On graphs whose Wiener complexity equals their order and on Wiener index of asymmetric graphs

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Abstract

If u is a vertex of a graph G, then the transmission of u is the sum of distances from u to all the other vertices of G. The Wiener complexity $C_W(G)$ of G is the number of different complexities of its vertices. G is transmission irregular if $C_W(G) = n(G)$. It is proved that almost no graphs are transmission irregular. Let T_{n_1,n_2,n_3} be the tree obtained from paths of respective lengths n_1, n_2, and n_3, by identifying an end-vertex of each of them. It is proved that T_{1,n_2,n_3} is transmission irregular if and only if $n_3 = n_2 + 1$ and $n_2 \notin \{(k^2-1)/2, (k^2-2)/2\}$ for some $k \geq 3$. It is also proved that if T is an asymmetric tree of order n, then the Wiener index of T is bounded by $(n^3-13n+48)/6$ with equality if and only if $T = T_{1,2,n-4}$. A parallel result is deduced for asymmetric uni-cyclic graphs.

Key words: Wiener index; Wiener complexity; asymmetric graphs; trees; uni-cyclic graphs

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1 Introduction

If $G = (V, E)$ is a graph and $u \in V$, then the *transmission* of u (also known as the *distance* of u or the *remoteness* of u) is defined as the sum of distances from

u to all the other vertices of G, that is, $\mathrm{Tr}_G(u) = \sum_{x \in V} d_G(u,x)$, see [1, 26, 28]. Here $d_G(u,x)$ is the standard shortest path distance between u and x in G. We will shortly write $\mathrm{Tr}(u)$ and $d(u,x)$, whenever G will be clear from the context. The *Wiener index* $W(G)$ of G is the sum of the distances between all pairs of vertices of G, in other words, $W(G) = \frac{1}{2}\sum_{u \in V(G)} \mathrm{Tr}(u)$. The papers [11,16,25,30] are some classical references on the Wiener index; to see the extent to which it has already been investigated we refer to surveys [9, 10, 20] and selected recent papers [4, 7, 8, 13, 15, 17, 18, 22, 24, 29]. Transmission of a vertex is also important elsewhere, notably in location theory where vertices with extremal transmission are of interest because they are target locations for facilities, cf. [5, 21, 27].

The fact that the sum of the transmissions of all the vertices of G is twice the Wiener index of G, led in [2] to the introduction of the *Wiener complexity* $C_W(G)$ as the number of different transmissions in G. Actually, C_W was named *Wiener dimension* and denoted $\dim_{\mathrm{W}}$ in [2], but here we rather follow the notation and terminology of a general approach from [3]. In this approach, the *I-complexity* C_I of an arbitrary summation-type topological index I is defined as the number of different contributions to I in its summation formula.

Call a graph G to be *transmission regular* [23] if all its vertices have the same transmission and *transmission irregular* if its vertices have pairwise different transmissions. In other words, transmission irregular graph are the graphs that have the largest possible Wiener complexity over all graphs of a given order. The reader can easily verify that each of the three graphs drawn in Fig. 1 is a transmission irregular graph.

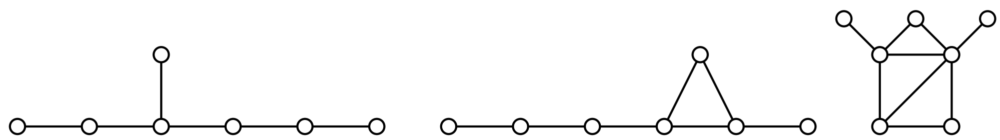

Figure 1: Sporadic examples of transmission irregular graphs

In this paper we are interested in transmission irregular graphs and proceed as follows. In the rest of the section terminology and notation needed are stated. In the next section we first show that almost all graphs are not transmission irregular. Then we introduce the trees T_{n_1,n_2,n_3} and characterize transmission irregular trees among the trees T_{1,n_2,n_3}. We also prove that if a graph G has at least three vertices of the same degree, then G and its complement cannot be both transmission irregular. In Section 3 we prove two extremal results on the Wiener index of asymmetric trees and of asymmetric uni-cyclic graphs and deduce corresponding consequences for transmission irregular graphs. In particular, if T is a transmission irregular tree of order n and $W(T) = (n^3 - 13n + 48)/6$, then $T = T_{1,2,3}$.

All graphs considered in this paper are connected. The order of a graph G is denoted with $n(G)$ and the degree of $u \in V(G)$ with $\deg(u)$. The *distance* $d_G(u,v)$ ($d(u,v)$ for short) is the number of edges on a shortest u,v-path. The *eccentricity* $\mathrm{ecc}_G(u)$ ($\mathrm{ecc}(u)$ for short) of a vertex u is the maximum distance between u and the other vertices. The *diameter* $\mathrm{diam}(G)$ of G is the maximum eccentricity of its vertices. The automorphism group of G is denoted with $\mathrm{Aut}(G)$. A graph is *asymmetric* if $|\mathrm{Aut}(G)| = 1$. Finally, for a positive integer n we use the notation $[n] = \{1, \ldots, n\}$.

2 Transmission irregular graphs are rare

An automorphism of a graph preserves the distance function. Hence, if u and v are vertices of a graph G such that $\alpha(u) = v$ holds for some $\alpha \in \mathrm{Aut}(G)$, then $\mathrm{Tr}(u) = \mathrm{Tr}(v)$. It follows that a transmission irregular graph is asymmetric and, as it well known, almost all graphs are asymmetric [12]. On the other hand, the fraction of transmission irregular graphs among asymmetric graphs is small as the next result asserts.

Theorem 2.1 *Almost all graphs are not transmission irregular.*

Proof. It is well known that almost every graph has diameter 2. Hence the conclusion of the theorem will follow after proving that a transmission irregular graph $G = (V, E)$ has $\mathrm{diam}(G) \geq 3$. Suppose then that $\mathrm{diam}(G) = k$. Clearly, $k \neq 1$ as complete graphs are not transmission irregular. Suppose that $k = 2$. Then for any vertex $u \in V$ we have $\mathrm{Tr}(u) = \deg(u) + 2(n(G) - 1 - \deg(u)) = 2n(G) - 2 - \deg(u)$. Since at least two vertices are of the same degree, they have the same transmission. We conclude that $k \geq 3$. $\square$

Transmission irregular graphs are thus rare. To increase the family of known such graphs, motivated by the leftmost transmission irregular graph from Fig. 1, we introduce the following family of trees. Let n_1, n_2, n_3 be integers for which $1 \le n_1 < n_2 < n_3$ holds. Then the tree T_{n_1,n_2,n_3} has the vertex set

$$\{u\} \cup \{x_1, \dots, x_{n_1}\} \cup \{y_1, \dots, y_{n_2}\} \cup \{z_1, \dots, z_{n_3}\},$$

and the edge set

$$\{ux_1, x_1x_2, \dots, x_{n_1-1}x_{n_1}\} \cup \{uy_1, y_1y_2, \dots, y_{n_2-1}y_{n_2}\} \cup \{uz_1, z_1z_2, \dots, z_{n_3-1}z_{n_3}\}.$$

The tree T_{n_1,n_2,n_3} can be described as the graph obtained from paths of respective lengths n_1, n_2, and n_3, by identifying an end-vertex of each of them. Note that $T_{1,2,3}$ is the leftmost transmission irregular graph from Fig. 1. Ideally, we would like to characterize transmission irregular trees among the trees T_{n_1,n_2,n_3}. For this sake it is not difficult to deduce the following equations:

$$\mathrm{Tr}(x_i) = \binom{n_1 - i + 1}{2} + \binom{n_2 + i + 1}{2} + \binom{n_3 + i + 1}{2} - \binom{i+1}{2}, \quad (1)$$

$$\mathrm{Tr}(y_j) = \binom{n_2 - j + 1}{2} + \binom{n_1 + j + 1}{2} + \binom{n_3 + j + 1}{2} - \binom{j+1}{2}, \quad (2)$$

$$\mathrm{Tr}(z_k) = \binom{n_3 - k + 1}{2} + \binom{n_1 + k + 1}{2} + \binom{n_2 + k + 1}{2} - \binom{k+1}{2}, \quad (3)$$

$$\mathrm{Tr}(u) = \binom{n_1 + 1}{2} + \binom{n_2 + 1}{2} + \binom{n_3 + 1}{2}, \quad (4)$$

where $i \in [n_1]$, $j \in [n_2]$, and $k \in [n_3]$. Hence T_{n_1,n_2,n_3} is transmission irregular if and only if the transmissions in Equations (1)-(4) are pairwise different. However, to characterize the triples (n_1, n_2, n_3) for which this is the case might be a difficult problem. This assertion is in part supported by Table 1, where a list of parameters (n_1, n_2, n_3) is given for $2 \le n_1 < n_2 < n_3 \le 15$ for which T_{n_1,n_2,n_3} is transmission irregular.

The case $n_1 = 1$ is not included in Table 1 because in this case we can give a complete characterization as follows.

Theorem 2.2 *If $1 = n_1 < n_2 < n_3$, then T_{1,n_2,n_3} is transmission irregular if and only if $n_3 = n_2 + 1$ and $n_2 \notin \{(k^2 - 1)/2, (k^2 - 2)/2\}$ for some $k \ge 3$.*

To prove Theorem 2.2 the following lemma will be useful. Its proof is straightforward and hence omitted. The notation of the lemma is illustrated in Fig. 2.

n_1	n_2	n_3	n_1	n_2	n_3	n_1	n_2	n_3	n_1	n_2	n_3	n_1	n_2	n_3
2	5	7	2	13	15	4	7	9	6	11	13	8	11	13
2	6	8	3	4	5	4	11	13	6	13	14	9	10	11
2	8	9	3	5	6	4	12	13	7	8	9	9	11	12
2	9	11	3	9	10	5	6	7	7	8	12	10	13	15
2	11	12	3	13	14	5	7	8	7	9	10	11	12	13
2	11	13	3	14	15	5	7	12	7	13	14	11	13	14
2	12	13	4	7	8	5	10	11	8	11	12	13	14	15

Table 1: Triples (n_1, n_2, n_3), $2 \leq n_1 < n_2 < n_3 \leq 15$, for which T_{n_1,n_2,n_3} is transmission irregular

Lemma 2.3 *Let u and v be vertices of a tree T and let P be the u,v-path in T. Let $Q = P - \{u, v\}$, and let $G - Q = T_u \bigcup T_v \bigcup S$, where T_u and T_v are the components containing u and v, respectively, and S is the union of the other components. Then*

$$\mathrm{Tr}(u) - \mathrm{Tr}(v) = (|T_v| - |T_u|)\, d(u, v) + \sum_{w \in V(S)} (d(u, w) - d(v, w)) \,.$$

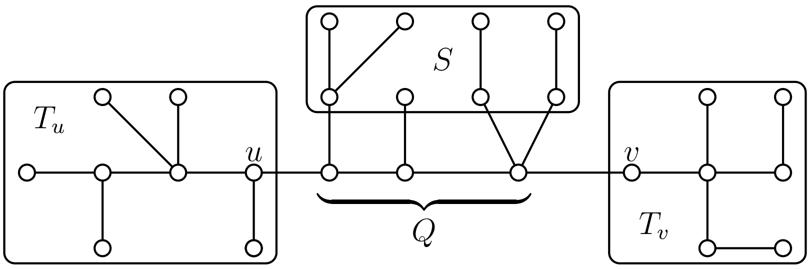

Figure 2: Example to the notation of Lemma 2.3

Proof. (of Theorem 2.2) Suppose first that $n_1 = 1$ and $n_3 = n_2 + 1$. Set $n = n(T_{1,n_2,n_2+1})$, that is, $n = 2n_2 + 3$. Then we can simplify the general notation of the vertices of T_{n_1,n_2,n_3} as follows. Let $V(T_{1,n_2,n_2+1}) = \{v_1, \ldots, v_n\}$, where $v_1, \ldots, v_{n-1}$ induce a path of order $n - 1$ and v_n is adjacent to $v_{\frac{n+1}{2}}$. This is indeed the tree T_{1,n_2,n_2+1}, where the vertices v_n and $v_{\frac{n+1}{2}}$ correspond to x_1 and u, respectively.

If $i \in [(n-1)/2]$, then Lemma 2.3 implies that

$$\mathrm{Tr}(v_i) - \mathrm{Tr}(v_{i+1}) = n - 2i \quad \text{and} \quad \mathrm{Tr}(v_i) - \mathrm{Tr}(v_{n-i}) = 1\,.$$

This implies that $\mathrm{Tr}(v_{i+1}) < \mathrm{Tr}(v_{n-i}) < \mathrm{Tr}(v_i)$ for $i \in [(n-1)/2]$ and consequently

$$\mathrm{Tr}(v_1) > \mathrm{Tr}(v_{n-1}) > \mathrm{Tr}(v_2) > \mathrm{Tr}(v_{n-2}) > \cdots > \mathrm{Tr}(v_{(n-1)/2}) > \mathrm{Tr}(v_{(n+1)/2})\,.$$

Hence the vertices $v_1, \ldots, v_{n-1}$ have pairwise distinct transmissions. It thus remains to show that $\mathrm{Tr}(v_n)$ is different from all other transmissions. By straightforward calculation we get that for $i \in [(n-1)/2]$,

$$\begin{aligned} \mathrm{Tr}(v_i) &= \frac{1}{2}\left(n^2 - 2in + 2i^2 - 2i + 3\right), \\ \mathrm{Tr}(v_{n-i}) &= \frac{1}{2}\left(n^2 - 2in + 2i^2 - 2i + 1\right), \end{aligned}$$

and that $\mathrm{Tr}(v_n) = (n^2 + 2n - 3)/4$. Suppose now that $\mathrm{Tr}(v_n) = \mathrm{Tr}(v_i)$ for some $i \in [n-1]$. Then $\mathrm{Tr}(v_n) = \mathrm{Tr}(v_i)$ or $\mathrm{Tr}(v_n) = \mathrm{Tr}(v_{n-i})$ for some $i \in [(n-1)/2]$ and

$$(n-1)^2 - 4in + (2i-1)^2 + 7 = 0 \tag{5}$$

or

$$(n-1)^2 - 4in + (2i-1)^2 + 3 = 0 \tag{6}$$

holds true. Solving (5), and having in mind that $i \leq (n-1)/2$, we get $i = (n - 2\sqrt{n-2} + 1)/2$. Since i is an integer this implies that n must be of the form $k^2 + 2$ for some integer k. Since $n = 2n_2 + 3$ this in turn implies that n_2 is of the form $(k^2-2)/2$. Similarly, the solution of (6) is $i = (n - 2\sqrt{n-1} + 1)/2$, hence in this case n must be of the form $k^2 + 1$, and consequently n_2 is of the form $(k^2-1)/2$.

To complete the proof we need to show that if $n_3 > n_2 + 1$, then T_{1,n_1,n_3} is not transmission irregular. Now, if $n_3 > n_2 + 1$, then using Lemma 2.3 one can indeed show that $\mathrm{Tr}(u) = \mathrm{Tr}(z_t)$ where $t = n_3 - n_2 - 1$. □

Note that the proof of Theorem 2.2 also reveals that if n_2 is of the form $(k^2-1)/2$ or $(k^2-2)/2$ for some $k \geq 3$, then $C_W(T_{1,n_2,n_2+1}) = 2n_2+2$. The smallest such integers are $n_2 = 4$ and $n_2 = 7$. For $T_{1,4,5}$ we have $\mathrm{Tr}(v_{11}) = \mathrm{Tr}(v_3) = 35$, while for $T_{1,7,8}$ we have $\mathrm{Tr}(v_{17}) = \mathrm{Tr}(v_{12}) = 80$.

We conclude the chapter with the following result that in a way supports Theorem 2.1. Recall that the *complement* $\bar{G}$ of a graph G is the graph with the same vertex set as G, and in which uv is an edge if and only if u is not adjacent to v in G.

Theorem 2.4 *If a graph G has three vertices of the same degree, then not both G and $\bar{G}$ are transmission irregular.*

Proof. If G is not transmission irregular, then there is nothing to prove. So assume in the rest that G is transmission irregular. We need to show that $\bar{G}$ is not transmission irregular.

From the proof of Theorem 2.1 we know that $\operatorname{diam}(G) \geq 3$. Then it follows that $\operatorname{diam}(\bar{G}) \leq 3$, see [6]. If $\operatorname{diam}(\bar{G}) = 2$, then $\bar{G}$ has at least two vertices of the same transmission and we are done. Hence assume in the rest that $\operatorname{diam}(\bar{G}) = 3$.

Let u, v, and w be vertices of G of the same degree in G (equivalently, of the same degree in $\bar{G}$). Since clearly the eccentricity of each vertex of $\bar{G}$ is either 2 or 3, at least two vertices among u, v, and w have the same eccentricity, say u and v. Let $\operatorname{ecc}_{\bar{G}}(u) = \operatorname{ecc}_{\bar{G}}(v) = k$, where $k \in \{2, 3\}$. If $k = 2$, then since u and v have the same degree, they also have the same transmission and we are done. So let $k = 3$. But then $\operatorname{ecc}_G(u) = \operatorname{ecc}_G(v) = 2$ which in turn implies that $\operatorname{Tr}_G(u) = \operatorname{Tr}_G(v)$, a contradiction with our assumption. $\square$

3 Two extremal results on the Wiener index

In this section we consider the graphs that have largest Wiener index among asymmetric trees and asymmetric uni-cyclic graphs. For the first class specific trees T_{n_1,n_2,n_3} appear as the extremal ones.

Theorem 3.1 *If T is an asymmetric tree of order $n = n(T)$, then*

$$W(T) \leq \frac{1}{6}\left(n^3 - 13n + 48\right) .$$

Moreover, equality holds if and only if $T = T_{1,2,n-4}$.

Proof. Let T be a tree that has the maximum Wiener index among all asymmetric trees of order n. Let P be a diametrical path in T. As T is asymmetric, $P \neq T$.

Let v be a leaf of T that does not lie on P. From the well known fact that the path P_n has the maximum Wiener index among all graphs of order n (and hence among all trees of the same order), we get

$$W(T) = W(T - v) + \mathrm{Tr}(v) \leq W(P_{n-1}) + \mathrm{Tr}(v)\,. \tag{7}$$

Since T is asymmetric and v does not lie on the diametrical path P, we have $\mathrm{ecc}(v) \leq n-3$. (Indeed, $\mathrm{ecc}(v) = n-2$ would mean that $T = T_{1,1,n-3}$ which has a non-trivial automorphism.) This in turn implies that $\mathrm{Tr}(v)$ is largest possible if v is adjacent to the third vertex of P (or the third before last vertex of P for that matter). As T has the maximum possible Wiener index, we must have equality in (7), which implies that $T - v = P_{n-1}$ and v is adjacent to the third (or the before last third vertex) of P_{n-1}, that is, $T = T_{1,1,n-4}$. Finally,

$$W(T_{1,1,n-4}) = W(P_{n-1}) + \mathrm{Tr}(v) = \binom{n}{3} + \left(\binom{n-2}{2} + 5\right) = \frac{n^3 - 13n + 48}{6}\,.$$

□

Combining Theorems 2.2 and 3.1 we get:

Corollary 3.2 *If T is a transmission irregular tree of order $n = n(T)$ and $W(T) = (n^3 - 13n + 48)/6$, then $n = 7$ and $T = T_{1,2,3}$.*

We now turn our attention to uni-cyclic graphs. Let U_n, $n \geq 7$, be the uni-cyclic graph with $V(U_n) = \{v_1, \ldots, v_n\}$, where the vertices $v_1, \ldots, v_{n-1}$ induce P_{n-1} and v_n is adjacent to v_{n-2} and v_{n-3}. Note that U_7 is the middle graph from Fig. 1.

Theorem 3.3 *If G is an asymmetric, uni-cyclic graph of order $n = n(G)$, then*

$$W(G) \leq \frac{1}{6}\left(n^3 - 13n + 36\right)\,.$$

Moreover, the equality holds if and only if $G = U_n$.

Proof. Since G is uni-cyclic and asymmetric, it contains at least two pendant vertices. Let v be a pendant vertex with the largest transmission among all pendant vertices of G and let w be another pendant vertex. Now consider the following transformation. Let G' be the graph obtained from G by removing the vertex w and attaching a new vertex w' to the vertex v. Then we have:

$$\begin{aligned} W(G') &= W(G-\{v,w\}) + \mathrm{Tr}_{G'}(v) + \mathrm{Tr}_{G'}(w') - 1 \\ &= W(G-\{v,w\}) + (\mathrm{Tr}_G(v) - d_G(v,w) + 1) + \\ &\quad (\mathrm{Tr}_G(v) - d_G(v,w) + n - 1) - 1\,, \\ W(G) &= W(G-\{v,w\}) + \mathrm{Tr}_G(v) + \mathrm{Tr}_G(w) - d(v,w)\,. \end{aligned}$$

Thus

$$W(G') - W(G) = \mathrm{Tr}(v) - \mathrm{Tr}(w) - d_G(v,w) + n - 1 \geq (n-1) - d_G(v,w)\,.$$

Since $d_G(v,w) < n-1$ it follows that $W(G') - W(G) > 0$.

Let C be the unique cycle of G. Since G is asymmetric, at least two vertices of C are of degree at least 3. Let $H(n,k,i)$ be the unicyclic graph constructed from the cycle C_k on the vertex set $\{v_1,\ldots,v_k\}$ by attaching the path P_{n-k-1} to the vertex v_1 and attaching a pendant vertex v to the vertex v_i. (Note that $H(n,3,2) = U_n$.)

Let $H = H(n,k,i)$. Using the above transformation we get that $W(G) \leq W(H_{n,k,i})$. Clearly $W(H) = W(H-v) + \mathrm{Tr}_H(v)$. Let H' be the graph obtained from H by removing the vertex v and connecting a new vertex v' to $v_{[k/2]}$. Since the vertex $v_{[k/2]+1}$ has the largest transmission among the vertices of C_k in the graph $H-v$, we have $W(H) \leq W(H')$. Let now $G(n,k)$ be the graph obtained from the cycle C_k by attaching an end vertex of the path of order $n-k$ to a vertex of C_k. In [31] it was proved that among the unicyclic graphs of order n, the graph $G(n,3)$ has the maximum Wiener index. Thus

$$\begin{aligned} W(G) &\leq W(H) \leq W(H') \\ &= W(H'-v) + \mathrm{Tr}_{H'}(v) \\ &\leq W(G(n-1,3)) + \mathrm{Tr}_{H'}(v)\,. \end{aligned}$$

Now, it is not difficult to see that $\mathrm{Tr}_{H'}(v) \leq \mathrm{Tr}_{H(n,3,2)}(v)$ and consequently

$$\begin{aligned} W(G) &\leq W(G(n-1,3)) + \mathrm{Tr}_{H(n,3,2)}(v) \\ &= W(H(n,3,2)) = W(U_n)\,. \end{aligned}$$

Moreover, the equality holds if and only if $G = U_n$. By a simple calculation we get $W(U_n) = \frac{1}{6}(n^3 - 13n + 36)$ and we are done. □

Corollary 3.4 *If G is a transmission irregular uni-cyclic graph of order $n = n(G)$ and $W(G) = (n^3 - 13n + 36)/6$, then $n = 7$ and $G = U_7$.*

Proof. By Theorem 3.3 we only need to prove that U_7 is the unique transmission irregular graph among the graphs U_n. We already know that U_7 is transmission irregular. On the other hand, if $n \geq 8$, then in U_n the vertices v_4 and v_{n-3} have the same transmission. □

We conclude the section with one more consequence of Theorem 3.3. For its statement recall that the *line graph* $L(G)$ of a graph G has the edge set of G as its vertex set, two different vertices of $L(G)$ being adjacent if the corresponding edges of G share a vertex. (We refer to [14,19] for a couple of recent investigations of the Wiener index of line graphs.)

Corollary 3.5 *Let G be a graph of size m let its line graph $L(G)$ be asymmetric. Then $W(L(G)) \leq \frac{1}{6}(m^3 - 13m + 36)$, where the equality holds if and only if $G = T_{1,2,m-3}$.*

Proof. If $\Delta(G) \leq 2$, then G is either a path or a cycle, hence $L(G)$ is not asymmetric. Hence $\Delta(G) \geq 3$ and thus $L(G)$ contains at least one cycle. By Theorem 3.3 we have $W(L(G)) \leq W(U_m)$ and the equality holds if and only if $L(G) = U_m$. This implies that $G = T_{1,2,m-3}$. □

4 Concluding remarks

In this paper we have introduced transmission irregular graphs as the graphs in which all vertices have pairwise different transmissions. Characterizing transmission irregular trees within the family of trees T_{1,n_2,n_3} an infinite family of transmission irregular graphs was constructed. All these trees are of odd order. Hence it would be of interest also to construct an infinite family of transmission irregular trees each tree being of even order. We also ask as an open problem whether there exist infinite families of 2-connected transmission irregular graphs, and whether there exist infinite families of regular graphs that are transmission irregular.

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