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On the Extremal Energies of Trees*

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Abstract. The energy of a graph is defined as the sum of the absolute values of its all eigenvalues. Gutman [Acyclic systems with extremal Hückel π-electron energy, Theoret. Chim. Acta 45(1977) 79-87] characterized the trees with n vertices having the minimal, the second-minimal, the third-minimal, the fourth-minimal, the maximal, and the second-maximal energies. In this paper, as the continuance of it, we determine the trees with n vertices having the fifth-minimal, the sixth-minimal, the seventh-minimal, and the third-maximal energies. As a consequence, we determine the tree with n vertices having extremal Hosoya index. And at the same time, we in part solve a conjecture proposed by Zhou and Li.

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1. Introduction

All graphs in this paper are finite, undirected and simple. Let G be a graph on n vertices. We denote the number of vertices in G by $|G|$, the number of edges in G by $||G||$, and the diameter of G by $d(G)$. The *characteristic polynomial* of G, denoted here by $P(G,x)$, is defined as $P(G,x) = \det(xI - A)$, where I is the identity matrix of order n and $A(G)$ is the adjacency matrix of G. The eigenvalues $x_1, x_2, \ldots, x_n$ of the adjacency matrix of G are called the *eigenvalues* of G. The *energy* of G, denoted by $E(G)$, is defined as

$$E(G) = \sum_{i=1}^{n} |x_i|.$$

Historically chemists used the model in which the experimental heats of formation of conjugated hydrocarbons are closely related to the total π-electron energy. Today such a model is over-simplistic, but nevertheless HMO has some value as it points to that part of the experimental heats of formation of conjugated hydrocarbons that can be viewed as due to molecular connectivity (molecular topology). The calculation of the total π-electron energy in a conjugated hydrocarbon can be reduced (within the framework of the HMO approximation; see e. g., [10, 11]) to $E(G)$ of the corresponding graph G. There are numerous results on $E(G)$ (e.g., see, [1, 3, 5-10, 12-24, 26-31, 33-38]), including on graphs with extremal energies [3,6,15,16,19,22-24,28,29,31,33-37,40-43].

For a graph G, let $m(G,k)$ be the number of the k-matchings of G, $k \geqslant 1$, and define $m(G,0) = 1$. If G is an acyclic graph on n vertices, then the energy of G can be expressed in terms of the Coulson integral formula [11] as

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left(\sum_{k=0}^{\lfloor n/2 \rfloor} m(G,k) x^{2k} \right) dx, \tag{1.1}$$

where

$$P(G,x) = x^n - m(G,1)x^{n-2} + m(G,2)x^{n-4} - \cdots + (-1)^k m(G,k) x^{n-2k} \tag{1.2}$$

is the characteristic polynomial of the corresponding acyclic graph G and n is the number of vertices in G.

Thus, by (1.1), $E(G)$ is a strictly monotonically increasing function of $m(G,k)$, $k = 1,\ldots,\lfloor n/2 \rfloor$. This observation led Gutman [6] to define a *quasi-order* over the set of all acyclic graphs: if G_1 and G_2 are two acyclic graphs, then

$$G_1 \succeq G_2 \Leftrightarrow m(G_1,k) \geqslant m(G_2,k) \text{ for all } k \geqslant 1.$$

If $G_1 \succeq G_2$, and there is a j such that $m(G_1,j) > m(G_2,j)$, then we write $G_1 \succ G_2$. Therefore,

$$G_1 \succ G_2 \Rightarrow E(G_1) > E(G_2).$$

If neither $G_1 \preceq G_2$ nor $G_2 \preceq G_1$, then G_1 and G_2 are said to be *incomparable.* This increasing property of energy has been used in the study of extremal values of energy over some significant classes of graphs. For instance, Gutman [6] determined trees with minimal, second-minimal, third-minimal and fourth-minimal energies, Zhang and Li characterized the trees with minimal energy [33] and maximal energy [34], respectively, among the trees with perfect matchings. Hou determined the graphs with minimal energy among all the trees with a given size of perfect matching [16] and all unicyclic graphs [15], respectively. Zhang et al. determined the graphs with maximal energy [35] and minimal energy [36], respectively, among the hexagonal chains. Yan and Ye characterized the tree with maximal energy among the trees with order n and at least $\lfloor \frac{n+2}{2} \rfloor$ pendent vertices [29]. Lin et al. [24] determined the tree with maximal energy among the trees with order n and maximum degree $\Delta(3 \leqslant \Delta \leqslant n-2)$ and the tree with minimal energy among the trees with order n and maximum degree $\Delta(\lceil \frac{n+1}{3} \rceil \leqslant \Delta \leqslant n-2)$. Recently, Yu and Lv [31] characterized the tree with minimal energy among the trees with k pendent vertices. Some most recent results along these lines are found in [40-43].

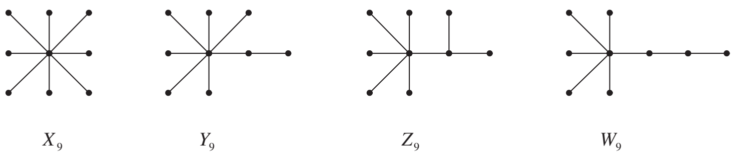

Figure 1: X_9, Y_9, Z_9, and W_9.

Let P_n denote the path with n vertices, where the vertices $1, 2, \ldots, n$ are labelled so that the vertices 1 and n are the terminal and the vertices j and $j+1$ are adjacent ($j = 1, 2, \ldots, n-1$), $P_n(i)m$ denote the graph obtained by joining the terminal vertex of P_m to the i-th vertex of P_n, where $1 \leqslant i \leqslant \lceil \frac{n}{2} \rceil$. For convenience we denote $P_n(i)m$ in an abbreviated manner as $n(i)m$. Let $\mathscr{T}_n$ be the collection of all trees with (exactly) n vertices. Gutman [6] proved that

$$E(X_n) < E(Y_n) < E(Z_n) < E(W_n) < E(T) < E(n-2(3)2) < E(P_n)$$

for any tree $T \in \mathscr{T}_n$ and $T \neq X_n, Y_n, Z_n, W_n, n-2(3)2, P_n$, where X_n is the star $K_{1,n-1}$, Y_n is the graph obtained by attaching a pendent edge to a pendent vertex of $K_{1,n-2}$, Z_n by attaching two pendent edges to a pendent vertex of $K_{1,n-3}$, and W_n by attaching a P_3 to a pendent vertex of $K_{1,n-3}$. Figure 1 shows X_9, Y_9, Z_9, and W_9. A *pendent vertex* is a vertex of degree one, and a *pendent edge* is an edge incident with a pendent vertex. A *caterpillar* is a tree in which a removal of all pendent vertices makes a path. Let $T(n, d; n_1, \ldots, n_{d-1}) \in \mathscr{T}_{n,d}$ be a caterpillar obtained from a path $v_0, v_1, \ldots, v_d$ by adding $n_i (n_i \geqslant 0)$ pendent edges to $v_i (i = 1, \ldots, d-1)$. And in this paper, if T_1 and T_2 are isomorphic, we denote it by $T_1 = T_2$. Let $\mathscr{T}_{n,d}$ denote the set of trees on n vertices and diameter d, where $2 \leqslant d \leqslant n-1$. Obviously, $T \in \mathscr{T}_{n,2}$ is a star $K_{1,n-1}$, while $T \in \mathscr{T}_{n,n-1}$ is a path P_n. So we assume in the following that $3 \leqslant d \leqslant n-2$.

Yan and Ye [28] proved that $T(n, d; n-d-1, 0, \ldots, 0)$ is the unique tree with minimal energy in $\mathscr{T}_{n,d}$. Zhou and Li [37] proved that the trees with the second-minimal energy in $\mathscr{T}_{n,d}$ are $T(n, d; 0, 0, n-d-1, 0, \ldots, 0)$ if $d \geqslant 6$, $T(n, 3; 1, n-5)$ if $d = 3$, $T(n, 4; 1, 0, n-6)$ or $T(n, 4; 0, n-5, 0)$ if $d = 4$, $(n \geqslant 7)$, $T(n, 5; 1, 0, 0, n-7)$ or $T(n, 5; 0, n-6, 0, 0)$ if $d = 5$ $(n \geqslant 8)$, and they also proposed the following conjecture

Conjecture 1.1. *$T(n, 4; 1, 0, n-6)$ $(n \geqslant 7)$ and $T(n, 5; 0, n-6, 0, 0)$ $(n \geqslant 9)$ achieve the second-minimal energy in the class of trees on n vertices and diameter d for $d = 4$ and $d = 5$, respectively.*

In this paper, we show that the Conjecture 1.1 is true for $d = 4$; while for $d = 5$ we has showed that the conjecture is also true [23].

Let G be a graph and st an edge of G, we denote by $G - st$ (respectively, $G - s$) the graph obtained from G by deleting the edge st (respectively, by deleting the vertex s and the edges incident with it).

Lemma 1.2 ([6]). *Let T be a tree with n vertices and uv an edge of T. Then*

$$m(T,k) = m(T - uv, k) + m(T - u - v, k - 1),$$

especially, if v is a pendent vertex of T with pendent edge uv, then $m(T,k) = m(T-v,k)+m(T - u - v, k - 1)$, where $k = 1, 2, \ldots, \lceil \frac{n}{2} \rceil$.

Lemma 1.3 ([6]). *$n - 1(i)1 \prec n - 1(3)1$, if $i \neq 1, 3$ and $1 \leqslant i \leqslant \lceil \frac{n-1}{2} \rceil$.*

Lemma 1.4 ([6]). *$P_l \succ P_2 \cup P_{l-2} \succ \cdots \succ P_{2k} \cup P_{l-2k} \succ P_{2k+1} \cup P_{l-2k-1} \succ P_{2k-1} \cup P_{l-2k+1} \succ \cdots \succ P_1 \cup P_{l-1}$, where $l = 4k + r, 0 \leqslant r \leqslant 3$.*

Lemma 1.5 ([6]). *If T is a tree with n vertices and $T \neq X_n, Y_n, Z_n, W_n, P_{n-2}(3)2, P_n$, then $E(X_n) < E(Y_n) < E(Z_n) < E(W_n) < E(T) < E(P_{n-2}(3)2) < E(P_n)$. Furthermore, $X_n \prec Y_n \prec Z_n \prec W_n \prec T \prec P_{n-2}(3)2 \prec P_n$.*

It is easy to see that $m(X_n, 1) = m(Y_n, 1) = m(Z_n, 1) = m(W_n, 1) = n-1$, $m(X_n, k) = 0$ if $k \geqslant 2$, $m(Y_n, 2) = n - 3$, $m(Y_n, k) = 0$ if $k \geqslant 3$, $m(Z_n, 2) = 2n - 8$, $m(Z_n, k) = 0$ if $k \geqslant 3$, $m(W_n, 2) = 2n - 7$, $m(W_n, k) = 0$ if $k \geqslant 3$.

Lemma 1.6 ([28]). *Let G be a forest of order $n(n > 1)$ and G' be a spanning subgraph (respectively, a proper spanning subgraph) of G, then $G \succeq G'$ (respectively, $G \succ G'$).*

This paper is organized as follows. In Section 1 we give the introduction and preliminary results. In Section 2 we determine the trees with n vertices having fifth-minimal, sixth-minimal, seventh-minimal energies and show that Conjecture 1.1 is true for $d = 4$. In Section 3 we characterize the tree with n vertices having the third-maximal energy. In the last section we study the trees with n vertices having extremal Hosoya index.

2. Trees with minimal energy

In this section we determine the trees in $\mathscr{T}_n$ with fifth-minimal, sixth-minimal, and seventh-minimal energies.

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be graphs with $V_1 \bigcap V_2 = \emptyset$. If G is obtained by joining a vertex u of G_1 to a vertex v of G_2 by an edge, we denote it by $G = G_1u : vG_2$, that is to say, $G = (V, E)$ for $V = V_1 \cup V_2$ and $E = E_1 \cup E_2 \cup \{uv\}$. We denote the star of n vertices by $K_{1,n-1}$ and denote the degree of a vertex v in G by $d_G(v)$. If e is an edge of the graph G, we denote it by $e \in G$. Let T be a tree and $e \in T$, then $T - e = T'_e \cup T''_e$, where T'_e and T''_e are the two components of $T - e$. Let $||T'_e|| = a_e$ and $||T''_e|| = b_e$. Without loss of generality, we always assume that $a_e \geqslant b_e$, $e = uv$, $u \in T'_e$ and $v \in T''_e$.

Theorem 2.1. *Among trees with n ($n \geqslant 6$) vertices, the graph with the fifth-minimal energy is D_n, where $D_n = K_{1,n-5}u : vK_{1,3}$; see Figure 2.*

Proof. By Lemma 1.2, we have

$$\begin{aligned} m(D_n, k) &= m(D_n - uv, k) + m(D_n - u - v, k-1) \\ &= m(K_{1,n-5} \cup K_{1,3}, k) + m((n-2)P_1, k-1) \\ &= m(K_{1,n-5} \cup K_{1,3}, k). \end{aligned}$$

So, $m(D_n, 1) = n - 1$, $m(D_n, 2) = 3n - 15$ and $m(D_n, k) = 0$ if $k \geqslant 3$. Similarly, we have

$$m(H_n, 1) = n - 1, m(H_n, 2) = 2n - 7, m(H_n, 3) = n - 5 \;\text{ and }\; m(H_n, k) = 0 \;\text{ if } k \geqslant 4, \tag{2.1}$$

where $H_n = X_{n-2}u : vP_2$; see Figure 2. At first we show that if $T \neq X_n, Y_n, Z_n$, W_n, D_n, H_n, then either $E(T) > E(D_n)$ or $E(T) > E(H_n)$. Finally, we will compare the energy of D_n and H_n. We distinguish between the following three cases to show $E(T) > E(D_n)$ or $E(T) > E(H_n)$.

Case 1. There exists an edge $e \in T$ such that $b_e \geqslant 3$. Note that $a_e + b_e = n - 2$ for all $e \in T$, and each edge in T'_e with an edge in T''_e form a 2-matching of T. Then

$$m(T, 2) \geqslant 3(n-5) = 3n - 15 = m(D_n, 2).$$

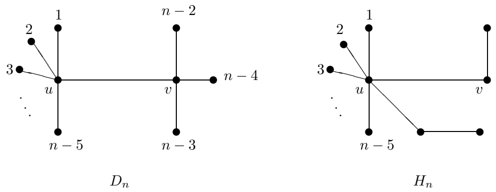

Figure 2: D_n and H_n

Since $T \neq D_n$, if $m(T,2) = m(D_n,2)$, then either $T'_e \neq K_{1,n-5}$ or $T''_e \neq K_{1,3}$. So we have $m(T,3) > m(D_n,3)$. Then $T \succ D_n$ follows easily, therefore $E(T) > E(D_n)$, and $E(T) = E(D_n)$ if and only if $T = D_n$.

Case 2. There exists an edge $e = uv \in T$ such that $b_e = 2$, i.e., $T''_e = P_3$. In order to prove the theorem in this case, we distinguish between the following two subcases.

Subcase 2.1. $T'_e \neq K_{1,n-4}$. By Lemma 1.5, we have $m(T'_e,k) \geqslant m(Y_{n-3},k)$ and $m(T'_e - u,k) \geqslant m(P_2,k)$ for all k and for any $u \in T'_e$.

If $d_{T''_e}(v) = 1$, then by Lemma 1.1, we have

$$\begin{aligned}
m(T,k) &= m(T-e,k) + m(T-u-v,k-1) \\
&= m(T'_e \cup T''_e,k) + m((T'_e-u) \cup (T''_e-v),k-1) \\
&= \sum_{j=0}^{k} m(T'_e,j)m(P_3,k-j) + \sum_{j=0}^{k-1} m(T'_e-u,j)m(P_2,k-1-j) \\
&\geqslant \sum_{j=0}^{k} m(Y_{n-3},j)m(P_3,k-j) + \sum_{j=0}^{k-1} m(P_2,j)m(P_2,k-1-j) \\
&= m(A_n,k),
\end{aligned}$$

where $A_n = Y_{n-3}u : vP_3$, $d_{Y_{n-3}}(u) = n-5$ and $d_{P_3}(v) \mp 1$. So $T \succeq A_n$ and $E(T) \geqslant E(A_n)$. Note that $m(A_n,1) = n-1$, $m(A_n,2) = 3n-12$, $m(A_n,3) = 2n-11$, and $m(A_n,k) = 0$ if $k \geqslant 4$. Then $m(H_n,k) \leqslant m(A_n,k)$, together with $m(H_n,2) < m(A_n,2)$. So it follows easily that $H_n \prec A_n$. Namely that $E(T) \geqslant E(A_n) > E(H_n)$.

Similarly, if $d_{T''_e}(v) = 2$, then we have $E(T) \geqslant E(B_n)$, where $B_n = Y_{n-3}u : vP_3$,

$d_{Y_{n-3}}(u) = n-5$ and $d_{P_3}(v) = 2$. So we have

$$m(B_n, k) = \sum_{j=0}^{k} m(Y_{n-3}, j)m(P_3, k-j) + m(P_2, k-1).$$

Then it follows easily that $m(B_n, 1) = n-1$, $m(B_n, 2) = 3n-13$, $m(B_n, 3) = 2n-12$ and $m(B_n, k) = 0$ if $k \geqslant 4$. Hence $H_n \prec B_n$, and it is easy to see that $B_n \prec A_n$, therefore

$$E(T) \geqslant E(B_n) > E(H_n) \text{ and } E(A_n) > E(B_n).$$

Subcase 2.2. $T'_e = K_{1,n-4}$. Note that $T \neq Z_n, W_n$. Then u is a pendent vertex of $K_{1,n-4}$. Let v' be the center vertex of $K_{1,n-4}$, it is easy to see that $b_{uv'} = 3$. Similar to Case 1, we have $E(T) \geqslant E(D_n)$ and $E(T) = E(D_n)$ if and only if $T = D_n$.

Case 3. There exists an edge $e = uv \in T$ such that $b_e = 1$. That is to say, $T''_e = P_2$. Note that $T \neq Y_n, Z_n$, then $T'_e \neq K_{1,n-3}$. By Lemma 1.5, we have $m(T'_e, k) \geqslant m(Y_{n-2}, k)$ and $m(T'_e - u, k) \geqslant m(P_2, k)$ for all k and for any $u \in T'_e$. Then we have

$$\begin{aligned} m(T, k) &= m(T-e, k) + m(T-u-v, k-1) \\ &= m(T'_e \cup T''_e, k) + m(T'_e - u, k-1) \\ &= \sum_{j=0}^{k} m(T'_e, j)m(T''_e, k-j) + m(T'_e - u, k-1) \\ &\geqslant \sum_{j=0}^{k} m(Y_{n-2}, j)m(P_2, k-j) + m(P_2, k-1) \\ &= m(H_n, k). \end{aligned}$$

Hence $E(T) > E(H_n)$, if $T \neq H_n$.

It is not difficult to calculate the spectra of the trees D_n and H_n. Then we get

$$E(D_n) = 2\sqrt{n-1+\sqrt{12n-60}}, \quad E(H_n) = 2 + 2\sqrt{n-2+\sqrt{4n-20}}.$$

¿From these formulas it is immediate to show that

$$E(D_n) < E(H_n)$$

holds for all $n \geqslant 5$. Hence, the fifth-minimal tree is D_n. □

Theorem 2.2. *Among trees with $n\,(n \geqslant 14)$ vertices, the graph of the sixth smallest energy is U_n, where $U_n = K_{1,n-5}u : vK_{1,3}$; see Figure 3.*

Proof. Note that $U_n = K_{1,n-5}u : vK_{1,3}$, where u is the center vertex of $K_{1,n-5}$ and v is the pendent vertex of $K_{1,3}$. Thus we have

$$\begin{aligned} m(U_n,k) &= m(U_n - uv, k) + m(U_n - u - v, k-1) \\ &= m(K_{1,n-5} \cup K_{1,3}, k) + m(P_3, k-1). \end{aligned}$$

Then $m(U_n,1) = n-1$, $m(U_n,2) = 3n-13$, and $m(U_n,k) = 0$ if $k \geqslant 3$.

At first, we will show that if $T \in \mathscr{T}_n$ and $T \neq X_n, Y_n, Z_n, W_n, D_n, H_n, U_n$, then $E(T) > E(U_n)$. We distinguish between the following three cases to prove it.

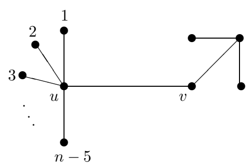

Figure 3: U_n

Case 1. There exists an edge $e \in T$ such that $b_e = 1$. Note that $T \neq Y_n, W_n$, then $T'_e \neq X_{n-2}$. We distinguish between the following two subcases in order to prove our result.

Subcase 1.1. $T'_e = Y_{n-2}$. If $d_{T'_e}(u) = n-4$, then $T = H_n$. Otherwise, we have $m(T'_e - u, k) \geqslant m(K_{1,n-5}, k)$ for all k and for any $u \in T'_e$. So,

$$\begin{aligned} m(T,k) &= m(T-e,k) + m(T-u-v,k-1) \\ &= m(Y_{n-2} \cup P_2, k) + m(T'_e - u, k-1) \\ &\geqslant m(Y_{n-2} \cup P_2, k) + m(K_{1,n-5}, k-1) \\ &= m(L_n, k), \end{aligned}$$

where $L_n = Y_{n-2}u : vP_2$ and $d_{Y_{n-2}}(u) = 2$. Therefore, $m(L_n,1) = n-1$, $m(L_n,2) = 3n-13$, $m(L_n,3) = n-5$ and $m(L_n,k) = 0$ if $k \geqslant 4$. It is easy to see that $U_n \prec L_n \preceq T$, hence $E(U_n) < E(L_n) \leqslant E(T)$.

Subcase 1.2. $T'_e \neq Y_{n-2}$. By Lemma 1.5, we have $m(T'_e, k) \geqslant m(Z_{n-2}, k)$ for all k and $m(T'_e - u, k) \geqslant m(P_3, k)$ for any $u \in T'_e$. Therefore

$$\begin{aligned} m(T,k) &= m(T-e,k) + m(T-u-v,k-1) \\ &= m(T'_e \cup T''_e, k) + m((T'_e - u) \cup (T''_e - v), k-1) \\ &= \sum_{j=0}^{k} m(T'_e, j) m(P_2, k-j) + m(T'_e - u, k-1) \\ &\geqslant \sum_{j=0}^{k} m(Z_{n-2}, j) m(P_2, k-j) + m(P_3, k-1) \\ &= m(R_n, k), \end{aligned}$$

where $R_n = Z_{n-2}u : vP_2$, and $d_{Z_{n-2}}(u) = n-5$. It is easy to see that $m(R_n, 1) = n-1$, $m(R_n, 2) = 3n-13$, $m(R_n, 3) = 2n-12$, and $m(R_n, k) = 0$ if $k \geqslant 4$. Hence $R_n \succ U_n$ and $E(R_n) > E(U_n)$.

Case 2. There exists an edge $e \in T$ such that $b_e = 2$, i.e., $T''_e = P_3$.

If $T'_e \neq K_{1,n-4}$, then, by the proof of Subcase 2.1 in Theorem 2.1, we have $E(T) \geqslant E(B_n)$ for $T \neq X_n, Y_n, Z_n, W_n, D_n$ and H_n. It is easy to see that $B_n \succ U_n$, then $E(T) \geqslant E(B_n) > E(U_n)$.

If $T'_e = K_{1,n-4}$, according to $T \neq Z_n, W_n$, then u is a pendent vertex of $K_{1,n-4}$. Furthermore, if $d_{T''_e}(v) = 2$, then $T = U_n$; otherwise, $d_{T''_e}(v) = 1$, and we denote the resulting graph by $\tilde{T}$. Then

$$\begin{aligned} m(\tilde{T},k) &= m(\tilde{T}-e,k) + m(\tilde{T}-u-v,k-1) \\ &= m(K_{1,n-4} \cup P_3, k) + m(K_{1,n-5} \cup P_2, k-1) \\ &= \sum_{j=0}^{k} m(K_{1,n-4}, j) m(P_3, k-j) + \sum_{j=0}^{k-1} m(K_{1,n-5}, j) m(P_2, k-1-j). \end{aligned}$$

Then, $m(\tilde{T}, 1) = n-1$, $m(\tilde{T}, 2) = 3n-12$, $m(\tilde{T}, 3) = n-5$ and $m(\tilde{T}, k) = 0$ if $k \geqslant 4$. Hence $\tilde{T} \succ U_n$ and $E(\tilde{T}) > E(U_n)$.

Case 3. There exists an edge $e \in T$ such that $b_e = 3$. Then T''_e is either P_4 or $K_{1,3}$. By Lemma 1.2, we have

$$\begin{aligned} m(T,k) &= m(T-e,k) + m(T-u-v,k-1) \\ &= m(T'_e \cup T''_e, k) + m((T'_e - u) \cup (T''_e - v), k-1) \\ &= \sum_{j=0}^{k} m(T'_e, j) m(T''_e, k-j) + m((T'_e - u) \cup (T''_e - v), k-1) \\ &\geqslant \sum_{j=0}^{k} m(K_{1,n-5}, j) m(K_{1,3}, k-j) + m((T'_e - u) \cup (T''_e - v), k-1). \end{aligned}$$

Subcase 3.1. $T''_e = K_{1,3}$ and $T'_e = K_{1,n-5}$. In this subcase if $d_{T'_e}(u) = n-5$, then $T = D_n$ or $T = U_n$. So we may assume that $d_{T'_e}(u) = 1$, thus

$$\begin{aligned} m(T,k) &= m(T-e,k) + m(T-u-v,k-1) \\ &= \sum_{j=0}^{k} m(T'_e, j) m(T''_e, k-j) + m((T'_e - u) \cup (T''_e - v), k-1) \\ &\geqslant \sum_{j=0}^{k} m(K_{1,n-5}, j) m(K_{1,3}, k-j) + m(K_{1,n-6}, k-1) \\ &= m(M_n, k), \end{aligned}$$

where $M_n = K_{1,n-5}u : vK_{1,3}$, $d_{K_{1,n-5}}(u) = 1$ and $d_{K_{1,3}}(v) = 3$. Since $m(M_n, 1) = n-1$, $m(M_n, 2) = 4n - 21$, and $m(M_n, k) = 0$ if $k \geqslant 3$, we have $U_n \prec M_n \preceq T$ and $E(U_n) < E(M_n) \leqslant E(T)$.

Subcase 3.2. $T''_e = K_{1,3}$ and $T'_e \neq K_{1,n-5}$. Then by Lemma 1.5, we have $m(T'_e, k) \geqslant m(Y_{n-4}, k)$ and $m(T'_e - u, k) \geqslant m(P_2, k)$ for all k and for any $u \in T'_e$. Thus

$$\begin{aligned} m(T,k) &= m(T-e,k) + m(T-u-v,k-1) \\ &= \sum_{j=0}^{k} m(T'_e, j) m(T''_e, k-j) + m((T'_e - u) \cup (T''_e - v), k-1) \\ &\geqslant \sum_{j=0}^{k} m(Y_{n-4}, j) m(K_{1,3}, k-j) + m(P_2, k-1) \\ &= m(R_n, k), \end{aligned}$$

where $R_n = Y_{n-4}u : vK_{1,3}$, $d_{Y_{n-4}}(u) = n-6$ and $d_{K_{1,3}}(v) = 3$. Since $m(R_n, 1) = n-1$,

$m(R_n,2) = 4n-21$ and $m(R_n,k) = 0$ if $k \geqslant 3$, we have $U_n \prec R_n \preceq T$, then $E(U_n) < E(R_n) \leqslant E(T)$.

Subcase 3.3. $T''_e = P_4$ and $d_{T''_e}(v) = 2$. Denote the tree with the minimal energy in this case by Q'_n. Then $Q'_n = K_{1,n-5}u : vP_4$; see Figure 4. So,

$$m(Q'_n,k) = \sum_{j=0}^{k} m(K_{1,n-5},j)m(P_4,k-j) + m(P_2,k-1).$$

Hence, we have

$$m(Q'_n,1) = n-1, m(Q'_n,2) = 3n-13, m(Q'_n,3) = n-5 \text{ and } m(Q'_n,k) = 0 \text{ if } k \geqslant 4. \tag{2.2}$$

Obviously, $U_n \prec Q'_n$ and $E(U_n) < E(Q'_n)$.

Subcase 3.4. $T''_e = P_4$ and $d_{T''_e}(v) = 1$. Denote the tree with the minimal energy in this case by I_n. Then $I_n = K_{1,n-5}u : vP_4$, where $d_{K_{1,n-5}}(u) = n-5$ and $d_{P_4}(v) = 1$. So,

$$m(I_n,k) = \sum_{j=0}^{k} m(K_{1,n-5},j)m(P_4,k-j) + m(P_3,k-1).$$

Therefore $m(I_n,1) = n-1$, $m(I_n,2) = 3n-12$, $m(I_n,3) = n-5$ and $m(I_n,k) = 0$ if $k \geqslant 4$. Hence, $U_n \prec I_n$ and $E(U_n) < E(I_n)$.

Case 4. There exists an edge $e \in T$ such that $b_e \geqslant 4$. Since $a_e + b_e = n-2$, we have $m(T,2) \geqslant 4(n-2-4) = 4n-24 > 3n-11$, if $n > 13$. Note that $m(T,3) \geqslant 0$. Then $T \succ U_n$, hence $E(T) > E(U_n)$.

On the other hand, we have to demonstrate that $E(U_n) < E(H_n)$. In fact, the spectrum of U_n can be calculated, resulting in

$$E(U_n) = 2\sqrt{n-1+\sqrt{12n-52}}.$$

Knowing this, the fact $E(U_n) < E(H_n)$ is immediate. Thus our result holds. □

Theorem 2.3 ([37]). *Let $T \in \mathscr{T}_{n,4}$ with $n \geqslant 7$, If $T \neq T(n,4;n-5,0,0)$, $T(n,4;1,0,n-6)$, $T(n,4;0,n-5,0)$, then $T \succ T(n,4;1,0,6)$.*

In the following we show that Conjecture 1.1 is true for $d = 4$, namely that the following holds:

Theorem 2.4. *$T(n, 4; 1, 0, n-6)(n \geqslant 7)$ achieves the second-minimal energy in the class of trees on n vertices and diameter d for $d = 4$.*

Proof. Note that the fact $d(X_n) = 2$, $d(Y_n) = d(Z_n) = 3$, $d(W_n) = 4$, $d(D_n) = d(H_n) = 3$, $d_{U_n} = 4$. Hence, by Lemma 1.2, Theorems 2.1, 2.2, we obtain that for $n \geqslant 14$, $U_n = T(n, 4; n-6, 0, 1)$ is the tree with the second-minimal energy of a prescribed diameter $d = 4$. So, by Theorem 2.3, it suffices to show that if $7 \leqslant n \leqslant 13$, $E(T(n, 4; n-6, 0, 1)) < E(T(n, 4; 0, n-5, 0))$. By direct calculation (rounded to three decimal places), we have

$$\begin{aligned}
&E(T(7,4;0,2,0)) = 7.596, && E(T(7,4;1,0,1)) = 6.828,\\
&E(T(8,4;0,3,0)) = 8.152, && E(T(8,4;2,0,1)) = 7.384,\\
&E(T(9,4;0,4,0)) = 8.632, && E(T(9,4;3,0,1)) = 7.870,\\
&E(T(10,4;0,5,0)) = 9.064, && E(T(10,4;4,0,1)) = 8.306,\\
&E(T(11,4;0,6,0)) = 8.899, && E(T(11,4;5,0,1)) = 8.705,\\
&E(T(12,4;0,7,0)) = 9.292, && E(T(11,4;6,0,1)) = 9.076,\\
&E(T(13,4;0,8,0)) = 9.657, && E(T(13,4;7,0,1)) = 9.423.
\end{aligned}$$

Thus, our result holds. □

Remark. In fact, Conjecture 1.1 for $d = 5$ is also true; see [23].

Theorem 2.5. *Among trees with n ($n \geqslant 14$) vertices, the graph of the seventh smallest energy is either Q_n or Q'_n, where $Q_n = K_{1,n-6}u : vK_{1,4}$, and $Q'_n = K_{1,n-5}u : vP_4$; see Figure 4. Furthermore, Q_n and Q'_n are incomparable.*

Proof. It is easy to see that $m(Q_n, 1) = n - 1$, $m(Q_n, 2) = 4n - 24$ and $m(Q_n, k) = 0$ if $k \geqslant 3$. By (2.2), we have Q_n and Q'_n are incomparable. For any tree $T \in \mathscr{T}_n$ and $T \neq X_n, Y_n, Z_n, W_n, D_n, H_n, U_n$, We distinguish between the following three cases to show our result.

Case 1. There exists an edge $e \in T$ such that $b_e \geqslant 4$. Similar to the proof of Case 1 in Theorem 2.1, we have $E(T) \geqslant E(Q_n)$, and

$$E(T) = E(Q_n) \Leftrightarrow T = Q_n.$$

Case 2. There exists an edge $e \in T$ such that $b_e = 3$. By the proof of Case 3 in Theorem 2.2, we have $E(T) \geqslant E(Q_n)$ and

$$E(T) = E(Q_n) \Leftrightarrow T = Q_n,$$

or $E(T) \geqslant E(Q'_n)$, and

$$E(T) = E(Q'_n) \Leftrightarrow T = Q'_n.$$

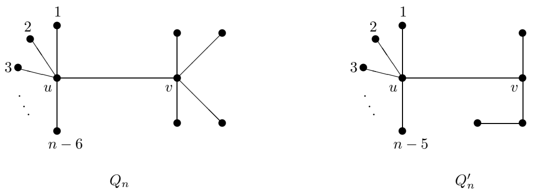

Figure 4: Q_n and Q'_n

Case 3. There exists an edge $e \in T$ such that $b_e \leqslant 2$. By the proof of Cases 1 and 2 in Theorem 2.2, we have

$$E(T) > E(Q'_n).$$

Finally we must demonstrate that $E(Q_n) < E(H_n)$ and $E(Q'_n) < E(H_n)$. In fact, the spectrum of Q_n can be calculated, resulting in $E(Q_n) = 2\sqrt{n-1+4\sqrt{n-6}}$. Knowing this, the fact $E(Q_n) < E(H_n)$ is immediate. On the other hand, by (2.1) and (2.2), we have $E(Q'_n) < E(H_n)$. Thereby, the theorem follows. $\square$

3. The third maximal energy among all n-vertex trees

In this section we determine the tree in $\mathscr{T}_n$ with the third-maximal energy.

Lemma 3.1. $n-1(i)1 \prec n-2(5)2$, *if* $i \neq 1, n-1$.

Proof. By Lemma 1.3, it suffices to prove that $n-1(3)1 \prec n-2(5)2$. It is easy to see that

$$\begin{aligned} m(n-2(4)2,k) &= m(n-2(4)1,k) + m(P_{n-2},k-1), \\ m(n-2(5)2,k) &= m(n-2(5)1,k) + m(P_{n-2},k-1). \end{aligned}$$

Since $m(n-2(4)1,k) = m(P_{n-2},k) + m(P_3 \cup P_{n-6},k-1)$, while $m(n-2(5)1,k) = m(P_{n-2},k) + m(P_4 \cup P_{n-7},k-1)$, by Lemma 1.4 we have $m(n-2(4)1,k) \leqslant m(n-2(5)1,k)$. Thus

$$n-2(4)2 \prec n-2(5)2. \tag{3.1}$$

Since

$$m(n-1(3)1,k) = m(P_2 \cup (n-3(3)1),k) + m(n-4(3)1,k-1),$$
$$m(n-2(4)2,k) = m(P_2 \cup (n-3(3)1),k) + m(P_{n-3},k-1).$$

Hence by Lemma 1.5, $m(n-1(3)1,k) \leqslant m(n-2(4)2,k)$. Therefore,

$$n-1(3)1 \prec n-2(4)2. \tag{3.2}$$

By Inequalities (3.1) and (3.2), we have $n-1(3)1 \prec n-2(5)2$. Thus our results hold. □

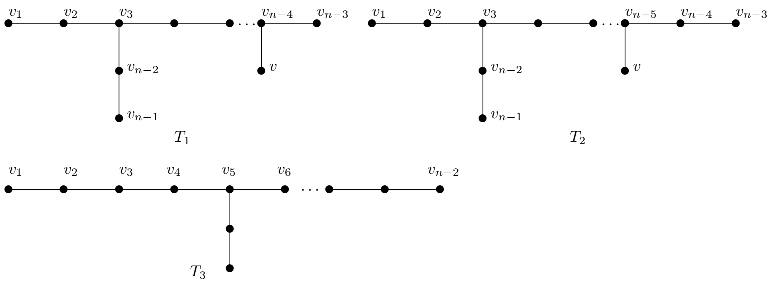

Figure 5: T_1, T_2 and T_3

Lemma 3.2. *Let T_1, T_2 and T_3 be as in Figure 5. Then $T_1 \prec T_2 \prec T_3$ for $n \geqslant 9$.*

Proof. By Lemma 1.2, we have

$$\begin{aligned} m(T_1,k) &= m(T_1 - v_{n-4}v,k) + m(T_1 - v_{n-4} - v,k-1) \\ &= m(n-3(3)2,k) + m(n-5(3)2,k-1) \\ &= m(n-3(3)2,k) + m(n-6(3)2,k-1) + m(n-7(3)2,k-2), \end{aligned}$$

while

$$\begin{aligned} m(T_2,k) &= m(T_2 - v_{n-5}v,k) + m(T_2 - v_{n-5} - v,k-1) \\ &= m(n-3(3)2,k) + m(P_2 \cup (n-6(3)2),k-1) \\ &= m(n-3(3)2,k) + m(n-6(3)2,k-1) + m(n-6(3)2,k-2). \end{aligned} \tag{3.3}$$

Note that $n-7(5)2$ is a proper subgraph of $n-6(3)2$. By Lemma 1.6, $n-7(3)2 \prec n-6(3)2$, then we have $m(T_1,k) \leqslant m(T_2,k)$. Hence, $T_1 \prec T_2$. On the other hand,

$$\begin{aligned} m(T_3,k) &= m(T_3-v_2v_3,k)+m(T_3-v_2-v_3,k-1) \\ &= m(P_2 \cup (n-4(3)2),k)+m(n-5(2)2,k) \\ &= m(n-4(3)2,k)+m(n-4(3)2,k-1)+m(n-5(2)2,k-1) \\ &= m(n-4(3)2,k)+m(n-4(3)2,k-1)+m(n-6(2)2,k-1) \\ &+ m(n-7(2)2,k-2). \end{aligned}$$

By Eq. (3.3), we have

$$\begin{aligned} m(T_2,\,k) &= m(n-4(3)2,k)+m(n-5(3)2,k-1)+m(n-6(3)2,k-1) \\ &+ m(n-6(3)2,k-2) \\ &= m(n-4(3)2,k)+m(n-4(3)2,k-1)+m(n-6(3)2,k-1) \\ &= m(n-4(3)2,k)+m(n-4(3)2,k-1)+m(n-7(2)2,k-1) \\ &+ m(P_{n-8},k-2). \end{aligned}$$

By Lemma 1.6, we have $n-7(2)2 \prec n-6(2)2$ and $P_{n-8} \prec n-7(2)2$. Hence $T_2 \prec T_3$, and the Lemma thus follows. □

Lemma 3.3. *Let* $|T| > 8$ *and* v *be a pendent vertex of* T*, where* $T \neq P_n, n-2(3)2, n-2(5)2$*, and* $T-v = n-3(3)2$*. Then* $T \preceq n-2(5)2$*, and* $E(T) = E(n-2(5)2) \Leftrightarrow T = n-2(5)2$*.*

Proof. We prove it by induction on $|T|$. Let $T-v := T_1-v$; see Figure 5. If $n=8,9$, the result can be checked by comparing the characteristic polynomial of T and $n-2(5)2$. Assume that the result holds for $9 \leqslant |T| < n$, and we consider the case $|T| = n$. Note that $T \neq n-2(3)2$. Then v is not adjacent to the vertex v_{n-3}, hence v_{n-3} is a pendent vertex of T. By Lemma 1.2 we have

$$m(T,k) = m(T-v_{n-3},k)+m(T-v_{n-3}-v_{n-4},k-1),$$
$$m(n-2(5)2,k) = m(n-3(5)2,k)+m(n-4(5)2,k-1).$$

Case 1. $T - v_{n-3} = n - 3(3)2$. In this case, $T = T_1$; see Figure 5. Then by Lemma 3.2, we have $T \prec n - 2(5)2$.

Case 2. $T - v_{n-3} - v_{n-4} = n - 4(3)2$. In this case, $T = T_2$; see Figure 5. Then by Lemma 3.2, we have $T \prec n - 2(5)2$.

Case 3. $T - v_{n-3} \neq n - 3(3)2$ and $T - v_{n-3} - v_{n-4} \neq n - 4(3)2$. Note that both $T - v_{n-3}$ and $n - 3(5)2$ have the same order $n - 1$ (respectively, both $T - v_{n-3} - v_{n-4}$ and $n - 4(5)2$ have the same order $n - 2$), and $T - v_{n-3} - v = n - 4(3)2$, $T - v_{n-3} \neq P_{n-1}, n - 3(3)2$ (respectively, $T - v_{n-3} - v_{n-4} - v = m - 5(3)2$, $T - v_{n-3} - v_{n-4} \neq P_{n-2}, n - 4(3)2$). By the induction assumption, we have $T - v_{n-3} \preceq n - 3(5)2$, and

$$E(T - v_{n-3}) = E(n - 3(5)2) \Leftrightarrow T - v_{n-3} = n - 3(5)2.$$

(Respectively, we have $T - v_{n-3} - v_{n-4} \preceq n - 4(5)2$, and

$$E(T - v_{n-3} - v_{n-4}) = E(n - 4(5)2) \Leftrightarrow T - v_{n-3} - v_{n-4} = n - 4(5)2.)$$

Therefore, $T \preccurlyeq n - 2(5)2$, and $E(T) = E(n - 2(5)2)$ if and only if $T = n - 2(5)2$. Thus our result follows. □

Lemma 3.4. *Let T_4, T_5 be as in Figure 6. Then $T_4 \prec 8(5)2$, and $T_5 \prec 9(5)2$.*

Proof. By Lemma 1.2, we have

$$\begin{aligned} m(T_4, k) &= m(T_4 - v_5 v, k) + m(T_4 - v_5 - v, k - 1) \\ &= m(P_2 \cup 6(5)2, k) + m(P_2 \cup P_4, k - 1), \end{aligned}$$

while $m(8(5)2, k) = m(P_2 \cup 6(5)2, k) + m(P_7, k - 1)$. By Lemma 1.6, we get $P_2 \cup P_4 \prec P_6 \prec P_7$. Then, $T_4 \prec 8(5)2$. Similarly, we have

$$\begin{aligned} m(T_5, k) &= m(T_5 - v_5 v, k) + m(T_4 - v_5 - v, k - 1) \\ &= m(P_2 \cup 7(5)2, k) + m(2P_2 \cup P_4, \text{k-1}), \text{ while} \end{aligned}$$

$m(9(5)2, k) = m(P_2 \cup 7(5)2, k) + m(6(5)2, k - 1)$. Note that $2P_2 \cup P_4$ is a proper subgraph of $6(5)2$. Then by Lemma 1.6, we have $2P_2 \cup P_4 \prec 6(5)2$. Hence, $T_5 \prec 9(5)2$. □

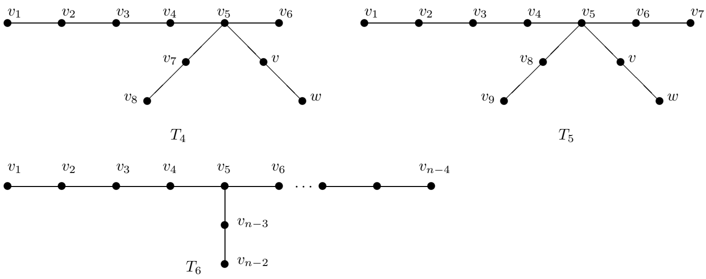

Figure 6: T_4, T_5 and T_6

Lemma 3.5. *Let vw be a pendent edge of T with pendent vertex v, where $T \neq P_n, n-2(3)2$, and $T-v-w = n-4(5)2$. Then $T \preceq n-2(5)2$, and $E(T) = E(n-2(5)2) \Leftrightarrow T = n-2(5)2$.*

Proof. We show it by induction on $|T|$. Let $T - v - w = T_6$; see Figure 6. If $n = 8, 9$, the result follows easily. Assume that the result holds for $|T| = 8, 9, 10, \ldots, n-1$, and consider the case $|T| = n$. Since $T \neq n-2(5)2$, w is not adjacent to v_{n-4}, so v_{n-4} is a pendent vertex of T. By Lemma 1.2, we get

$$m(T, k) = m(T - v_{n-4}, k) + m(T - v_{n-5} - v_{n-4}, k-1),$$

$$m(n-2(5)2, k) = m(n-3(5)2, k) + m(n-4(5)2, k-1).$$

(i) $T - v_{n-4} = n-3(3)2$. In this case, $n = 10$ and $T = T_4$; see Figure 6. By Lemma 3.4, $T \prec n-2(5)2$.

(ii) $T - v_{n-4} - v_{n-5} = n-4(3)2$. In this case, $n = 11$ and $T = T_5$; see Figure 6. By Lemma 3.4, $T \prec n-2(5)2$.

1

(iii) $T - v_{n-4} \neq n-3(3)2$ and $T - v_{n-4} - v_{n-5} \neq n-4(3)2$. Note that both $T - v_{n-4}$ and $n-3(5)2$ have the same order $n-1$ (respectively, both $T - v_{n-5} - v_{n-4}$ and $n-4(5)2$ have the same order $n-2$), and $T - v_{n-4} - v - w = n-5(5)2$, $T - v_{n-4} \neq P_{n-1}, n-3(3)2$, $T - v_{n-5} - v_{n-4} \neq P_{n-2}, n-4(3)2$ (respectively, $T - v_{n-5} - v_{n-4} - v - w = n-6(5)2$). By the induction hypothesis, we have $m(T - v_{n-5}v_{n-4}, k) \leqslant m(n-3(5)2, k)$ and $m(T - v_{n-5} - v_{n-4}, k-1) \leqslant m(n-4(5)2, k-1)$. Therefore, $T \preccurlyeq n-2(5)2$ and $E(T) = E(n-2(5)2)$ if and only if $T = n-2(5)2$. Hence the result follows. $\square$

Theorem 3.6. *Let $T \in \mathscr{T}_n$, and $T \neq P_n, n-2(3)2, n-2(5)2$, then $n-2(5)2 \succ T$.*

Proof. For $|T| = 8, 9$, the result can be checked and suppose the result holds for all $|T| = 8, 9, \ldots, n-1$. Now let $|T| = n$, we show that $n-2(5)2 \succ T$ if $T \neq P_n, n-2(3)2, n-2(5)2$. Let v be a pendent vertex of T, being adjacent to w. By Lemma 1.2, we have

$$m(T, k) = m(T - v, k) + m(T - v - w, k - 1),$$

$$m(n - 2(5)2, k) = m(n - 3(5)2, k) + m(n - 4(5)2, k - 1).$$

If $T - v = P_{n-1}$, i.e., $T = n-1(i)1$, where $i \neq 1, n-1$, then by Lemma 3.1, $T \prec n-2(5)2$. If $T - v = n - 3(3)2$, then by Lemma 3.3, $T \prec n - 2(5)2$. So, we assume that $T - v \neq P_{n-1}, n - 3(3)2$. Note that the order of $T - v$ is $n - 1$, then by the induction hypothesis, if $T - v \neq n - 3(5)2$ then we have $n - 3(5)2 \succ T - v$.

If $T - v - w = P_{n-2}$, then $T = n-2(i)2$, and it is easy to see that $n-2(5)2 \succ T$, since $T \neq P_n, n-2(3)2$. If $T-v-w = n-4(5)2$, by Lemma 3.5, we have $T \prec n-2(5)2$. So we assume that $T - v - w \neq P_{n-2}, n - 4(5)2$. Note that the order of $T - v - w$ is $n - 2$, then by the induction hypothesis, if $T - v - w \neq n-4(5)2$ then we have $n-4(5)2 \succ T - v - w$. Note that if $T - v = n-3(5)2$, and $T - v - w = n-4(5)2$, then $T = n-2(5)2$. Therefore, the theorem holds. □

4. Inequalities for topological index of Hosoya

Hosoya [17] introduced the topological index $Z = Z(G)$, which is by definition

$$Z(G) = 1 + m(G, 1) + m(G, 2) + \cdots + m(G, k),$$

where, as before, $m(G, j)$ is the number of ways in which j non-incident edges can be selected in a graph G.

Hence, as shown already in [6], $T_1 \succ T_2$ implies also $Z(T_1) > Z(T_2)$, unless T_1 and T_2 are cospectral (when, of course, it is $Z(T_1) = Z(T_2)$). Every relation between trees which has been derived in the present paper results in a corresponding inequality for the topological index. We list such inequalities which generalize those of Gutman in [6].

For sufficient large n, if $T \in \mathscr{T}_n$ and $T \neq X_n, Y_n, Z_n, W_n, D_n, Q_n, Q'_n, U_n, n-2(5)2$, $n-2(3)2$, and P_n, then by Lemma 1.4 and Theorems 2.1, 2.2, 2.5 and 3.6 we have

$$Z(X_n) < Z(Y_n) < Z(Z_n) < Z(W_n) < Z(D_n) < Z(U_n) < Z(Q_n) < Z(T) < Z(n-2(5)2) < Z(n-2(3)2) < Z(P_n),$$

or

$$Z(X_n) < Z(Y_n) < Z(Z_n) < Z(W_n) < Z(D_n) < Z(U_n) < Z(Q'_n) < Z(T) < Z(n-2(5)2) < Z(n-2(3)2) < Z(P_n).$$

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