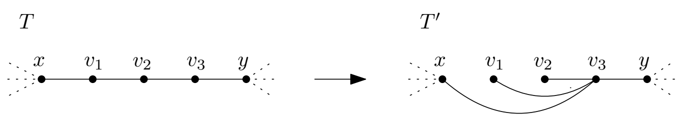

Figure 4. The transformation from the assertion (i) of the proof of Lemma 2. The dotted segment lines are optional.

$$\sigma(T') - \sigma(T) = (d(x) - 4)^2 + (d(y) - 4)^2 + 18 - (d(x) - 2)^2 - (d(y) - 2)^2$$
$$= 42 - 4d(x) - 4d(y) > 0,$$

since $d(x), d(y) \leq 4$, and therefore, T is not extremal.

(ii) To prove this claim, suppose that there is a path $uv_1v_2w \dots xv_3v_4y$ with $d(v_i) = 2$, $i = 1, 2, 3, 4$. Let T' be the chemical tree obtained from T by applying the transformation $[v_1v_2 \xrightarrow{v_1} v_3]$. Then,

$$\begin{aligned}\sigma(T') - \sigma(T) &= (d(w) - 1)^2 + (d(x) - 3)^2 + 1 + 1 \\ &\quad - (d(w) - 2)^2 - (d(x) - 2)^2 \\ &= 4 + 2d(w) - 2d(x) > 0,\end{aligned}$$

since $d(x) \leq 4$ and $d(w) \geq 3$. Again, we obtain that T is not extremal. Note that w could be equal to x.

(iii) Suppose that there is a path $v_1v_2 \dots v_3v_4$ with $d(v_1) = d(v_2) = 2$, and $d(v_3), d(v_4) \geq 3$ and let $T' = T - \{v_1v_2, v_3v_4\} + \{v_1v_3, v_2v_4\}$ (see Figure 5 for an illustration).

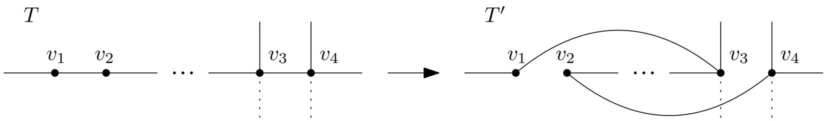

Figure 5. The transformation from the assertion (iii) of the proof of Lemma 2.

It holds that

$$\begin{aligned}\sigma(T') - \sigma(T) &= (d(v_3) - 2)^2 + (d(v_4) - 2)^2 - (d(v_3) - d(v_4))^2 \\ &= 2(d(v_3) - 2))(d(v_4) - 2)) > 0,\end{aligned}$$

since $d(v_3), d(v_4) \in \{3, 4\}$, which means that T is not extremal.

If T is an extremal chemical tree with $m_{22} \neq 0$, then by the assertions (i) and (ii) it follows that $m_{22} = 1$. Let $v_1v_2 \in E(T)$, $d(v_1) = d(v_2) = 2$. Consider a path $xv_1v_2yv_3z$ in T. By assertions (i), (ii), and (iii), it follows that $d(x), d(y), d(z)$ are 3 or 4 and $d(v_3) = 2$. Observe that such a path in T exists, since we consider chemical trees of order $n \geq 14$. Let $T' = T - \{xv_1, v_1v_2, v_2y\} + \{xy, v_1v_3, v_2v_3\}$ (see Figure 6 for an illustration).

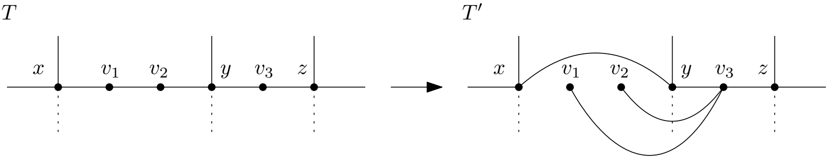

Figure 6. The final transformation from the proof of Lemma 2.

Then,

$$\begin{aligned}\sigma(T') - \sigma(T) &= 18 + (d(x) - d(y))^2 + (d(y) - 4)^2 + (d(z) - 4)^2 \\ &\quad - (d(x) - 2)^2 - 2(d(y) - 2)^2 - (d(z) - 2)^2 \\ &= 34 - 2(d(x)d(y) + 2d(z) - 2d(x)) \geq 34 - 32 = 2 > 0,\end{aligned}$$

and hence, T is not extremal. ■

Lemma 3. *If T is an extremal chemical tree, then $n_3 = 0$.*

Proof. Firstly, we prove the following assertion.

Claim 1. *An extremal chemical tree cannot have more than one* 3*-vertex.*

Proof of Claim 1. Assume that the claim is false and that an extremal chemical tree T has at least two 3-vertices. Denote two of them by v_1 and v_2. Regarding the neighborhood relation between v_1 and v_2, one can distinguish the following three cases.

Case 1.1. *v_1 are v_2 adjacent.* Let vertices a_1 and b_1 be adjacent to v_1, and a_2 and b_2 be adjacent to v_2. We may assume that $d(a_1) \geq d(b_1)$, $d(a_2) \geq d(b_2)$ and $d(a_1) \geq d(a_2)$. Let T' be obtained from T by applying the transformation $[b_1 v_1 \xrightarrow{b_1} v_2]$. It holds that

$$\begin{aligned}\sigma(T') - \sigma(T) &= (2 - d(a_1))^2 + (4 - d(b_1))^2 + (4 - d(a_2))^2 \\ &\quad + (4 - d(b_2))^2 + 4 - (3 - d(a_1))^2 - (3 - d(b_1))^2 \\ &\quad - (3 - d(a_2))^2 - (3 - d(b_2))^2 \\ &= 2(10 + d(a_1) - d(a_2) - d(b_1) - d(b_2)) \\ &\geq 2(10 - d(b_1) - d(b_2)) > 0,\end{aligned}$$

which is a contradiction of the optimality of T.

Case 1.2. *v_1 and v_2 are not adjacent and they share a common neighbor.* Let vertices a_1 and b_1 be adjacent to v_1, and a_2 and b_2 be adjacent to v_2. By c, we denote the common neighbor of v_1 and v_2. We may assume that $d(a_1) \geq d(a_2)$. After applying the transformation $[b_1 v_1 \xrightarrow{b_1} v_2]$ on T, we get a chemical tree T'. It holds that

$$\begin{aligned}\sigma(T') - \sigma(T) &= (2 - d(a_1))^2 + (4 - d(b_1))^2 + (2 - d(c))^2 \\ &\quad + (4 - d(a_2))^2 + (4 - d(b_2))^2 + (4 - d(c))^2 \\ &\quad - (3 - d(a_1))^2 - (3 - d(b_1))^2 - (3 - d(c))^2 \\ &\quad - (3 - d(a_2))^2 - (3 - d(b_2))^2 - (3 - d(c))^2 \\ &= 2(9 + d(a_1) - d(a_2) - d(b_1) - d(b_2)) \\ &\geq 2(9 - d(b_1) - d(b_2)) > 0,\end{aligned}$$

which is again a contradiction of the optimality of T.

Case 1.3. *v_1 and v_2 are not adjacent and they do not share a common neighbor.* Let vertices a_1, b_1 and c_1 be adjacent to v_1, and a_2, b_2 and c_2 be adjacent to v_2. It will be assumed that the degrees of a_1, b_1, c_1, a_2, b_2 and c_2 are not equal to 3, otherwise we proceed with Case 1.1. We may assume also that $d(a_1) \geq d(b_1) \geq d(c_1)$, $d(a_2) \geq d(b_2) \geq d(c_2)$ and $d(a_1) \geq d(a_2)$. In the case when c_1 is not on the path $v_1 \ldots v_2$ apply the transformation $[c_1 v_1 \xrightarrow{c_1} v_2]$ to T obtaining a chemical tree T'. It holds that

$$\begin{aligned}\sigma(T') - \sigma(T) &= (2 - d(a_1))^2 + (2 - d(b_1))^2 + (4 - d(c_1))^2 \\ &\quad + (4 - d(a_2))^2 + (4 - d(b_2))^2 + (4 - d(c_2))^2 \\ &\quad - (3 - d(a_1))^2 - (3 - d(b_1))^2 - (3 - d(c_1))^2 \\ &\quad - (3 - d(a_2))^2 - (3 - d(b_2))^2 - (3 - d(c_2))^2 \\ &= 2(9 + d(a_1) - d(a_2) + d(b_1) - d(b_2) - d(c_1) - d(c_2)) \\ &\geq 2(9 - d(b_2) - d(c_2)) > 0.\end{aligned}$$

If c_1 is on the path $v_1 \ldots v_2$, then we have two possibilities: $d(c_1) = d(b_1)$ and $d(c_1) < d(b_1)$. In the first case, $d(c_1) = d(b_1)$, we swap the labels of the vertices b_1 and c_1 such that now c_1 is not on the path $v_1 \ldots v_2$, and we proceed with the previous transformation. If $d(c_1) < d(b_1)$, then it must hold that $d(c_1) = 2$ and $d(a_1) = d(b_1) = 4$. Denote by x the neighbor of c_1 different than v_1. By applying the transformation $[c_1 x \xrightarrow{x} v_1]$ to T, we obtain the chemical tree T'. It holds that $\sigma(T') - \sigma(T) = 18 - 4d(x) > 0$, and therefore, T is not optimal. This concludes the proof of Claim 1.

Now, we assume that an extremal tree T has one 3-vertex. We denoted it by v.

Next, we claim that *if there is a 2-vertex in T, then its both neighbors cannot be v and a 4-vertex.* Assume the opposite, that both neighbors of a 2-vertex w are v and a 4-vertex u. Let denote by a and b the two vertices adjacent to v, which are different from w. By applying transformation $[wu \xrightarrow{u} v]$ to T, we obtain the chemical tree T'. It holds that

$$\begin{aligned}\sigma(T') - \sigma(T) &= 9 + (d(a) - 4)^2 + (d(b) - 4)^2 \\ &\qquad - 1 - 4 - (d(a) - 3)^2 - (d(b) - 3)^2 \\ &= 2(9 - d(a) - d(b)) > 0,\end{aligned}$$

which is a contradiction of the maximality of T. This establish the claim.

In addition, having by Lemmas 1 and 2 that $m_{12} = 0$ and $m_{22} = 0$, it follows that the 3-vertex v can be adjacent only to a pendant vertex or to a 4-vertex. Concerning the number of pendant neighbors to v three different cases can be distinguished.

Case 1. *v has no pendant neighbors.* In this case, all neighbors of v are 4-vertices. Let $P : avx \dots uz$ be a path in T such that $d(u) = 4$ and $d(z) = 1$. Such a path exists due to Lemma 1 and previously proved claims. Let b be a neighbor of v not in P. Denote by T' the tree obtained by transformation $[vb \xrightarrow{b} z]$ of T. Then, $\sigma(T') - \sigma(T) = 16 - 12 = 4 > 0$, and therefore, T is not extremal.

Case 2. *v has one pendant neighbor.* Let a be the pendant vertex and u one 4-vertex adjacent to v. Consider the tree T' obtained from T by applying the transformation $[uv \xrightarrow{u} a]$. The change of the σ-irregularity after this transformation is $\sigma(T') - \sigma(T) = 2 > 0$. Thus, T is not extremal.

Case 3. *v has two pendant neighbors.* Let x and y be the two pendant neighbors of v and z be the 4-vertex adjacent to v. Consider a path $vzwu$ of T. Observe that, such a path exists since $n \geq 14$. We distinguish two possible cases regarding the degree of w. When $d(w) = 4$, then $d(z) = 4$, and we consider the tree $T' = T - \{xv, yv, zw, wu\} + \{zx, xw, wy, yu\}$, depicted in Figure 7. It holds that

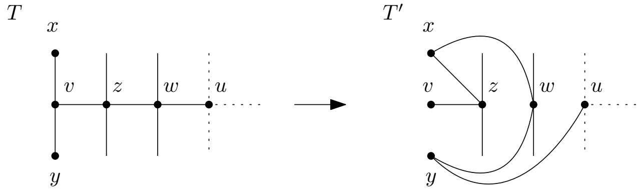

Figure 7. The transformation from the proof of Lemma 3, Case 3 when $d(w) = 4$.

$$\begin{aligned}\sigma(T') - \sigma(T) &= (d(u) - 2)^2 + 4 + 4 + 4 + 9 - (d(u) - 4)^2 - 1 - 4 - 4 \\ &= 4d(u) > 0.\end{aligned}$$

Therefore, T is not extremal.

When $d(w) = 2$, then, by Lemma 2 we have that $d(u) = 4$ and $d(z) = 4$. Let now $T' = T - \{zw, wu\} + \{zu, wv\}$ (see Figure 8 for an illustration). Then,

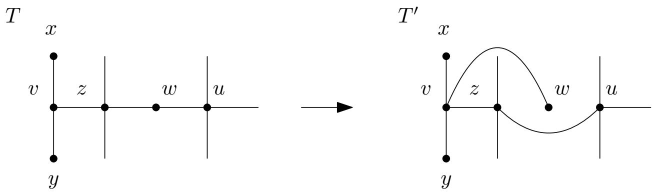

Figure 8. The transformation from the proof of Lemma 3, Case 3 when $d(w) = 2$.

$$\sigma(T') - \sigma(T) = 27 - 17 = 10,$$

and thus, again T is not extremal, and we may finally conclude that $n_3 = 0$. ■

Now, we are ready to prove the main result.

Proof of Theorem 1. The extremal trees with $n = 8, 9, 11, 12, 13$ vertices, obtained by computer-based search and presented in Figure 1, satisfy the theorem. Therefore, we proceed with the proof for $n \geq 14$.

Since by Lemma 3 $n_3 = 0$, an extremal chemical tree T of order n satisfies the following two equations:

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

$$n_1 + 2n_2 + 4n_4 = 2(n-1). \tag{2}$$

Lemmas 1-3 assert that in any extremal chemical tree T, $m_{12} = m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = 0$. It follows that

$$\sigma(T) = \sum_{uv \in E(T)} (d(u) - d(v))^2 = 9m_{14} + 4m_{24}.$$

Moreover, each 2-vertex in T is adjacent to two 4-vertices, and thus, $2n_2 = m_{24}$, and

$$\sigma(T) = 9m_{14} + 8n_2. \tag{3}$$

Note that $n_1 = m_{14}$. From (1) and (2), we obtain $3n_1 = 2n - 2n_2 + 2$, or $3m_{14} = 2n - 2n_2 + 2$, and therefore, (3) can be rewritten as

$$\sigma(T) = 6n + 2n_2 + 6.$$

It follows that the maximal value of $\sigma(T)$ is achieved when n_2 is maximal.

Now if T is an extremal chemical tree, let H be the chemical tree obtained from T using the following transformation: (i) remove every 2-vertex (if there is any), (ii) add an edge between the 4-vertices, which were adjacent to a removed 2-vertex. Note that $H \in \mathcal{H}(n - n_2)$. For the order of H it can be deduced that the relation $n - n_2 \equiv 2 \pmod{3}$ must hold. Let m_{44}^H be the number of edges in H with end-vertices of degree 4. Then, $m_{44}^H = (n - n_2 - 5)/3$ also holds. Since $n_2 \leq m_{44}^H$, we obtain

$$4n_2 \leq n - 5.$$

Thus, the number of 2-vertices, for which the maximal σ-irregularity is obtained is

$$n_2^* = \max\{k \in \mathbb{N}_0 \,|\, 4k \le n-5 \text{ and } n-k \equiv 2 \pmod{3}\}. \qquad \blacksquare$$

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References

[1] H. Abdo, N. Cohen, D. Dimitrov, Graphs with maximal irregularity, *Filomat* **28** (2014) 1315–1322.

[2] H. Abdo, D. Dimitrov, The irregularity of graphs under graph operations, *Discuss. Math. Graph Theory* **34** (2014) 263–278.

[3] H. Abdo, D. Dimitrov, I. Gutman, Graphs with maximal σ-irregularity, *Discr. Appl. Math.* **250** (2018) 57–64.

[4] M. O. Albertson, The irregularity of a graph, *Ars Comb.* **46** (1997) 219–225.

[5] A. Ali, A. M. Albalahi, A. M. Alanazi, A. A Bhatti, A. E. Hamza, On the maximum sigma index of k-cyclic graphs, *Discr. Appl. Math.* **352** (2023) 58–62.

[6] R. Criado, J. Flores, A. G. del Amo, M. Romance, Centralities of a network and its line graph: an analytical comparison by means of their irregularity, *Int. J. Comput. Math.* **91** (2014) 304–314.

[7] E. Estrada, Quantifying network heterogeneity, *Phys. Rev. E* **82** (2010) #066102.

[8] E. Estrada, Randić index, irregularity and complex biomolecular networks, *Acta Chim. Slov.* **57** (2010) 597–603.

[9] I. Gutman, P. Hansen, H. Mélot, Variable neighborhood search for extremal graphs. 10. Comparison of irregularity indices for chemical trees, *J. Chem. Inf. Model.* **45** (2005) 222–230.

[10] I. Gutman, M. Togan, A. Yurttas, A. S. Cevik, I. N. Cangul, Inverse problem for sigma index, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 491–508.

[11] P. Hansen, H. Mélot, Variable neighborhood search for extremal graphs. 9. Bounding the irregularity of a graph, *DIMACS Ser. Discr. Math. Theor. Comput. Sci.* **69** (2005) 253–264.

[12] T. Réti, On some properties of graph irregularity indices with a particular regard to the σ-index, *Appl. Math. Comput.* **344** (2019) 107–115.

[13] T. Réti, R. Sharafdini, Á. Drégelyi-Kiss, H. Haghbin, Graph irregularity indices used as molecular descriptors in QSPR studies, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 509–524.

[14] T. A. B. Snijders, The degree variance: an index of graph heterogeneity, *Soc. Netw.* **3** (1981) 163–174.