New transmission irregular chemical graphs

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Abstract

The transmission of a vertex v of a (chemical) graph G is the sum of distances from v to other vertices in G. If any two vertices of G have different transmissions, then G is a transmission irregular graph. It is shown that for any odd number $n \geq 7$ there exists a transmission irregular chemical tree of order n. A construction is provided which generates new transmission irregular (chemical) trees. Two additional families of chemical graphs are characterized by property of transmission irregularity and two sufficient condition provided which guarantee that the transmission irregularity is preserved upon adding a new edge.

Key words: graph distance; transmission; transmission irregular graph; chemical graph; tree

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1 Introduction

In chemical graph theory, molecules are naturally represented by (chemical) graphs. In the next step, the graph distance function is an obvious tool for exploring chemical graphs, which in turn reflect the physico-chemical properties of the corresponding (organic) compounds, cf. [32]. The Wiener index [36] is a famous example, but many other distance-based (possibly combined with vertex degrees) topological indices have been studied such as Schultz index [33, 29], hyper-Wiener index [31], Gutman index [23, 29], vertex-Szeged index [23], PI index [26], edge-Wiener index [27], edge-Szeged index [24], Wiener polarity index [2, 25], and more. The area is still very active; for a survey on graphs extremal with respect to distance-based topological indices see [39], and for a selection of recent developments with a focus on applications see [8, 9, 15, 17, 34, 35, 40, 41].

Exploring all these indices can be interesting from a mathematical point of view, but it is also much important from a chemical point of view, as it turns out in practice that several indices need to be combined to determine the properties of molecules. Moreover, this approach has found applications in many other areas such as communication theory, facility location, crystallography, and even in ornithology. As a point of interest for the latter we mention that it was shown in [11] that the interaction between a flock of birds depends more intimately on the topological distance rather than the Euclidian distance.

If $G = (V(G), E(G))$ is a graph and $x, y \in V(G)$, then $d_G(x, y)$ denotes the shortest-path distance between x and y in G. The sum of all distances from a vertex x to other vertices is a basic building block in exploration of metric properties of a graph and is called the *transmission* of x and denoted by ${\rm Tr}_G(x)$. That is,

$$
{\rm Tr}_G(x) = \sum_{u \in V(G) \setminus \{x\}} d_G(x, u)\,.
$$

That the transmission of a vertex is indeed a fundamental concept is demonstrated by the fact that it is also known by several other names, such as the status of a vertex [1, 30] and the total distance of a vertex [16, 28].

The *transmission set* of G is

$$
{\rm Tr}(G) = \{{\rm Tr}_G(x) :\ x \in V(G)\}\,.
$$

If $|{\rm Tr}(G)| = n(G)$ holds, where $n(G)$ denotes the order of G, then G is *transmission irregular*, TI for short. Recalling that the Wiener complexity of a G is the number of different transmission of its vertices [3], see also [22, 37], we can equivalently say that TI graphs are the graphs with maximum Wiener complexity.

Since almost no graph is transmission irregular [4], the search for such graphs has become of interest to several groups of researchers. Results to date have been presented in [5, 6, 7, 12, 13, 18, 19, 20, 21, 38]. In this paper we continue this line of research with a focus on chemical graphs. In the next section we list definitions needed, recall some known results, and prove a couple of results to be used later. In Section 3 we investigate transmission irregularity of chemical trees while in Section 4 we consider families of chemical graphs containing a few short cycles. We conclude the paper with some open problems.

2 Preliminaries

All graphs considered in this paper are finite, simple and, unless stated otherwise, also connected. For $X \subseteq V(G)$, let $G - X$ be the subgraph of G obtained from G by removing the vertices from X and the edges incident with them, in particular, $G - \{v\}$ will be briefly denoted by $G-v$. Similarly, for $F \subseteq E(G)$, $G-F$ is the spanning subgraph of G obtained by removing the edges of F and if $e \in E(G)$ then we will write $G-e$ for $G-\{e\}$. The *eccentricity* $\mathrm{ecc}_G(v)$ of a vertex $v \in V(G)$ is the maximum distance from v to all other vertices in G. If $uv \in E(G)$, then n_u (or $n_G(u)$ if the graph G is necessarily mentioned) is the number of vertices in G closer to u than to v and n_v (or $n_G(v)$ for completeness) is similarly defined.

A vertex v with $\deg_G(v) = 1$ is called a *pendant vertex* (also *leaf* when G is a tree) in G, and the edge incident with a pendant vertex is called a *pendant edge*. A path $P := u_k u_{k-1} \cdots u_2 u_1$ with natural adjacency relation in a graph G is a *proper pendant path* in G if $\deg_G(u_k) \geq 3$, $\deg_G(u_1) = 1$, and $\deg_G(u_i) = 2$ for $i \in \{2, 3, \ldots, k-1\}$, where u_k is its root. If both u_k and u_1 in P have degrees at least 3 and each of u_j with $j \in \{2, 3, \ldots, k-1\}$ has degree 2, then P is an *internal path* in G with two *terminals* u_k and u_1. Specially, if u_1 and u_k have degrees at least 2, then the above P is a *weak internal path* with two weak terminals u_1 and u_k.

The definition of a chemical graph is still a matter of debate, but we will stick to the most common and simple one: A graph G is a *chemical graph* if its maximum degree is at most 4. A vertex of degree at least 3 is a *branching vertex*. A tree with a unique branching vertex v is *starlike*. A starlike tree T with branching vertex v will be denoted by $T = T(n_1, \ldots, n_k)$ if $T - v$ consists of k disjoint paths of orders $n_1, \ldots, n_k$, respectively. And the pendant path of length n_i from v is called an n_i-*arm* in it.

For an induced subgraph H of G, we say that the transmission set of H in G is $\mathrm{Tr}_G(H) = \{\mathrm{Tr}_G(u) : u \in V(H)\}$. In particular, $\mathrm{Tr}_G(G) = \mathrm{Tr}(G)$. For an induced subgraph H of a graph G, if $|\mathrm{Tr}_G(H)| = n(H)$, then H is a *partially transmission irregular* subgraph of G.

For a positive integer k we use the notation $[k] = \{1, \ldots, k\}$ and $[k]_0 = \{0, 1, \ldots, k\}$. For a set A of integers and $i \in \mathbb{Z}$, we denote by $A+i$ the usual coset, that is, $A+i = \{a+i : a \in A\}$.

For any tree T and its subtree T_0 with a non-leaf vertex $v \in V(T_0)$, we denote by V_j the set of vertices at distance j from v in T_0. Let $a = \mathrm{ecc}_{T_0}(v)$. Then $V(T^*) = \cup_{j=1}^{a} V_j$ is a *distance-based partition* of the forest $T_0 - v$ at v. If $\min\limits_{u \in V_{j+1}} \mathrm{Tr}_T(u) \geq \max\limits_{u \in V_j} \mathrm{Tr}_T(u)$ for any $j \in [a-1]$ in the above partition, then T_0 is a *distance-based transmission monotonic (DBTM for short) subtree* of T at v. See an example of a DBTM subtree in Fig. 1. In particular, if $T_0 = T$, then T is a DBTM tree. If $\min\limits_{u \in V_{j+1}} \mathrm{Tr}_T(u) \geq \max\limits_{u \in V_{j-1}} \mathrm{Tr}_T(u)$ for any $j \in [a-1] \setminus [1]$ in the above distance-based partition of T at $v \in V(T)$, then T is a 2-DBTM tree at v. If T is a DBTM tree at $v \in V(T)$, then $\min\limits_{u \in V_{j+1}} \mathrm{Tr}_T(u) \geq \max\limits_{u \in V_j} \mathrm{Tr}_T(u) \geq \min\limits_{u \in V_j} \mathrm{Tr}_T(u) \geq \max\limits_{u \in V_{j-1}} \mathrm{Tr}_T(u)$, which implies that T is a 2-DBTM tree at v. Therefore DBTM tree is a special 2-DBTM tree with the same root.

A set of positive integers is odd (even, resp.) if it consists of odd (even, resp.) integers. A family $A = \cup_{i=1}^{k} A_i$ of sets of positive integers has *intersecting parity* if A_p and A_{p+1} have different parities for any $p \in [k-1]$. Moreover, similarly as above, if $\min A_{j+1} \geq \max A_{j-1}$ for any $j \in [k-1] \setminus [1]$, then A is 2-*distance monotonic*.

Lemma 2.1 *Let $A = \cup_{i=1}^{k} A_i$ be a 2-distance monotonic family of sets of positive integers. If A has intersecting parity, then the sets A_i are pairwise disjoint.*

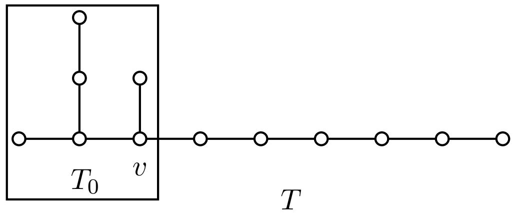

Figure 1: Tree T with a DBTM subtree T_0 rooted at v.

Proof. Without loss of generality, we assume that A_1 is odd. From the condition that A has intersecting parity, we deduce that A_j has the same parity with its subscript j for any $j \in [k]$. Then $A_p \cap A_q = \emptyset$ if $p, q \in [k]$ have different parities. It follows that $A^{(1)} \cap A^{(2)} = \emptyset$ where $A^{(1)}$ is the union of sets A_i with odd $i \in [k]$ and $A^{(2)}$ is the union of sets A_i with even $i \in [k]$. In view of the 2-distance monotonic property of A, we conclude that both $A^{(1)}$ and $A^{(2)}$ are pairwise disjoint. Thus the result follows immediately. $\square$

From Lemma 2.1, the following result is obvious.

Corollary 2.2 *Let $A = \cup_{i=1}^{k} A_i$ be a 2-distance monotonic family of sets of positive integers, and let t be an even positive integer. If A has intersecting parity, then both $\cup_{i=1}^{k}(A_i + it)$ and $\cup_{i=1}^{k}(A_i + a)$ are pairwise disjoint, where a is a constant.*

Lemma 2.3 [10] *If G is a graph with $n(G) > 2$ and $uv \in E(G)$, then $\mathrm{Tr}(u) - \mathrm{Tr}(v) = n_v - n_u$.*

Lemma 2.4 [38] *Let G be a graph with $n(G) = n$ and v a vertex with $\deg(v) \geq 3$. If $P = uv_1v_2 \cdots v_{x-1}v$ is a pendant path with natural adjacency relation attaching at v, where $\deg(u) = 1$ and $x < \frac{n}{2}$, then $\mathrm{Tr}(v_{x-1}) - \mathrm{Tr}(v) = n - 2x$.*

Lemma 2.5 *Let G be a graph with $n(G) = n$ and $P = vv_1v_2 \cdots v_kv^*$ is a weak internal path in G with two weak terminals v and v^* such that each edge in P is a cut edge. If $\mathrm{Tr}(v_1) - \mathrm{Tr}(v) = a > 0$, then $\mathrm{Tr}(v_j) - \mathrm{Tr}(v) = j(a + j - 1)$ for any $j \in [k]$.*

Proof. By Lemma 2.3, we have $n_v - n_{v_1} = a$. Since each edge in P is a cut edge, we have $n_{v_1} - n_{v_2} = a + 2$, $n_{v_2} - n_{v_3} = a + 4$, $\ldots$, $n_{v_{j-1}} - n_{v_j} = a + 2(j - 1)$. From Lemma 2.3, we have $\mathrm{Tr}(v_2) - \mathrm{Tr}(v_1) = a + 2$, $\mathrm{Tr}(v_3) - \mathrm{Tr}(v_2) = a + 4$, $\ldots$, $\mathrm{Tr}(v_j) - \mathrm{Tr}(v_{j-1}) = a + 2(j - 1)$. Note that $v_{p-1} = v$ if $p = 1$. It follows that

$$\begin{aligned}\mathrm{Tr}(v_j) - \mathrm{Tr}(v) &= \sum_{p=1}^{j} \Big(\mathrm{Tr}(v_p) - \mathrm{Tr}(v_{p-1})\Big) \\ &= j(a + j - 1),\end{aligned}$$

completing the proof. $\square$

3 Transmission irregular chemical trees

In [5, 38] some TI starlike trees are determined, in particular, the TI starlike trees with maximum degree 3 are characterized in [5] with a complicated condition. It is proved in [38] that $T = T(a, a+1, \ldots, a+k)$ is TI if $n(T)$ is odd. A tree $H^k(a_1, a_2; b_1, b_2)$ is obtained by attaching two pendant paths of lengths b_1, b_2, respectively, at a leaf on the k-arm of $T(a_1, a_2, k)$, see Fig. 2.

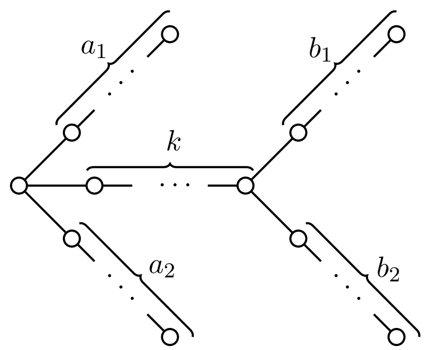

Figure 2: The tree $H^k(a_1, a_2; b_1, b_2)$

Before stating our first main result, we make the following comment which will be used frequently in the subsequent proof.

Remark 3.1 *Let $a < b$ be two positive integers. If $b^2 - a^2$ is even (odd, resp.), then $b - a$ and $b + a$ are both even (odd, resp.).*

Proof. Clearly, $b^2 - a^2 = (b+a)(b-a)$. Note that $b+a$ and $b-a$ have a same parity since $(b+a)+(b-a) = 2b$ is even. Thus our result follows immediately. $\square$

By a computer search we find that there is no TI tree of order at most 6. On the other hand, we have the following result.

Theorem 3.2 *If $n \geq 7$ is an odd integer, then there exists a TI chemical tree of order n.*

Proof. TI chemical trees of order 7 and 9 are displayed in Fig. 3, where, for each vertex, we also give its transmission.

In the rest we assume that $n \geq 11$ is odd.

If $n = 4a+3$, then $a \geq 2$. Now we consider the tree $T = H^2(a-1, a; a, a+1)$ and prove that T is TI. Let u be the vertex of degree 3 in T at which two pendant paths of lengths a, $a+1$, respectively, are attached. Assume that $\mathrm{Tr}_T(u) = x$ and $uv \in E(T)$ with $\deg_T(v) = 2$ and $vw \in E(T)$. Then w is the other vertex of degree 3 in T with $\mathrm{Tr}_T(v) = x+1$, and $\mathrm{Tr}_T(w) = x+4$. Let A_1 and A_3 be the sets of transmissions of vertices on the pendant

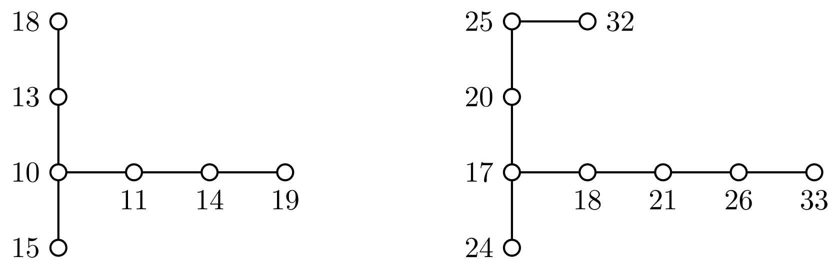

Figure 3: Sporadic TI chemical trees

paths of lengths $a-1$ and a, respectively, attached at w, and let A_2 and A_4 be the sets of transmissions of vertices on the pendant paths of lengths a and $a+1$, respectively, attached at u. From the structure of T and Lemma 2.5 we have

$$\begin{aligned} A_1 &= \{2ka + (k+2)^2 : \ k \in [a-1]\} + x, \\ A_2 &= \{2ka + (k+1)^2 - 1 : \ k \in [a]\} + x, \\ A_3 &= \{2ka + (k+1)^2 - 1 : \ k \in [a]\} + 4 + x, \\ A_4 &= \{2ka + k^2 : \ k \in [a+1]\} + x. \end{aligned}$$

Next we prove that $A_i \cap A_j = \emptyset$ for any $i, j \in [4]$. If $2k_1a + (k_1+2)^2 = 2k_2a + (k_2+1)^2 - 1$ with $k_1 \in [a-1]$ and $k_2 \in [a]$, then $k_1 < k_2$. It follows that $2(k_2-k_1)a - 1 = (k_1+2)^2 - (k_2+1)^2$. By Remark 3.1, $k_1 - k_2 + 1$ is odd, that is, $k_1 - k_2 \leq -2$ is even. However, we have $2(k_2-k_1)a - 1 > 0 > (k_1+k_2+3)(k_1-k_2+1)$ as a contradiction. Thus $A_1 \cap A_2 = \emptyset$. Similarly as above, we have $A_1 \cap A_3 = \emptyset$. If $2k_1a + (k_1+2)^2 = 2k_2a + k_2^2$ with $k_1 \in [a-1]$ and $k_2 \in [a+1]$, then $2(k_2-k_1)a = (k_1+2)^2 - k_2^2$ with $k_2 > k_1$. Note that $k_1 - k_2 \leq -2$ is even from Remark 3.1. But $2(k_2-k_1)a > 0 \geq (k_1+k_2+2)(k_1-k_2+2)$ is a clear contradiction. Therefore $A_1 \cap A_4 = \emptyset$. Note that $A_3 = A_2 + 4$. Then $A_2 \cap A_3 = \emptyset$ since $|s-t| > 2a \geq 4$ for any $s, t \in A_2$. If $2k_1a + (k_1+1)^2 - 1 = 2k_2a + k_2^2$ with $k_1 \in [a]$ and $k_2 \in [a+1]$, then $(k_1+1)^2 - k_2^2 = 2(k_2-k_1)a + 1$ with $k_2 > k_1$, which implies that $k_1 - k_2 \leq -2$ is even from Remark 3.1. But $2(k_2-k_1)a + 1 > 0 > (k_1+k_2+1)(k_1-k_2+1)$ occurs contradictorily. Thus $A_2 \cap A_4 = \emptyset$. Similarly as above, we have $A_3 \cap A_4 = \emptyset$ as desired.

If $n = 4b+1$, then $b \geq 3$. We consider the tree $T = H^2(b-2, b-1; b, b+1)$ and prove that T is TI. Let z_1 be the vertex of degree 3 in T at which two pendant paths of lengths b, $b+1$, respectively, are attached, $z_1z_2 \in E(T)$ with $\deg_T(z_2) = 2$ and $z_2z_3 \in E(T)$. Assume that $\mathrm{Tr}_T(z_1) = y$. Then, by Lemma 2.3, we have $\mathrm{Tr}_T(z_2) = y+3$ and $\mathrm{Tr}_T(z_3) = y+8$. Denote by B_i the set of transmissions of vertices on the pendant path of length $b+2-i$ attached at z_1

or z_3 with $i \in [4]$. From the structure of T and Lemma 2.5 we have

$$
\begin{aligned}
B_1 &= \{2ka + k^2 - 2k :\ k \in [b+1]\} + y,\\
B_2 &= \{2ka + k^2 :\ k \in [b]\} + y,\\
B_3 &= \{2ka + (k+1)^2 - 1 :\ k \in [b-1]\} + 8 + y,\\
B_4 &= \{2ka + (k+2)^2 - 4 :\ k \in [b-2]\} + 8 + y.
\end{aligned}
$$

Now it suffices to prove that $B_i \cap B_j = \emptyset$ for any $i, j \in [4]$. If $2k_1b + k_1^2 - 2k_1 = 2k_2b + k_2^2$ with $k_1 \in [b+1]$ and $k_2 \in [b]$, then $2(k_1 - k_2)b - 1 = k_2^2 - (k_1 - 1)^2$ with $k_1 > k_2$. By Remark 3.1, $k_2 - k_1 \leq -2$ is even, which implies that $2(k_1 - k_2)b - 1 > 0 > (k_2 - k_1 + 1)(k_2 + k_1 - 1)$ as a contradiction. This yields that $B_1 \cap B_2 = \emptyset$. If $2k_1b + k_1^2 - 2k_1 = 2k_2b + (k_2 + 1)^2 + 7$ with $k_1 \in [b+1]$ and $k_2 \in [b-1]$, then $2(k_1 - k_2)b - 8 = (k_2 + 1)^2 - (k_1 - 1)^2$ with $k_1 > k_2$. Using Remark 3.1 again, we find that $k_2 - k_1 \leq -2$ is even. If $k_2 - k_1 = -2$, then we have $b = 2$, contradicting to the fact that $b \geq 3$. If $k_2 - k_1 \leq -4$, we have $2(k_1 - k_2)b - 8 \geq 8b - 8 > 0 > (k_2 - k_1 + 2)(k_2 + k_1)$ as a contradiction, again. Thus we get $B_1 \cap B_3 = \emptyset$. If $2k_1b + k_1^2 - 2k_1 = 2k_2b + (k_2 + 2)^2 + 4$ with $k_1 \in [b+1]$ and $k_2 \in [b-2]$, then $2(k_1 - k_2)b - 5 = (k_2 + 2)^2 - (k_1 - 1)^2$ with $k_1 > k_2$. By Remark 3.1, we observe that $k_2 - k_1 \leq -2$ is even. If $k_2 - k_1 = -2$, then $2(k_1 - k_2)b - 5 = 4b - 5 = 2k_2 + 3$, that is, $k_2 = 4b - 8 > b - 2$, contradicting to the fact $k_2 \in [b-2]$ with $b \geq 3$. If $k_2 - k_1 \leq -4$, then $2(k_1 - k_2)b - 5 \geq 4b - 5 > 0 > (k_2 + 2)^2 - (k_1 - 1)^2$ as a clear contradiction again. Therefore $B_1 \cap B_4 = \emptyset$. If $2k_1b + k_1^2 = 2k_2b + (k_2 + 1)^2 + 7$ with $k_1 \in [b]$ and $k_2 \in [b-1]$, then $2(k_1 - k_2)b - 7 = (k_2 + 1)^2 - k_1^2$ with $k_1 > k_2$, which implies that $k_2 - k_1 \leq -2$ is even from Remark 3.1. But we deduce that $2(k_1 - k_2)b - 7 \geq 4b - 7 > 0 > (k_2 + 1)^2 - k_1^2$ as a contradiction. Thus $B_2 \cap B_3 = \emptyset$. Similarly as above, we have $B_2 \cap B_4 = \emptyset$. If $2k_1b + (k_1 + 1)^2 + 7 = 2k_2b + (k_2 + 2)^2 + 4$ with $k_1 \in [b-1]$ and $k_2 \in [b-2]$, then we have $2(k_1 - k_2)b + 3 = (k_2 + 2)^2 - (k_1 + 1)^2$ with $k_1 > k_2$. Taking Remark 3.1 into account, we observe that $k_2 - k_1 \leq -2$ is even. However, $2(k_1 - k_2)b + 3 \geq 4b + 3 > 0 > (k_2 + 2)^2 - (k_1 + 1)^2$ is a contradiction, again, implying that $B_3 \cap B_4 = \emptyset$. $\square$

We next provide a method for constructing a TI tree from a tree with a DBTM subtree.

Theorem 3.3 *Let T_0 be a tree of order $n \geq 7$ containing a proper pendant path P of length k, where v_{k+1} is its root. Let T_0^* be the subtree of T_0 obtained by removing all the vertices of P but v_{k+1}, and let T_0' be a copy of T_0 with the vertex $v_1' \in V(T_0')$ corresponding to v_1. Let T be the tree obtained by joining the vertices v_1 and v_1', and by attaching a new leaf w at v_1. See Fig. 4. If T_0^* is a partially transmission irrgular DBTM subtree of T_0 and $2n \in \left(j^2 + 1, (j+1)^2\right)$ with $j \in [k]$, then T is transmission irregular.*

Proof. From the structure of T, we have $n(T) = 2n + 1$. Set $\mathrm{Tr}_T(v_1) = x$. Let $P = v_{k+1}v_k \cdots v_2v_1$ and let $P' = v_{k+1}'v_k' \cdots v_2'v_1'$ be the corresponding pendant path in T_0'. Then $\mathrm{Tr}_T(w) = x + 2n - 1$ and $\mathrm{Tr}_T(v_1') = x + 1$ by Lemma 2.3.

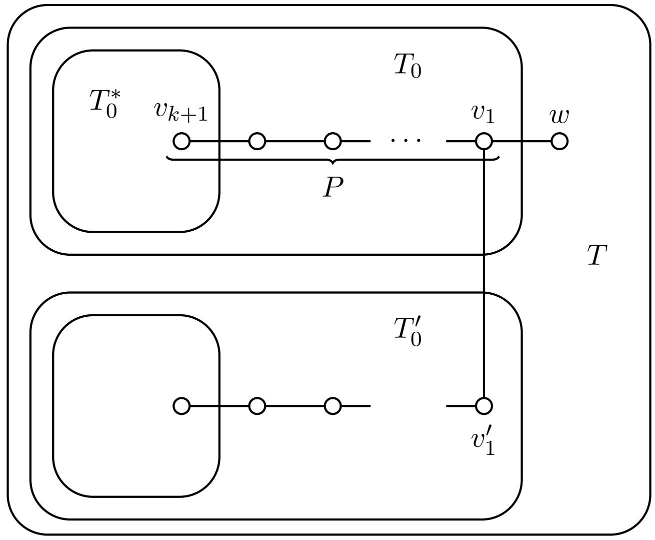

Figure 4: The construction of the tree T in Theorem 3.3

Note that P and $v_1v_1'P'$ are two internal paths of lengths k and $k+1$, respectively, in T. Then $n_T(v_i) - n_T(v_{i+1}) = n_T(v_i') - n_T(v_{i+1}') = 2i+1$ for $i \in [k]$ from the structure of T. In view of Lemma 2.3 and $\mathrm{Tr}_T(v_1) = x$, we have $\mathrm{Tr}_T(v_i') = x + i^2$ and $\mathrm{Tr}_T(v_i) = x + i^2 - 1$ for $i \in [k+1]$, that is, $\mathrm{Tr}_T(P) = \{i^2 - 1 : i \in [k+1]\} + x$ with $\mathrm{Tr}_T(P') = \mathrm{Tr}_T(V(P)) + 1$.

Next we consider the transmissions of vertices from $V(T) \setminus (V(P) \cup V(P') \cup \{w\})$. Set $V_0^* = V(T_0^*)$ and let V_i be the set of vertices in V_0^* at distance i from v_{k+1} in T_0. Then $V_0^* = \cup_{j=0}^{a} V_j$, where $a = \mathrm{ecc}_{T_0^*}(v_{k+1})$. For any edge $st \in E(T_0^*)$, without loss of generality, we may assume that $d_{T_0}(s, v_{k+1}) > d_{T_0}(t, v_{k+1})$. Since $n_T(t) = n_{T_0}(t) + n + 1$ and $n_T(s) = n_{T_0}(s)$, we have

$$n_T(t) - n_T(s) = n_{T_0}(t) - n_{T_0}(s) + n + 1. \tag{1}$$

Assume that $\mathrm{Tr}_{T_0}(u) - \mathrm{Tr}_{T_0}(v_{k+1}) = h$ for any vertex $u \in V_j \subseteq V(T_0^*)$. By Lemma 2.3 and (1) we have $\mathrm{Tr}_T(u) = \mathrm{Tr}_T(v_{k+1}) + h + j(n+1)$ with $\mathrm{Tr}_T(v_{k+1}) = \mathrm{Tr}_{T_0}(v_{k+1}) + (k+1)(n+1) + \mathrm{Tr}_{T_0}(v_1)$, that is, $\mathrm{Tr}_T(u) = \mathrm{Tr}_{T_0}(v_{k+1}) + (k+j+1)(n+1) + \mathrm{Tr}_{T_0}(v_1) + h$. It follows that

$$\mathrm{Tr}_T(u) = \mathrm{Tr}_{T_0}(u) + j(n+1) + c \tag{2}$$

for any vertex $u \in V_j$ where $c = (k+1)(n+1) + \mathrm{Tr}_{T_0}(v_1)$.

Note that $\mathrm{Tr}_{T_0}(T_0^*)$ is pairwise disjoint by the assumption. Let s, t be arbitrary vertices of T_0^*. Then $\mathrm{Tr}_T(s) \neq \mathrm{Tr}_T(t)$ for any $\{s, t\} \subseteq V_j$ with $j \in [a]$ because of (2) and the fact that $\mathrm{Tr}_{T_0}(s) \neq \mathrm{Tr}_{T_0}(t)$. Assume that $s \in V_j$, $t \in V_\ell$ with $j, \ell \in [a]$ and $j \neq \ell$. Then $\mathrm{Tr}_T(s) \neq \mathrm{Tr}_T(t)$ holds by (2) and the fact that T_0^* is a DBTM subtree of T_0. Therefore $\mathrm{Tr}_T(T_0^*)$ is pairwise disjoint.

Note that $V(T_0) = V(T_0^*) \cup V(P)$. Set $A_0 = \mathrm{Tr}_T(T_0)$. From the structure of T, we have $\mathrm{Tr}_T(u) > \mathrm{Tr}_T(v_{k+1}) = x + (k+1)^2 - 1$ for any vertex $u \in V(T_0^*) \setminus \{v_{k+1}\}$. Then A_0 is pairwise disjoint. By symmetry, we have $\mathrm{Tr}_T(T_0') = A_0 + 1$, which is also pairwise disjoint. In view of Lemma 2.3 and the structure of T, the absolute value of the difference between any two elements in A_0 is greater than 1. Therefore $A_0 \cap A_1 = \emptyset$ where $A_1 = A_0 + 1$. Recall that $\mathrm{Tr}_T(w) = x + 2n - 1$. Since $2n \in \left(j^2 + 1, (j+1)^2\right)$ with $j \in [k]$, we have $\mathrm{Tr}_T(w) \cap A = \emptyset$ with $A = A_0 \cup A_1$. □

Let T be a transmission irregular chemical tree of order n with a DBTM subtree T_0 obtained by removing all the non-root vertices of a pendant path of length k such that $2n \in \left(j^2 + 1, (j+1)^2\right)$ with $j \in [k]$. By using the method in Theorem 3.3, we can construct another transmission irregular chemical tree of order $2n + 1$.

The condition that T_0^* is a DBTM subtree of T_0 in Theorem 3.3 is not necessary for obtaining a transmission irregular tree T. See an example in Fig. 5 of T_0 with a subtree T_0^* rooted at vertex v which is not DBTM. It is routine that the tree T, constructed from T_0 with the method in Theorem 3.3, is transmission irregular.

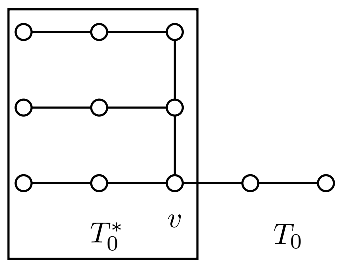

Figure 5: Tree T_0 with a non-DBTM subtree T_0^* rooted at v.

4 Cycle-containing TI graphs

Let Z_0 be the graph obtained from K_4 be removing one of its edges. For an integer $a \geq 2$, we denote by $Z_0(a-1, a+1; a-2, a+2)$ the graph obtained from Z_0 by attaching a pendant path of length $a-1$ to a vertex of degree 3, a pendant path of length $a+1$ at the other vertex of degree 3, a pendant path of length $a-2$ at a vertex of degree 2, and a pendant path of length $a+2$ at the other vertex of degree 2, see Fig. 6.

Theorem 4.1 *If $a \geq 2$, then $Z_0(a-1, a+1; a-2, a+2)$ is TI if and only if a is odd with $a \neq 1 \bmod 3$.*

Proof. Set $Z = Z_0(a-1, a+1; a-2, a+2)$. It is straightforward to check that Z is not TI for $a = 2$. Assume in the rest that $a \geq 3$. Let u_1 and u_2 be the vertices in Z of degree 3, and let P_1 and P_2 be the paths of lengths $a+2$ and $a-2$ attached at u_1 and u_2, respectively. Let

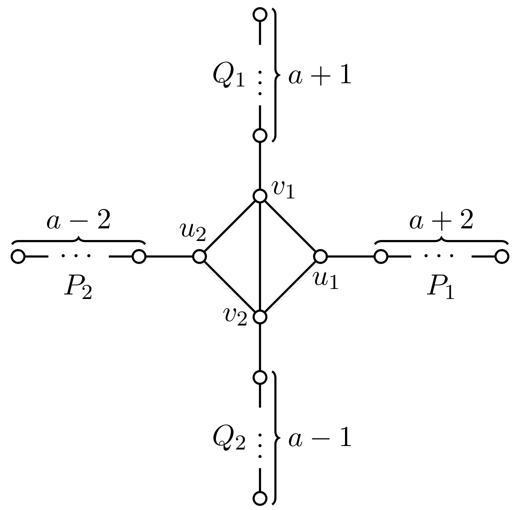

Figure 6: The graph $Z_0(a-1, a+1; a-2, a+2)$

v_1 and v_2 be the vertices of degree 4, and let Q_1 and Q_2 be the paths of lengths $a+1$ and $a-1$ attached to v_1 and v_2, respectively. See Fig. 6 again.

Note that $n(Z) = 4a + 4$. Let $\mathrm{Tr}_Z(v_1) = x$. From the structure of Z and Lemma 2.3, we have $\mathrm{Tr}_Z(v_2) = x + 2$, $\mathrm{Tr}_Z(u_1) = a - 2 + x$, and $\mathrm{Tr}_Z(u_2) = a + 6 + x$. By Lemma 2.4, the transmissions of vertices lying on the pendant paths P_1, P_2, Q_1, and Q_2 including their roots, respectively form the following sets:

$$\begin{aligned}
A_1 &= \{(2j+1)a + (j-2)(j+1) : \ j \in [a+2]_0\} + x, \\
A_2 &= \{(2j+1)a + (j+6)(j+1) : \ j \in [a-2]_0\} + x, \\
B_1 &= \{2ja + j(j+1) : j \in [a+1]_0\} + x, \\
B_2 &= \{2ja + j(j+5) + 2 : \ j \in [a-1]_0\} + x.
\end{aligned}$$

Set $A = A_1 \cup A_2$ and $B = B_1 \cup B_2$. Therefore Z is transmission irregular if and only if $A \cup B$ is pairwise disjoint.

If a is even, we select $(2k+1)a + (k-2)(k+1) \in A_1$ and $2ka + k(k+1) \in B_1$ with $k \in [a+1]$. Then $(2k+1)a + (k-2)(k+1) = 2ka + k(k+1)$ if $k = \frac{a-2}{2} \in [a+1]$. It follows that $A \cap B \neq \emptyset$, that is, Z is not transmission irregular. Next we turn to the case when a is odd. Note that A consists of odd numbers and B consists of even numbers in this case. Therefore $A \cap B = \emptyset$ holds. To characterizing the TI property of Z for odd a, it suffices to determine the condition of a such that $A_1 \cap A_2 = \emptyset$ and $B_1 \cap B_2 = \emptyset$.

For any two elements $2sa + s(s+1) \in B_1$ with $s \in [a+1]_0$ and $2ta + t(t+5) + 2 \in B_2$ with $t \in [a-1]_0$, if $2sa + s(s+1) = 2ta + t(t+5) + 2$, then

$$(s-t)(2a+s+t+1) = 4t+2 \tag{3}$$

with $s-t>0$. If $s-t=1$, then $2a+2t+2=4t+2$, that is, $t=a$. This contradicts the range of t. If $s-t=2$, we have $2(2a+2t+3)=4t+2$, which implies that $a=-1$. This is impossible. While $s-t\geq 3$, we have $s+t\geq 3$. From (3) we have $(s-t)(2a+s+t+1)\geq 3(2a+4)=6a+12>4a-2=4(a-1)+2\geq 4t+2$. A clear contradiction occurs again. Therefore $B_1\cap B_2=\emptyset$ holds for any odd number a.

For any two elements $(2s+1)a+(s-2)(s+1)\in A_1$ with $s\in[a+2]_0$ and $(2t+1)a+(t+1)(t+6)\in A_2$ with $t\in[a-2]_0$, if $(2s+1)a+(s-2)(s+1)=(2t+1)a+(t+1)(t+6)$, then

$$(s-t)(2a+t+s-1)=8t+8 \tag{4}$$

with $s>t$. If $s-t\geq 4$, then $s+t\geq 4$, which implies that

$$(s-t)(2a+t+s-1)\geq 4(2a+3)=8a+12>8a-8\geq 8(a-2)+8\geq 8t+8.$$

Therefore, (4) does not hold. If $s-t=3$, then by (4) we have $3(2a+2t+2)=8t+8$, that is, $t=3a-1>a-2$, contradicting the fact that $t\in[a-2]_0$. If $s-t=2$, from (4), we have $2(2a+2t+1)=8t+8$, that is, $t=a-\frac{3}{2}$. This is impossible since t is an integer. For $s-t=1$, similarly as above, we have $2a+2t=8t+8$, that is, $t=\frac{a-4}{3}$. Therefore, $A_1\cap A_2=\emptyset$ if and only if $a\neq 1 \bmod 3$. This completes the proof. $\square$

Denote by $K_4(k_1,k_2,k_3,k_4)$ the graph obtained from the complete graph K_4 by respectively attaching pendant paths of lengths $k_i\geq 0$, $i\in[4]$, to its vertices.

Theorem 4.2 *If $a\geq 2$, then $K_4(a-2,a-1,a+1,a+2)$ is TI if and only if $a\neq 2 \bmod 3$.*

Proof. Set $K=K_4(a-2,a-1,a+1,a+2)$. For $a=2$, it can be easily checked that the vertex of degree 3 has the same transmission as the vertex of degree 2 adjacent to the vertex of degree 4 at which a pendant path of length 4 is attached. Therefore K is not TI for $a=2$.

In the following assume that $a\geq 3$. Let v_1, v_2, v_3, and v_4 be the vertices of degree 4, and let $P^{(1)}$, $P^{(2)}$, $P^{(3)}$, and $P^{(4)}$ be respective attached paths of lengths $a+2$, $a+1$, $a-1$, and $a-2$. Let $\mathrm{Tr}(v_1)=x$. By Lemma 2.3, we have $\mathrm{Tr}(v_2)=x+1$, $\mathrm{Tr}(v_3)=x+3$, and $\mathrm{Tr}(v_4)=x+4$. Note that $n(K)=4a+4$. By Lemma 2.4, the set of transmissions of vertices on $P^{(1)}$ including v_1 is $\{2ja+j(j-1):\ j\in[a+2]_0\}+x$. Similarly, the sets of transmissions of vertices on $P^{(2)}$, $P^{(3)}$, and $P^{(4)}$, respectively including v_2, v_3, and v_4, are $\{2ja+j(j+1)+1:\ j\in[a+1]_0\}+x$, $\{2ja+(j+1)(j+4)-1:\ j\in[a-1]_0\}+x$ and $\{2ja+j(j+7)+4:\ j\in[a-2]_0\}+x$. For convenience, we set $A_1=\{2ja+j(j-1):\ j\in[a+2]_0\}$, $A_2=\{2ja+j(j+1)+1:\ j\in[a+1]_0\}$, $A_3=\{2ja+(j+1)(j+4)-1:\ j\in[a-1]_0\}$, $A_4=\{2ja+j(j+7)+4:\ j\in[a-2]_0\}$, and $A=\cup_{i=1}^4 A_i$. Then K is transmission irregular if and only if the sets A_i, $i\in[4]$, are pairwise disjoint.

Note that each of A_1 and A_4 consists of even numbers and each of A_2 and A_3 consists of odd numbers. Clearly $A_p\cap A_q=\emptyset$ for any $p\in\{1,4\}$ and $q\in\{2,3\}$. Next we show that $A_2\cap A_3=\emptyset$. Otherwise, there are two elements $s=2ka+k(k+1)+1\in A_2$ and

$t = 2ja + (j+1)(j+4) - 1 \in A_3$ with $k \in [a+1]_0$, $j \in [a-1]_0$ and $s = t$. Clearly, we have $k > j$. Then $(k-j)(2a+k+j) = 5j - k + 2$, that is,

$$(k-j)(2a+k+j-1) = 4j+2. \tag{5}$$

If $k - j \geq 2$, then $(k-j)(2a+k+j-1) > 4a+2$ and $4j+2 \leq 4a-2$ since $j \in [a-1]_0$. Therefore (5) does not hold. If $k-j = 1$, we have $2a+2j = 4j+2$ from (5). Then $a = j+1$, which is impossible since $j \in [a-1]_0$. Therefore $A_2 \cap A_3 = \emptyset$ follows immediately.

Now we determine the non-empty property of $A_1 \cap A_4$. Choosing any two elements $s = 2ka + k(k-1) \in A_1$ and $t = 2ja + j(j+7) + 4 \in A_4$ with $k \in [a+2]_0$ and $j \in [a-2]_0$, we have $s - t = (k-j)(2a+k+j+7) - (8k+4)$. If $s = t$, then

$$(k-j)(2a+k+j+7) = 8k+4 \tag{6}$$

with $k > j$. If $k - j \geq 4$, then $(k-j)(2a+k+j+7) > 8a+28$ and $8k+4 \leq 8a+20$ since $k \in [a+2]_0$. So (6) does not hold. If $k-j = 3$, then $6a+6j+30 = 8j+28$ from (6), that is, $6a = 2j-2$. Since $j \in [a-2]_0$, we have $6a \leq 2a-6$, contradicting the assumption $a \geq 3$. If $k-j = 2$, similarly as above, we have $4a \leq 4a-6$ as a contradiction, again. If $k-j = 1$, from Equality (6), we have $2a+2j+8 = 8j+12$, that is, $a = 3j+2$. Therefore $s \neq t$, that is, $A_1 \cap A_4 = \emptyset$ if and only if $a \neq 2 \bmod 3$. $\square$

$Z_0(a-1, a+1; a-2, a+2)$ can be changed into $K_4(a-2, a-1, a+1, a+2)$ by adding an edge between the two vertices of degree 3. By Theorems 4.1 and 4.2, if a is an odd multiple of 3, the TI property remains from $Z_0(a-1, a+1; a-2, a+2)$ to $K_4(a-2, a-1, a+1, a+2)$ by inserting a new edge. In our last result we provide two sufficient conditions which guarantee that the transmission irregularity is preserved after inserting a new edge.

Theorem 4.3 *Let G be a TI graph with $\mathrm{Tr}_G(v_1) > \mathrm{Tr}_G(v_2) > \mathrm{Tr}_G(v_3)$ as the first three largest transmissions.*

(i) *If v_1, v_2, and v_3 lie on a pendant path $v_4v_3v_2v_1$ with natural adjacency relation, where v_4 is the root and v_1 is a pendant vertex, then $G + v_2v_4$ is transmission irregular.*

(ii) *If v_1 and v_2 are both pendant vertices with $v_1v_3 \in E(G)$, v_2 and v_3 have a common neighbor and $\mathrm{Tr}_G(v_3) - 1 > \mathrm{Tr}_G(z)$ for any $z \in V(G) \setminus \{v_1, v_2, v_3\}$, then $G + v_2v_3$ is transmission irregular.*

Proof. We first deal with (i). For convenience, we set $G' = G + v_2v_4$ and let G_0 be the subgraph of G induced by V_0, where $V_0 = V(G) \setminus \{v_1, v_2, v_3\}$. Note that the vertices v_2, v_3, v_4 form a triangle in G'. For any vertex $u \in V_0$, we have $d_{G'}(u, v_i) = d_G(u, v_i) - 1$ for $i \in [2]$, and $d_{G'}(u, w) = d_G(u, w)$ for any vertex w in $(V_0 \cup \{v_3\}) \setminus \{v_1, v_2, u\}$. Therefore we have $\mathrm{Tr}_{G'}(u) = \mathrm{Tr}_G(u) - 2$ for any vertex $u \in V_0$, that is, $\mathrm{Tr}_{G'}(G_0) = \mathrm{Tr}_G(G_0) - 2$. Set $\mathrm{Tr}_G(v_4) = x$. Then, by Lemma 2.3, we have $\mathrm{Tr}_G(v_3) = x + n - 6$, $\mathrm{Tr}_G(v_2) = x + 2n - 10$, and $\mathrm{Tr}_G(v_1) = x + 3n - 12$. Thus we have $\mathrm{Tr}(G) = \mathrm{Tr}_G(G_0) \cup \Big(\{n-6, 2n-10, 3n-12\} + x\Big)$.

From the structure of G' and the above argument, we have $\mathrm{Tr}_{G'}(v_4) = x - 2$, $\mathrm{Tr}_{G'}(v_3) = x + n - 6$, $\mathrm{Tr}_{G'}(v_2) = x + n - 7$, and $\mathrm{Tr}_{G'}(v_1) = x + 2n - 9$, which imply that

$$\mathrm{Tr}(G') = \Big(\mathrm{Tr}_G(G_0) - 2\Big) \cup \Big(\{n-6, n-7, 2n-9\} + x\Big).$$

From the assumption, we have $x + n - 6 > y$ for any $y \in \mathrm{Tr}_G(G_0)$, that is,

$$x + n - 7 > y - 1 > y - 2$$

for any $y - 2 \in \mathrm{Tr}_G(G_0) - 2$. Moreover, $\Big(\mathrm{Tr}_G(G_0) - 2\Big) \cap \Big(\{n-6, n-7, 2n-9\} + x\Big) = \emptyset$ with $\mathrm{Tr}_G(G_0) - 2$ being pairwise disjoint. So G' is transmission irregular as desired.

Now we turn to (ii). Assume that v_4 is the unique common neighbor of v_2 and v_3. Let $G^* = G + v_2v_3$ and $\mathrm{Tr}_G(v_4) = y$. By Lemma 2.3, we have $\mathrm{Tr}_G(v_3) = y + n - 4$, $\mathrm{Tr}_G(v_2) = y + n - 2$, and $\mathrm{Tr}_G(v_1) = y + 2n - 6$. Note that v_2, v_3, and v_4 form a triangle in G^*. From the structure of G^*, we have $d_{G^*}(u, w) = d_G(u, w)$ for any two vertices $u, w \in V(G) \setminus \{v_1, v_2, v_3\}$ and $d_{G^*}(u, z) = d_G(u, z)$ for any $z \in \{v_1, v_2, v_3\}$. Thus $\mathrm{Tr}_{G^*}(u) = \mathrm{Tr}_G(u)$ for any vertex $u \in V(G) \setminus \{v_1, v_2, v_3\}$ with $\mathrm{Tr}_{G^*}(v_3) = y + n - 5$, $\mathrm{Tr}_{G^*}(v_2) = y + n - 4$, and $\mathrm{Tr}_{G^*}(v_1) = y + 2n - 7$.

Let $G_1 = G - \{v_1, v_2, v_3\}$. Then $\mathrm{Tr}_{G^*}(G) = \mathrm{Tr}_G(G_1) \cup \Big(\{n-5, n-4, 2n-7\} + y\Big)$ from the above argument. From the assumptions, $\mathrm{Tr}_G(G_1)$ is pairwise disjoint and $y + n - 5 > t$ for any $t \in \mathrm{Tr}_G(G_1)$. Therefore G^* is transmission irregular. $\square$

Two examples of graphs of order 21 satisfying the conditions of (i) and (ii), respectively, in Theorem 4.3 are provided in Figs. 7 and 8 where a specific vertex v is given with $\mathrm{Tr}_G(v) = x$ and $\mathrm{Tr}(G) = \{a_u : u \in V(G)\} + x$ for all the values of a_u being labelled. That is, the transmission of v is x, and the transmission of every other vertex is equal to the sum of x and the value next to the vertex.

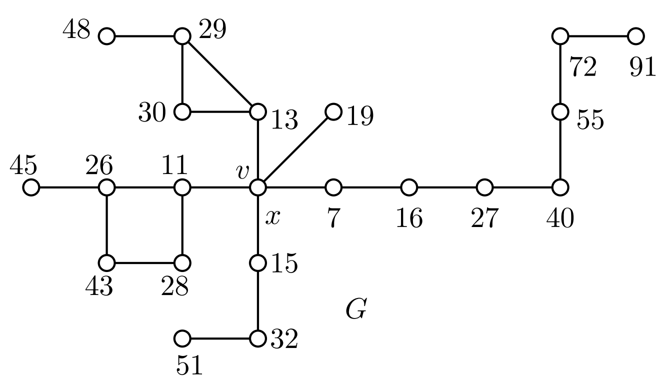

Figure 7: Graph G satisfying the condition (i) in Theorem 4.3.

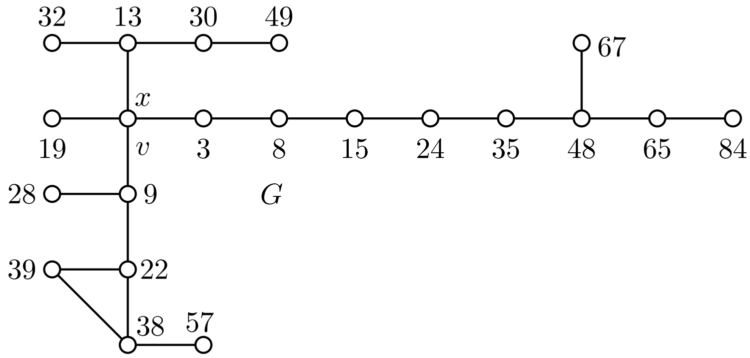

Figure 8: Graph G satisfying the condition (ii) in Theorem 4.3.

5 Concluding remarks

In this paper we prove the TI property of some chemical graphs and provide the method of construct new TI graphs.

Note that there are some transmission irregular chemical graphs of even order $n = 4a + 4$ with $a \neq 2 \bmod 3$. Combining this fact with Theorem 3.2, we pose the following problem.

Problem 5.1 *Does there exist a TI chemical graph of every even order?*

Note that Theorem 3.2 implicitly provides a method constructing TI chemical trees from known TI ones by attaching a pendant vertex at each of their leaves. Theorem 4.3 naturally leads to the following two problems.

Problem 5.2 *Establish additional methods for constructing TI graphs from known TI graphs.*

Problem 5.3 *Characterize TI chemical graphs G which preserve TI property after joining two nonadjacent vertices.*

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