J Math Chem (2010) 47:937–958
DOI 10.1007/s10910-009-9616-3

ORIGINAL PAPER

Ordering of the trees by minimal energies

Wen-Huan Wang · Li-Ying Kang

Received: 7 May 2009 / Accepted: 3 October 2009 / Published online: 24 October 2009

Abstract The ordering of the trees with n vertices according to their minimal energies is investigated by means of a quasi-ordering relation and the theorem of zero points. We deduce the first 9 trees for a general case with $n \geq 46$. We obtain the first 12, 11, $n+6$, 17, 15, and 12 trees for $7117598 \geq n \geq 26$, $25 \geq n \geq 18$, $17 \geq n \geq 11$, $n = 10$, $n = 9$, and $n = 8$, respectively. For $n = 7$, we list all the trees in the increasing order of their energies. The maximal diameters of the trees with minimal energies obtained here are 4 for $n \geq 18$ and 5 for $17 \geq n \geq 8$, respectively. For the trees under consideration, the ones with smaller diameters have smaller energies. In addition, we in part prove a conjecture proposed by Zhou and Li (J. Math. Chem. 39:465–473, 2006).

Keywords Trees · Matching · Ordering · Minimal energy

1 Introduction

Let T be a tree with n vertices and $A(T)$ its adjacent matrix. The characteristic polynomial of T is [1]

$$\phi(T, x) = \det[x\mathbf{I} - A(T)] = \sum_{i=0}^{n} a_i x^{n-i} = \sum_{k=0}^{[n/2]} (-1)^k m(T, k) x^{n-2k}, \qquad (1)$$

where $\mathbf{I}$ is the unit matrix of order n, $a_0, a_1, \ldots, a_n$ are the coefficients of the characteristic polynomial of T and $m(T, k)$ is the number of k-matchings in T. The n

W.-H. Wang (✉) · L.-Y. Kang
Department of Mathematics, Shanghai University, Shanghai 200444, China
e-mail: whwang@shu.edu.cn

roots of $\phi(T, x) = 0$ are denoted by $\lambda_1, \ldots, \lambda_n$, which are the eigenvalues of the corresponding graph T.

As is well known, the experimental heats due to the formation of conjugated hydrocarbons are closely connected to the total π-electron energy. The total energy $E(T)$ of all π-electrons in conjugated hydrocarbons, within the framework of Hückel molecular orbital (HMO) approximation [1,2], can be reduced to

$$E(T) = \sum_{i=1}^{n} |\lambda_i|. \tag{2}$$

$E(T)$ can also be expressed as the Coulson integral formula [2, p. 141]

$$E(T) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left[1 + \sum_{k=1}^{[n/2]} m(T, k) x^{2k} \right] \mathrm{d}x. \tag{3}$$

The fact that $E(T)$ is a strictly monotonously increasing function of $m(T, k)$ provides us a useful way to compare the energies of the trees under consideration.

For two trees T_1 and T_2, Gutman and Zhang [3,4] introduced a quasi-ordering relation as follows

$$m(T_1, k) \leq m(T_2, k) \iff T_1 \preceq T_2. \tag{4}$$

Furthermore, if $m(T_1, k) < m(T_2, k)$ for an arbitrary k, we have $T_1 \prec T_2$. If neither $T_1 \prec T_2$ nor $T_1 \succ T_2$, we say that T_1 and T_2 are incomparable. According to (3), we have $E(T_1) \leq E(T_2)$ and $E(T_1) < E(T_2)$ from $T_1 \preceq T_2$ and $T_1 \prec T_2$, respectively. For the sake of conciseness, we introduce the symbols "$\rightharpoonup$", "$\rightleftharpoons$" and "$\rightrightarrows$" as follows:

$$\begin{aligned} &E(T_1) < E(T_2) \iff T_1 \rightharpoonup T_2, \quad E(T_1) = E(T_2) \iff T_1 \rightleftharpoons T_2, \\ &E(T_1) \leq E(T_2) \iff T_1 \rightrightarrows T_2. \end{aligned} \tag{5}$$

Based on the above method of quasi-ordering, a number of results have been reached for the ordering of graphs with extremal energies. For example, acyclic [3–9], unicyclic [10–13], bicyclic [14] and tricyclic [15] graphs were considered.

We denote by $\mathcal{T}_n$ the set of trees with n vertices and by $\mathcal{T}_n^d$ the subset of $\mathcal{T}_n$ in which the trees have diameter d with $2 \leq d \leq n-1$. Let P_n be a path with n vertices and the vertices of P_n are labelled consecutively by $v_0, v_1, \ldots, v_{n-1}$. Let $T_n^d(n_1, n_2, \ldots, n_{d-1})$ be a caterpillar obtained from a path P_{d+1} by attaching n_i ($n_i \geq 0$) pendant edges to v_i ($i = 1, 2, \ldots, d-1$), where a caterpillar is a tree in which a removal of all pendant vertices makes a path [16]. Obviously, $\sum_{i=1}^{d-1} n_i = n - d - 1$ and $T_n^d(n_1, n_2, \ldots, n_{d-1}) \in \mathcal{T}_n^d$. We have one tree only in $\mathcal{T}_n^d$ for $d = 2$ and $d = n-1$, namely $\mathcal{T}_n^2 = \{K_{1,n-1}\}$ and $\mathcal{T}_n^{n-1} = \{P_n\}$, where $K_{1,n-1} = T_n^2(n-3)$ with $n \geq 3$. In Ref. [7], $K_{1,n-1}$ is denoted by X_n. Gutman [3] found that the non-branched path P_n has maximal, and the maximally branched star X_n has minimal energy in $\mathcal{T}_n$.

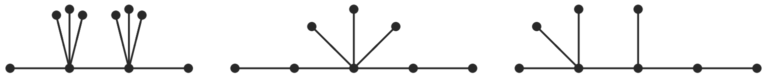
(a) (b) (c)

Fig. 1 (**a**) Q_{10}; (**b**) H_8; (**c**) Q'_8

For $T_n^3(n_1, n_2)$, we suppose $n_1 \geq n_2$. For example, the trees Y_n, Z_n, D_n, and Q_n in Ref. [7] can be re-written as $Y_n = T_n^3(n-4, 0)$ with $n \geq 4$, $Z_n = T_n^3(n-5, 1)$ with $n \geq 6$, $D_n = T_n^3(n-6, 2)$ with $n \geq 8$, and $Q_n = T_n^3(n-7, 3)$ with $n \geq 10$, respectively.

For $T_n^4(n_1, 0, n_3)$, we suppose $n_1 \geq n_3$. For example, the trees W_n and U_n in Ref. [7] can be re-written as $W_n = T_n^4(n-5, 0, 0)$ with $n \geq 5$ and $U_n = T_n^4(n-6, 0, 1)$ with $n \geq 7$, respectively. In addition, the trees H_n and Q'_n in Ref. [7] can be re-written as $H_n = T_n^4(0, n-5, 0)$ with $n \geq 6$ and $Q'_n = T_n^4(n-6, 1, 0)$ with $n \geq 7$, respectively. For example, Q_{10}, H_8 and Q'_8 are shown in Fig. 1.

For the sake of conciseness, "the k-th minimal tree" is referred to as "the tree with k-th minimal energy". In $\mathcal{T}_n$, Gutman [3] deduced $X_n < Y_n < Z_n < W_n < T$ for $n \geq 6$, where $T \neq X_n, Y_n, Z_n, W_n$ and $T \in \mathcal{T}_n$. Recently, using the quasi-ordering relation, Li and Li [7] extended Gutman's result [3] by determining D_n and U_n are the fifth- and sixth-minimal trees in $\mathcal{T}_n$ with $n \geq 6$ and $n \geq 14$, respectively. Li and Li [7] found two trees Q_n and Q'_n and suggested that either Q_n or Q'_n is the seventh-minimal tree in $\mathcal{T}_n$ with $n \geq 14$. The quasi-ordering relation, however, can not be used to compare the energies of Q_n and Q'_n. By use of a systematic computer-aided search, Gutman et al. [17] provided a slight correction of the claim in Ref. [7] that D_n is the fifth one for $n \geq 9$ only. By numerical calculation, Gutman et al. [17] claimed, but did not prove, that Q_n is the seventh one for $n \geq 12$ and Q'_n is not the seventh one for any value of n. Gutman et al. [17] listed the first 7 trees for $11 \geq n \geq 7$ and all the trees for $n = 6$ in the increasing order of their minimal energies within $\mathcal{T}_n$. A rigor mathematical proof for the seventh-minimal tree and further ordering of trees for $n \geq 7$ remain a task.

In this paper, we use a straightforward method to extend Gutman's [3] and Li and Li's [7] results for $n \geq 7$. We mathematically prove that Q_n is the seventh-minimal tree for $n \geq 12$ and Q'_n is not the seventh one for any value of n. We find that Q'_n is the twelfth-minimal tree for $7117598 \geq n \geq 59$. The method employed here is simple, which makes it easy to find new trees with minimal energy within $\mathcal{T}_n$. Thus we derive the first 9 trees for a general case with $n \geq 46$ and series of trees in the increasing order of their energies for $n \geq 7$. The first 7 trees are consistent with those obtained by Gutman [3] and Li and Li [7] for $n \geq 7$.

2 Preliminaries

For $T \in \mathcal{T}_n$, it is consistent to define $m(T, 0) = 1$ and $m(T, k) = 0$ for $k > n/2$. Obviously, $m(T, 1) = n-1$. We assume $2 \leq k \leq n/2$ hereinafter. The trees in $\mathcal{T}_n$ can be partitioned into two subsets $\mathcal{T}_n^{\mathrm{A}}$ and $\mathcal{T}_n^{\mathrm{B}}$ according to the numbers of the k-matchings of the

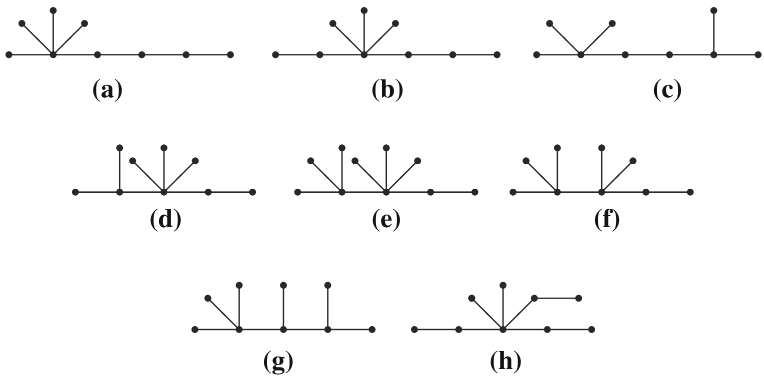

Fig. 2 (**a**) A_9; (**b**) B_9; (**c**) C_9; (**d**) I_9; (**e**) J_{10}; (**f**) K_9; (**g**) L_9; (**h**) M_9

trees with $3 \leq k \leq n/2$. For the first subset, $\mathcal{T}_n^{\mathrm{A}} = \{X_n,\ T_n^3(n_1, n_2),\ T_n^4(n_1, 0, n_3)\}$ where the numbers of the k-matchings with $3 \leq k \leq n/2$ are zero. Thus, $\mathcal{T}_n^{\mathrm{B}} = \mathcal{T}_n - \mathcal{T}_n^{\mathrm{A}}$.

For simplicity, we introduce some notations for trees in $\mathcal{T}_n^{\mathrm{B}}$. Let $A_n = T_n^5(n-6, 0, 0, 0)$ with $n \geq 7$, $B_n = T_n^5(0, n-6, 0, 0)$ with $n \geq 7$, $C_n = T_n^5(n-7, 0, 0, 1)$ with $n \geq 8$, $I_n = T_n^4(1, n-6, 0)$ with $n \geq 8$, $J_n = T_n^4(2, n-7, 0)$ with $n \geq 10$, $K_n = T_n^4(n-7, 2, 0)$ with $n \geq 8$, and $L_n = T_n^4(n-7, 1, 1)$ with $n \geq 8$. Let M_n be a tree obtained from P_5 by attaching $n-7$ pendant edges and a path of length two to v_2, where $n \geq 7$. For example, A_9, B_9, C_9, I_9, J_{10}, K_9, L_9, and M_9 are given in Fig. 2.

To deduce the final results of this paper, Lemmas 1–3 and Conjecture 1 are simply quoted here from Refs. [1,2,16,18].

Lemma 1 [1] *Let $e = uv$ be an edge of a tree T. Then the characteristic polynomial $\Phi(T, x)$ satisfies*

$$\Phi(T, x) = \Phi(T - e, x) - \Phi(T - u - v, x).$$

Lemma 2 [2] *Let $e = uv$ be an edge of G and k a positive integer. Then we have*

$$m(G, k) = m(G - e, k) + m(G - u - v, k - 1). \tag{6}$$

Lemma 3 [18] *Let d be a positive integer more than one and T a tree with n vertices having diameter at least d. Then $T_n^d(n-d-1, 0, 0, \ldots, 0) \rightrightarrows T$ with equality if and only if (iff) $T = T_n^d(n-d-1, 0, 0, \ldots, 0)$.*

Zhou and Li [16] characterized the second-minimal trees in $\mathcal{T}_n^d$ are $T_n^d(0, 0, n-d-1, 0, \ldots, 0)$ if $d \geq 6$, Y_n if $d = 3$, U_n or H_n if $d = 4$ and $n \geq 7$, B_n or C_n if $d = 5$ and $n \geq 9$. Zhou and Li [16] proposed the following conjecture.

Conjecture 1 [16] *U_n with $n \geq 7$ and B_n with $n \geq 9$ are the second-minimal trees in $\mathcal{T}_n^4$ and $\mathcal{T}_n^5$, respectively.*

Recently, Li and Li [7] showed that Conjecture 1 holds for $d = 4$. In Sect. 3, we will prove that Conjecture 1 is also true for $d = 5$.

3 Main results

In this section, we assume that T appearing in the last terms of all the inequalities does not contain the preceding terms and the calculation for comparing the energies of two trees is directly performed on the basis of (2).

In Lemmas 4–12, we provide the inequalities which can not be proved by the quasi-ordering relation. However, these inequalities can be obtained by using the theorem of zero points.

Lemma 4 *$A_n \rightharpoonup I_n$ for $n \geq 8$.*

Proof Straightforward derivation by Lemma 1 yields

$$\Phi(A_n, x) = x^{n-6}\left[-(n-5) + (3n-12)x^2 - (n-1)x^4 + x^6\right] \triangleq x^{n-6} f_1(x),$$
$$\Phi(I_n, x) = x^{n-6}\left[-(2n-12) + (3n-13)x^2 - (n-1)x^4 + x^6\right] \triangleq x^{n-6} f_2(x).$$

It is noted that the exact solutions for the roots of $f_1(x) = 0$ and $f_2(x) = 0$ with respect to x can be obtained. However, the exact representations for the energies of A_n and I_n are too complex to compare their quantities for an arbitrary n. As it is, approximate roots of $f_1(x) = 0$ and $f_2(x) = 0$ can be used instead.

Obviously, we have

$$f_1\left(\sqrt{0.37}\right) = 0.747553 - 0.0269n < 0, \quad (n \geq 28),$$
$$f_1\left(\sqrt{0.39}\right) = 0.531419 + 0.0179n > 0, \quad (n \geq 7),$$
$$f_1\left(\sqrt{2.58}\right) = -2.13009 + 0.0836n > 0, \quad (n \geq 26),$$
$$f_1\left(\sqrt{2.7}\right) = -0.427 - 0.19n < 0, \quad (n \geq 7),$$
$$f_1\left(\sqrt{n-4}\right) = 5 - n < 0, \quad (n \geq 7),$$
$$f_1\left(\sqrt{n-3.9}\right) = 0.1(-15.9902 + n)(-4.80983 + n) > 0, \quad (n \geq 16).$$

According to the theorem of zero points, we have, for $n \geq 28$,

$$E(A_n) < 2\left(\sqrt{0.39} + \sqrt{2.7} + \sqrt{n-3.9}\right). \tag{7}$$

Obviously, we have

$$f_2\left(\sqrt{0.92}\right) = 1.66509 - 0.0864n < 0, \quad (n \geq 20),$$
$$f_2(1) = 1 > 0, \quad (n \geq 7),$$
$$f_2\left(\sqrt{1.9}\right) = -2.231 + 0.09n > 0, \quad (n \geq 25),$$
$$f_2\left(\sqrt{2}\right) = -2 < 0, \quad (n \geq 7),$$
$$f_2\left(\sqrt{n-4}\right) = 16 - 3n < 0, \quad (n \geq 7),$$
$$f_2\left(\sqrt{n-3.9}\right) = 0.1(-35.574 + n)(-5.22601 + n) > 0, \quad (n \geq 36).$$

According to the theorem of zero points, we have, for $n \geq 36$,

$$2\left(\sqrt{0.92} + \sqrt{1.9} + \sqrt{n-4}\right) < E(I_n). \tag{8}$$

It follows from $\sqrt{0.39} + \sqrt{2.7} + \sqrt{n-3.9} < \sqrt{0.92} + \sqrt{1.9} + \sqrt{n-4}$ that the right-hand side (RHS) of (7) is less than the left-hand side (LHS) of (8) as $n \geq 36$. Therefore, $A_n \rightharpoonup I_n$ for $n \geq 36$.

The calculation yields $A_n \rightharpoonup I_n$ for $35 \geq n \geq 8$. □

Next, we simply provide the necessary equations and inequalities in the proofs for Lemmas 5–12 since the method involved is similar to that for Lemma 4.

Lemma 5 *$B_n \rightharpoonup K_n$ for $n \geq 11$ and $K_n \rightharpoonup B_n$ for $10 \geq n \geq 8$.*

Proof Straightforward derivation by Lemma 1 yields

$$\Phi(B_n, x) = x^{n-6}\left[-(2n-11) + (3n-12)x^2 - (n-1)x^4 + x^6\right] \triangleq x^{n-6} f_3(x),$$
$$\Phi(K_n, x) = x^{n-6}\left[-(2n-12) + (4n-21)x^2 - (n-1)x^4 + x^6\right] \triangleq x^{n-6} f_4(x).$$

Since

$$f_3\left(\sqrt{0.97}\right) = 1.21357 - 0.0309n < 0, \quad (n \geq 40),$$
$$f_3(1) = 1 > 0, \quad (n \geq 7),$$
$$f_3\left(\sqrt{1.98}\right) = -1.07721 + 0.0196n > 0, \quad (n \geq 55),$$
$$f_3\left(\sqrt{2}\right) = -1 < 0, \quad (n \geq 7),$$
$$f_3\left(\sqrt{n-4}\right) = 11 - 2n < 0, \quad (n \geq 6),$$
$$f_3\left(\sqrt{n-3.9}\right) = 0.1(-25.4125 + n)(-5.38751 + n) > 0, \quad (n \geq 26),$$

we have, for $n \geq 55$,

$$E(B_n) < 2\left(1 + \sqrt{2} + \sqrt{n - 3.9}\right). \tag{9}$$

Since

$$\begin{aligned}
f_4\left(\sqrt{0.55}\right) &= 0.918875 - 0.1025n < 0, \quad (n \geq 9),\\
f_4\left(\sqrt{0.59}\right) &= 0.163479 + 0.0119n > 0, \quad (n \geq 7),\\
f_4\left(\sqrt{3.3}\right) &= -10.473 + 0.31n > 0, \quad (n \geq 34),\\
f_4\left(\sqrt{3.42}\right) &= -8.12191 - 0.0164n < 0, \quad (n \geq 7),\\
f_4\left(\sqrt{n-5}\right) &= 17 - 3n < 0, \quad (n \geq 7),\\
f_4\left(\sqrt{n-4.7}\right) &= 0.3(-18.0509 + n)(-5.34915 + n) > 0, \quad (n \geq 19),
\end{aligned}$$

we have, for $n \geq 34$,

$$2\left(\sqrt{0.55} + \sqrt{3.3} + \sqrt{n-5}\right) < E(K_n). \tag{10}$$

It follows from $1 + \sqrt{2} + \sqrt{n-3.9} < \sqrt{0.55} + \sqrt{3.3} + \sqrt{n-5}$ that the RHS of (9) is less than the LHS of (10) as $n \geq 55$. Therefore, $B_n \rightharpoonup K_n$ for $n \geq 55$.

The calculation yields $B_n \rightharpoonup K_n$ for $54 \geq n \geq 11$ and $K_n \rightharpoonup B_n$ for $10 \geq n \geq 8$. □

Lemma 6 *$C_n \rightharpoonup M_n$ for $n \geq 8$.*

Proof Straightforward derivation by Lemma 1 yields

$$\begin{aligned}
\Phi(C_n, x) &= x^{n-6}\left[-(2n-12) + (4n-19)x^2 - (n-1)x^4 + x^6\right] \triangleq x^{n-6} f_5(x),\\
\Phi(M_n, x) &= x^{n-8}\left[(n-7) - (3n-17)x^2 + (3n-12)x^4 - (n-1)x^6 + x^8\right]\\
&\triangleq x^{n-8} f_6(x).
\end{aligned}$$

Since

$$\begin{aligned}
f_5\left(\sqrt{0.55}\right) &= 2.01887 - 0.1025n < 0, \quad (n \geq 20),\\
f_5\left(\sqrt{0.59}\right) &= 1.34348 + 0.0119n > 0, \quad (n \geq 8),\\
f_5\left(\sqrt{3.3}\right) &= -3.873 + 0.31n > 0, \quad (n \geq 13),\\
f_5\left(\sqrt{3.42}\right) &= -1.28191 - 0.0164n < 0, \quad (n \geq 8),
\end{aligned}$$

$$f_5\left(\sqrt{n-5}\right) = 7 - n < 0, \quad (n \geq 8),$$
$$f_5\left(\sqrt{n-4.9}\right) = 0.1(-17.0962 + n)(-6.70385 + n) > 0, \quad (n \geq 18),$$

we have, for $n \geq 20$,

$$E(C_n) < 2\left(\sqrt{0.59} + \sqrt{3.42} + \sqrt{n-4.9}\right). \tag{11}$$

Since

$$f_6\left(\sqrt{0.94}\right) = -0.011867 + 0.000216n > 0, \quad (n \geq 55),$$
$$f_6\left(\sqrt{1-1/n}\right) = (1 - 5n - 2n^2)/n^4 < 0, \quad (n \geq 8),$$
$$f_6\left(\sqrt{1-2/n}\right) = -4(-4 + 10n + n^2)/n^4 < 0, \quad (n \geq 8),$$
$$f_6\left(\sqrt{1-10/n}\right) = 100(100 - 50n + 7n^2)/n^4 > 0, \quad (n \geq 8),$$
$$f_6(1) = 0, \quad (n \geq 8),$$
$$f_6\left(\sqrt{n-4}\right) = -3(-5 + n)^2 < 0, \quad (n \geq 8),$$
$$f_6\left(\sqrt{n-3.9}\right) = 0.1(-34.9 + n)(24.01 - 9.8n + n^2) > 0, \quad (n \geq 35),$$

we have, for $n \geq 55$,

$$2\left(\sqrt{0.94} + \sqrt{1-2/n} + 1 + \sqrt{n-4}\right) < E(M_n). \tag{12}$$

It follows from $\sqrt{0.59} + \sqrt{3.42} + \sqrt{n-4.9} < \sqrt{0.94} + \sqrt{1-2/n} + 1 + \sqrt{n-4}$ that the RHS of (11) is less than the LHS of (12) as $n \geq 55$. Therefore, $C_n \rightharpoonup M_n$ for $n \geq 55$.

The calculation yields $C_n \rightharpoonup M_n$ for $54 \geq n \geq 8$. □

Lemma 7 $C_n \rightharpoonup J_n$ *for* $n \geq 11$.

Proof Straightforward derivation by Lemma 1 yields

$$\Phi(J_n, x) = x^{n-6}\left[-(3n-21) + (4n-21)x^2 - (n-1)x^4 + x^6\right] \triangleq x^{n-6} f_7(x).$$

Since

$$f_7\left(\sqrt{0.95}\right) = 2.80988 - 0.1025n < 0, \quad (n \geq 40),$$
$$f_7(1) = 2 > 0, \quad (n \geq 10),$$
$$f_7\left(\sqrt{2.8}\right) = -8.008 + 0.36n > 0, \quad (n \geq 23),$$
$$f_7\left(\sqrt{3}\right) = -6 < 0, \quad (n \geq 10),$$

$$f_7\left(\sqrt{n-5}\right) = 26 - 4n < 0, \quad (n \geq 10),$$
$$f_7\left(\sqrt{n-4.9}\right) = 0.1(-47.4183 + n)(-6.38172 + n) > 0, \quad (n \geq 48),$$

we have, for $n \geq 48$,

$$2\left(\sqrt{0.95} + \sqrt{2.8} + \sqrt{n-5}\right) < E(J_n). \tag{13}$$

It follows from $\sqrt{0.59} + \sqrt{3.42} + \sqrt{n-4.9} < \sqrt{0.95} + \sqrt{2.8} + \sqrt{n-5}$ that the RHS of (11) is less than the LHS of (13) as $n \geq 48$. Therefore, $C_n \rightharpoonup J_n$ for $n \geq 48$.
The calculation yields $C_n \rightharpoonup J_n$ for $47 \geq n \geq 11$. □

By Lemma 5, we will show that Conjecture 1 holds for $d = 5$, as given in Lemma 8.

Lemma 8 *Let $T \in \mathcal{T}_n^5$. Then $A_n \rightharpoonup B_n \rightharpoonup C_n \rightharpoonup T$ for $n \geq 9$ and $A_n \rightharpoonup C_n \rightharpoonup B_n \rightharpoonup T$ for $n = 8$.*

Proof By Lemma 3, we have $A_n \rightharpoonup B_n$ for $n \geq 9$ and $A_n \rightharpoonup C_n$ for $n = 8$. As $n \geq 9$, $K_n \rightharpoonup C_n$ follows from $m(K_n, 2) = 4n - 21 < 4n - 19 = m(C_n, 2)$, $m(K_n, 3) = m(C_n, 3) = 2n - 12$ and $m(K_n, k) = m(C_n, k) = 0$ with $4 \leq k \leq n/2$. Furthermore, by Lemma 5, we have $B_n \rightharpoonup C_n$ for $n \geq 11$. The calculation yields $B_n \rightharpoonup C_n$ for $n = 10, 9$. $C_n \rightharpoonup T$ for $n \geq 9$ was proved by Zhou and Li [16]. The calculation yields $C_n \rightharpoonup B_n \rightharpoonup T$ for $n = 8$. In conclusion, Lemma 8 holds. □

Lemma 9 *$T_n^4(n-7, 0, 2) \rightharpoonup H_n$ for $n \geq 9$.*

Proof Straightforward derivation by Lemma 1 yields

$$\Phi(T_n^4(n-7,0,2), x) = x^{n-4}\left[(4n-21) - (n-1)x^2 + x^4\right] \triangleq x^{n-4} f_8(x),$$
$$\Phi(H_n, x) = x^{n-6}\left[-(n-5) + (2n-7)x^2 - (n-1)x^4 + x^6\right] \triangleq x^{n-6} f_9(x).$$

Since

$$f_8\left(\sqrt{3.8}\right) = -2.76 + 0.2n > 0, \quad (n \geq 14),$$
$$f_8(2) = -1 < 0, \quad (n \geq 7),$$
$$f_8\left(\sqrt{n-5}\right) = -1 < 0, \quad (n \geq 7),$$
$$f_8\left(\sqrt{n-4.95}\right) = -1.4475 + 0.05n > 0, \quad (n \geq 29),$$

we have, for $n \geq 29$,

$$E(T_n^4(n-7,0,2)) < 2\left(2 + \sqrt{n-4.95}\right). \tag{14}$$

Since

$$f_9\left(\sqrt{1-3/n}\right) = -3(9-12n+n^2)/n^3 < 0, \quad (n \geq 12), \tag{15}$$

$$f_9\left(\sqrt{1-1/n}\right) = (-1+4n+n^2)/n^3 > 0, \quad (n \geq 6), \tag{16}$$

$$f_9(1) = 0, \quad (n \geq 6), \tag{17}$$

$$f_9\left(\sqrt{n-3}\right) = 8-2n < 0, \quad (n \geq 6), \tag{18}$$

$$f_9\left(\sqrt{n-2.9}\right) = 0.1(-23.9+n)(-3.9+n) > 0, \quad (n \geq 24), \tag{19}$$

we have, for $n \geq 24$,

$$2\left(\sqrt{1-3/n}+1+\sqrt{n-3}\right) < E(H_n). \tag{20}$$

It follows from $2+\sqrt{n-4.95} < \sqrt{1-3/n}+1+\sqrt{n-3}$ that the RHS of (14) is less than the LHS of (20) as $n \geq 29$. Therefore, $T_n^4(n-7,0,2) \rightharpoonup H_n$ for $n \geq 29$.

The calculation yields $T_n^4(n-7,0,2) \rightharpoonup H_n$ for $28 \geq n \geq 9$. □

Lemma 10 $H_n \rightharpoonup T_n^3(n-8,4)$ *for* $n \geq 46$ *and* $T_n^3(n-8,4) \rightharpoonup H_n$ *for* $45 \geq n \geq 12$.

Proof It follows from (15)–(19) that, for $n \geq 24$,

$$E(H_n) < 2\left(\sqrt{1-1/n}+1+\sqrt{n-2.9}\right). \tag{21}$$

Straightforward derivation by Lemma 1 yields

$$\Phi(T_n^3(n-8,4),x) = x^{n-4}\left[(5n-35)-(n-1)x^2+x^4\right] \triangleq x^{n-4}f_{10}(x).$$

Since

$$f_{10}\left(\sqrt{4.86}\right) = -6.5204+0.14n > 0, \quad (n \geq 47),$$

$$f_{10}\left(\sqrt{5}\right) = -5 < 0, \quad (n \geq 12),$$

$$f_{10}\left(\sqrt{n-6}\right) = -5 < 0, \quad (n \geq 12),$$

$$f_{10}\left(\sqrt{n-5.5}\right) = -10.25+0.5n > 0, \quad (n \geq 21),$$

we have, for $n \geq 47$,

$$2\left(\sqrt{4.86}+\sqrt{n-6}\right) < E(T_n^3(n-8,4)). \tag{22}$$

It follows from $\sqrt{1-1/n}+1+\sqrt{n-2.9} < \sqrt{4.86}+\sqrt{n-6}$ that the RHS of (21) is less than the LHS of (22) as $n \geq 58$. Therefore, $H_n \rightharpoonup T_n^3(n-8,4)$ for $n \geq 58$.

The calculation yields $H_n \rightharpoonup T_n^3(n-8,4)$ for $57 \geq n \geq 46$ while $T_n^3(n-8,4) \rightharpoonup H_n$ for $45 \geq n \geq 12$. □

Lemma 11 $T_n^4(n-8,0,3) \rightharpoonup Q'_n$ *for* $7117598 \geq n \geq 11$.

Proof Straightforward derivation by Lemma 1 yields

$$\Phi(T_n^4(n-8,0,3),x) = x^{n-4}[(5n-31)-(n-1)x^2+x^4] \triangleq x^{n-4}f_{11}(x),$$
$$\Phi(Q'_n,x) = x^{n-6}[-(n-5)+(3n-13)x^2-(n-1)x^4+x^6] \quad \triangleq x^{n-6}f_{12}(x).$$

Since

$$f_{11}\left(\sqrt{4.94}\right) = -1.6564+0.06n > 0, \quad (n \geq 28),$$
$$f_{11}\left(\sqrt{5-1/10n}\right) = (1-110n-90n^2)/100n^2 < 0, \quad (n \geq 11),$$
$$f_{11}\left(\sqrt{n-6}\right) = -1 < 0, \quad (n \geq 11),$$
$$f_{11}\left(\sqrt{n-5.99}\right) = -1.1099+0.01n > 0, \quad (n \geq 111),$$

we have, for $n \geq 111$,

$$E(T_n^4(n-8,0,3)) < 2\left(\sqrt{5-1/10n}+\sqrt{n-5.99}\right). \tag{23}$$

Since

$$f_{12}\left(\sqrt{0.3819}\right) = 0.236847-0.00014761n < 0, \quad (n \geq 1605), \tag{24}$$
$$f_{12}\left(\sqrt{0.389}\right) = 0.153185+0.015679n > 0, \quad (n \geq 11), \tag{25}$$
$$f_{12}\left(\sqrt{2.617}\right) = -4.24929+0.002311n > 0, \quad (n \geq 1839), \tag{26}$$
$$f_{12}\left(\sqrt{2.7}\right) = -3.127-0.19n < 0, \quad (n \geq 11), \tag{27}$$
$$f_{12}\left(\sqrt{n-4}\right) = 9-2n < 0, \quad (n \geq 11), \tag{28}$$
$$f_{12}\left(\sqrt{n-3.9}\right) = 0.1(-26.4114+n)(-4.38864+n) > 0, \quad (n \geq 27), \tag{29}$$

we have, for $n \geq 1839$,

$$2\left(\sqrt{0.3819}+\sqrt{2.617}+\sqrt{n-4}\right) < E(Q'_n). \tag{30}$$

It follows from $\sqrt{5-1/10n}+\sqrt{n-5.99} < \sqrt{0.3819}+\sqrt{2.617}+\sqrt{n-4}$ that the RHS of (23) is less than the LHS of (30) as $7117598 \geq n \geq 1839$. Therefore, $T_n^4(n-8,0,3) \rightharpoonup Q'_n$ for $7117598 \geq n \geq 1839$.

The calculation yields $T_n^4(n-8,0,3) \rightharpoonup Q'_n$ for $1838 \geq n \geq 11$. □

It should be noted that the theorem of zero points is not applicable for the mathematical proof of $T_n^4(n-8,0,3) \rightharpoonup Q_n'$ with $n \geq 7117599$. However, the calculation and graphical representation allow us to make a conjecture for $n \geq 7117599$ as follows. A rigorous proof for Conjecture 2 remains a mathematical task for the future.

Conjecture 2 *$T_n^4(n-8,0,3) \rightharpoonup Q_n'$ for $n \geq 7117599$.*

Lemma 12 *$Q_n' \rightharpoonup T_n^3(n-9,5)$ for $n \geq 59$ while $T_n^3(n-9,5) \rightharpoonup Q_n'$ for $58 \geq n \geq 14$.*

Proof We have

$$f_{12}\left(\sqrt{0.37}\right) = 0.377553 - 0.0269n < 0, \quad (n \geq 14), \tag{31}$$

$$f_{12}\left(\sqrt{2.5}\right) = -5.625 + 0.25n > 0, \quad (n \geq 23). \tag{32}$$

It follows from (31), (25), (32), and (27)–(29) that, for $n \geq 27$,

$$E(Q_n') < 2\left(\sqrt{0.389} + \sqrt{2.7} + \sqrt{n-3.9}\right). \tag{33}$$

Straightforward derivation by Lemma 1 yields

$$\Phi(T_n^3(n-9,5),x) = x^{n-4}\left[(6n-48) - (n-1)x^2 + x^4\right] \triangleq x^{n-4} f_{13}(x).$$

Since

$$f_{13}\left(\sqrt{5.83}\right) = -8.1811 + 0.17n > 0, \quad (n \geq 49),$$
$$f_{13}\left(\sqrt{6}\right) = -6 < 0, \quad (n \geq 7),$$
$$f_{13}\left(\sqrt{n-7}\right) = -6 < 0, \quad (n \geq 7),$$
$$f_{13}\left(\sqrt{n-6.5}\right) = -12.25 + 0.5n > 0, \quad (n \geq 25),$$

we have, for $n \geq 49$,

$$2\left(\sqrt{5.83} + \sqrt{n-7}\right) < E(T_n^3(n-9,5)). \tag{34}$$

It follows from $\sqrt{0.389} + \sqrt{2.7} + \sqrt{n-3.9} < \sqrt{5.83} + \sqrt{n-7}$ that the RHS of (33) is less than the LHS of (34) as $n \geq 116$. Therefore, $Q_n' \rightharpoonup T_n^3(n-9,5)$ for $n \geq 116$.

The calculation yields $Q_n' \rightharpoonup T_n^3(n-9,5)$ for $115 \geq n \geq 59$ while $T_n^3(n-9,5) \rightharpoonup Q_n'$ for $58 \geq n \geq 14$. □

We introduce Property 1 and Lemma 13 to deduce the increasing orders of the trees in $\mathcal{T}_n^{\mathrm{A}}$ which are given in Lemmas 14 and 15 for $n \geq 18$ and $17 \geq n \geq 7$, respectively.

Property 1 *Let $n \geq 7$. (i) $E(T_n^3(n_1, n_2))$ is a monotonously increasing function of n_2. (ii) $E(T_n^4(n_1, 0, n_3))$ is a monotonously increasing function of n_3.*

Proof Since $n_1 + n_2 = n - 4$ for $T_n^3(n_1, n_2)$, we have

$$m(T_n^3(n_1, n_2), 2) = (n_1 + 1)(n_2 + 1) = -n_2^2 + (n-4)n_2 + (n-3). \quad (35)$$

As $0 \leq n_2 \leq (n-4)/2$, it follows from (35) that $m(T_n^3(n_1, n_2), 2)$ is a monotonously increasing function of n_2. Since $m(T_n^3(n_1, n_2), k) = 0$ for $3 \leq k \leq n/2$, Property 1(i) holds.

Since $n_1 + n_3 = n - 5$ for $T_n^4(n_1, 0, n_3)$, we have

$$\begin{aligned} m(T_n^4(n_1, 0, n_3), 2) &= (n_1 + 1)(n_3 + 2) + (n_3 + 1) \\ &= -n_3^2 + (n-5)n_3 + (2n-7). \end{aligned} \quad (36)$$

As $0 \leq n_3 \leq (n-5)/2$, it follows from (36) that $m(T_n^4(n_1, 0, n_3), 2)$ is a monotonously increasing function of n_3. Since $m(T_n^4(n_1, 0, n_3), k) = 0$ for $3 \leq k \leq n/2$, Property 1(ii) holds. □

Lemma 13 *Let $n \geq 12$.*

(i) If $0 \leq a \leq (n-11)/3$, then

$$\begin{aligned} T_n^4(n-5-a, 0, a) &\rightharpoonup T_n^3(n-6-a, a+2) \rightharpoonup T_n^4(n-6-a, 0, a+1) \\ &\rightrightarrows T_n^3(n-7-a, a+3) \end{aligned}$$

with equality iff $a = (n-11)/3$.

(ii) If $(n-11)/3 < a < (n-8)/3$, then

$$\begin{aligned} T_n^4(n-5-a, 0, a) &\rightharpoonup T_n^3(n-6-a, a+2) \rightharpoonup T_n^3(n-7-a, a+3) \\ &\rightharpoonup T_n^4(n-6-a, 0, a+1). \end{aligned}$$

(iii) If $(n-8)/3 \leq a \leq (2n-17)/5$, then

$$\begin{aligned} T_n^3(n-6-a, a+2) &\rightrightarrows T_n^4(n-5-a, 0, a) \rightrightarrows T_n^3(n-7-a, a+3) \\ &\rightharpoonup T_n^4(n-6-a, 0, a+1). \end{aligned}$$

The first and second equalities hold iff $a = (n-8)/3$ and $a = (2n-17)/5$, respectively.

(iv) If $a > (2n-17)/5$, then

$$\begin{aligned} T_n^3(n-6-a, a+2) &\rightharpoonup T_n^3(n-7-a, a+3) \rightharpoonup T_n^4(n-5-a, 0, a) \\ &\rightharpoonup T_n^4(n-6-a, 0, a+1). \end{aligned}$$

Proof It is obvious that, for $3 \leq k \leq n/2$, the k-matchings for the trees considered in Lemma 13 are zero. Next we compare the numbers of their 2-matchings. By (35) and (36), we deduce

$$m(T_n^4(n-5-a,0,a),2) - m(T_n^3(n-6-a,a+2),2) = 3a-(n-8), \quad (37)$$
$$m(T_n^3(n-6-a,a+2),2) - m(T_n^4(n-6-a,0,a+1),2) = -(a+2), \quad (38)$$
$$m(T_n^4(n-6-a,0,a+1),2) - m(T_n^3(n-7-a,a+3),2) = 3a-(n-11), \quad (39)$$
$$m(T_n^4(n-5-a,0,a),2) - m(T_n^3(n-7-a,a+3),2) = 5a-(2n-17). \quad (40)$$

As $0 \leq a \leq (n-11)/3$, by (37)–(39), we have Lemma 13(i).

As $(n-11)/3 < a < (n-8)/3$, by (37), Property 1(i) and (39), we have Lemma 13(ii).

As $(n-8)/3 \leq a \leq (2n-17)/5$, by (37), (40) and (39), we have Lemma 13(iii).

As $a > (2n-17)/5$, by Property 1(i), (40) and Property 1(ii), we have Lemma 13(iv). □

Lemma 13 shows that $T_n^3(n_1,n_2)$ and $T_n^4(n_1,0,n_3)$ are staggered in the increasing order of their energies.

Obviously, the k-matchings with $3 \leq k \leq n/2$ for X_n, Y_n, Z_n, W_n, D_n, and U_n are zero. For $n \geq 7$, we deduce $m(X_n,2) = 0 < m(Y_n,2) = n-3 < 2n-8 = m(Z_n,2) < m(W_n,2) = 2n-7 \leq 3n-15 = m(D_n,2) < 3n-13 = m(U_n,2)$. This inequality still holds without "$\leq 3n-15 = m(D_n,2)$" for $n = 7$. Therefore, we have

$$X_n \rightharpoonup Y_n \rightharpoonup Z_n \rightharpoonup W_n \rightrightarrows D_n \rightharpoonup U_n, \qquad (n \geq 8), \quad (41)$$
$$X_n \rightharpoonup Y_n \rightharpoonup Z_n \rightharpoonup W_n \rightharpoonup U_n, \qquad (n = 7). \quad (42)$$

The equality in (41) holds iff $n = 8$. The inequalities in (42) and (41) were also reported by Gutman [3] and Li and Li [7]. For the sake of conciseness, the symbols (∇) and ($\triangle$) denote hereinafter (41) and $X_n \rightharpoonup Y_n \rightharpoonup Z_n \rightharpoonup W_n \rightharpoonup D_n$, respectively.

As $n \geq 14$ and $a = 1 \leq (n-11)/3$, by Lemma 13(i), we get $U_n \rightharpoonup Q_n \rightharpoonup T_n^4(n-7,0,2) \rightrightarrows T_n^3(n-8,4)$ with equality iff $n = 14$. For the sake of conciseness, the inequalities

$$(\nabla) \rightharpoonup Q_n \rightharpoonup T_n^4(n-7,0,2), \quad (n \geq 14), \quad (43)$$
$$(\nabla) \rightharpoonup Q_n \rightharpoonup T_n^4(n-7,0,2) \rightrightarrows T_n^3(n-8,4), \quad (n \geq 14) \quad (44)$$

are hereinafter denoted by the symbols ($\diamond$) and ($\perp$), respectively.

Lemma 14 *Let $T \in \mathcal{T}_n^A$ with $n \geq 18$, we have*

$$(\perp) \rightharpoonup T_n^4(n-8,0,3) \rightharpoonup T_n^3(n-9,5) \rightharpoonup T. \quad (45)$$

Proof As $n \geq 18$ and $a = 2 < (n-11)/3$, by Lemma 13(i), we have the first and second inequalities in (45). By Property 1(i), we obtain $T_n^3(n-9,5) \rightharpoonup T$ for

$T = T_n^3(n_1, n_2)$ with $n_2 \geq 6$. Since $m(T_n^3(n-9,5),2) = 6n-48 < 6n-43 = m(T_n^4(n-9,0,4),2)$ and $m(T_n^3(n-9,5),k) = m(T_n^4(n-9,0,4),k) = 0$ for $3 \leq k \leq n/2$, we get $T_n^3(n-9,5) \rightharpoonup T_n^4(n-9,0,4)$. Furthermore, by Property 1(ii), we obtain $T_n^3(n-9,5) \rightharpoonup T$ for $T = T_n^4(n_1,0,n_3)$ with $n_3 \geq 4$. In conclusion, $T_n^3(n-9,5) \rightharpoonup T$ holds for $T \in \mathcal{T}_n^{\mathrm{A}}$. □

Lemma 15 *The increasing order by their energies of all the trees in $\mathcal{T}_n^A$ are*

$$(\perp) \rightharpoonup T_n^4(n-8,0,3) \leftrightarrows T_n^3(n-9,5) \rightharpoonup T_n^3(n-10,6) \rightharpoonup T_n^4(n-9,0,4) \rightharpoonup T_n^4(n-10,0,5) \rightharpoonup T_n^4(n-11,0,6), \quad (n=17), \tag{46}$$

$$(\perp) \rightharpoonup T_n^3(n-9,5) \rightharpoonup T_n^4(n-8,0,3) \leftrightarrows T_n^3(n-10,6) \rightharpoonup T_n^4(n-9,0,4) \rightharpoonup T_n^4(n-10,0,5), \qquad (n=16), \tag{47}$$

$$(\perp) \rightharpoonup T_n^3(n-9,5) \rightharpoonup T_n^4(n-8,0,3) \rightharpoonup T_n^4(n-9,0,4) \rightharpoonup T_n^4(n-10,0,5), \quad (n=15), \tag{48}$$

$$(\perp) \rightharpoonup T_n^3(n-9,5) \rightharpoonup T_n^4(n-8,0,3) \rightharpoonup T_n^4(n-9,0,4), \quad (n=14), \tag{49}$$

$$(\nabla) \rightharpoonup Q_n \rightharpoonup T_n^3(n-8,4) \rightharpoonup T_n^4(n-7,0,2) \rightharpoonup T_n^4(n-8,0,3) \rightharpoonup T_n^4(n-9,0,4), (n=13), \tag{50}$$

$$(\nabla) \rightharpoonup Q_n \rightharpoonup T_n^3(n-8,4) \rightharpoonup T_n^4(n-7,0,2) \rightharpoonup T_n^4(n-8,0,3), \quad (n=12), \tag{51}$$

$$(\nabla) \leftrightarrows Q_n \rightharpoonup T_n^4(n-7,0,2) \rightharpoonup T_n^4(n-8,0,3), \quad (n=11), \tag{52}$$

$$(\triangle) \rightharpoonup Q_n \rightharpoonup U_n \rightharpoonup T_n^4(n-7,0,2), \quad (n=10), \tag{53}$$

$$(\nabla) \rightharpoonup T_n^4(n-7,0,2), \quad (n=9). \tag{54}$$

Proof Let $n = 17$. As $a = 2 = (n-11)/3$, by Lemma 13(i), we get the first inequalities and the equality in (46). As $a = 3 = (n-8)/3$, by Lemma 13(iii), we get the second and third inequalities in (46). By Property 1(ii), we have the remaining inequalities in (46).

Let $n = 16$. As $(n-11)/3 < a = 2 < (n-8)/3$, by Lemma 13(ii), we get the first and second inequalities in (47). As $a = 3 = (2n-17)/5$, by Lemma 13(iii), we get the equality and the third inequality in (47). By Property 1(ii), we have the last inequality in (47).

Let $n = 15$. As $(n-11)/3 < a = 2 < (n-8)/3$, by Lemma 13(ii), we get the first and second inequalities in (48). By Property 1(ii), we have the remaining inequalities in (48).

Let $n = 14$. As $a = 2 = (n-8)/3$, by Lemma 13(iii), we get the first and second inequalities in (49). By Property 1(ii), we have the last inequality in (49).

Let $n = 13, 12$. As $(n-11)/3 < a = 1 < (n-8)/3$, by Lemma 13(ii), we get the first to the third inequalities in (50) and (51). By Property 1(ii), we have the remaining inequalities in (50) and (51).

Since $m(D_n,2) = 3n-15$, $m(U_n,2) = 3n-13$, $m(Q_n,2) = 4n-24$, $m(T_n^4(n-7,0,2),2) = 4n-21$, $m(T_n^4(n-8,0,3),2) = 5n-31$, we deduce $m(U_n,2) = m(Q_n,2) < m(T_n^4(n-7,0,2),2) < m(T_n^4(n-8,0,3),2)$ for $n = 11$ and

$m(D_n, 2) < m(Q_n, 2) < m(U_n, 2) < m(T_n^4(n-7, 0, 2), 2)$ for $n = 10$. Furthermore, the k-matchings for $D_n, U_n, Q_n, T_n^4(n-7, 0, 2)$, and $T_n^4(n-8, 0, 3)$ are zero for $3 \le k \le n/2$. Therefore, we obtain (52) and (53).

Let $n = 9$. By Property 1(ii), we get (54). □

We introduce Lemmas 16–18 to deduce the increasing order of the trees in $\mathcal{T}_n^{\mathrm{B}}$ with $n \ge 7$ which is given in Lemma 19.

Let $D_n^4(n_1; n_2 - 2p, p; n_3)$ be a tree obtained from P_5 by attaching n_1 and n_3 pendant edges to v_1 and v_3, respectively, and then attaching p paths of length two and $n_2 - 2p$ pendant edges to v_2, where $n_1 + n_2 + n_3 = n - 5$, $n_1 \ge n_3$, $0 \le n_2 \le n - 5$ and $0 \le p \le [n_2/2]$. Obviously, the trees in $\mathcal{T}_n^4$ are represented by $D_n^4(n_1; n_2 - 2p, p; n_3)$. If $p = 0$, then $D_n^4(n_1; n_2 - 2p, p; n_3) = T_n^4(n_1, n_2, n_3)$. If $n_2 = 0$, then $T_n^4(n_1, n_2, n_3) \in \mathcal{T}_n^{\mathrm{A}}$. If $n_2 \ne 0$, then $D_n^4(n_1; n_2 - 2p, p; n_3) \in \mathcal{T}_n^{\mathrm{B}}$. For example, $D_n^4(0; 2, 1; 0) = M_9$. For $D_n^4(n_1; n_2 - 2p, p; n_3)$, we simply quote Lemma 16 presented by Gutman and Zhang [4].

Lemma 16 [4] *Let $q = n - 5 - n_2$ with $n_2 \le n - 5$. Then* $D_n^4(q; n_2 - 2p, p; 0) \rightharpoonup D_n^4(q-1; n_2 - 2p, p; 1) \rightharpoonup D_n^4(q-2; n_2 - 2p, p; 2) \rightharpoonup \cdots \rightharpoonup D_n^4(q - [q/2]; n_2 - 2p, p; [q/2])$.

Lemma 17 $D_n^4(n_1; n_2 - 2p, p; n_3) \rightharpoonup D_n^4(n_1; n_2 - 2p - 2, p + 1; n_3)$ *with* $n_2 \ge 2$ *and* $0 \le p \le [n_2/2]$.

Proof Let the pendant edge attached at v_2 of $T_n^4(n_1, n_2, n_3)$ and the pendant edge of a path of length two attached at v_2 of $D_n^4(n_1; n_2 - 2, 1; n_3)$ be the edge e in (6). It follows from Lemma 2 that

$$\begin{aligned} m(T_n^4(n_1, n_2, n_3), k) &= m(T_n^4(n_1, n_2 - 1, n_3), k) \\ &\quad + m(K_{1,n_1+1} \cup K_{1,n_3+1}, k - 1), \qquad (55) \\ m(D_n^4(n_1; n_2 - 2, 1; n_3), k) &= m(T_n^4(n_1, n_2 - 1, n_3), k) \\ &\quad + m(T_n^4(n_1, n_2 - 2, n_3), k - 1). \qquad (56) \end{aligned}$$

Since $K_{1,n_1+1} \cup K_{1,n_3+1}$ is a subgraph of $T_n^4(n_1, n_2 - 2, n_3)$, we have $m(K_{1,n_1+1} \cup K_{1,n_3+1}, k-1) \le m(T_n^4(n_1, n_2 - 2, n_3), k-1)$ where the equality does not hold for all values of k. For example, $m(K_{1,n_1+1} \cup K_{1,n_3+1}, 1) = n_1 + n_3 + 2 < n_1 + n_2 + n_3 + 2 = m(T_n^4(n_1, n_2 - 2, n_3), 1)$ since $n_2 \ge 2$. By comparing (55) with (56), we have Lemma 17 for $p = 0$. By recursion, Lemma 17 holds for $1 \le p \le [n_2/2]$. □

Since $m(C_n, 2) = 4n - 19$, $m(C_n, 3) = 2n - 12$ and $m(C_n, k) = 0$ with $4 \le k \le n/2$, we have Lemma 18.

Lemma 18 *Let $T \in \mathcal{T}_n$. If $m(T, 2) \ge 4n - 19$ and $m(T, 3) \ge 2n - 12$, then $C_n \rightrightarrows T$, with equality iff the equalities in the two conditions hold simultaneously and $m(T, k) = 0$ with $4 \le k \le n/2$.*

Lemma 19 *For $T \in \mathcal{T}_n^B$, we have*

$$H_n \rightharpoonup Q'_n \rightharpoonup A_n \rightharpoonup I_n \rightharpoonup B_n \rightharpoonup K_n \rightharpoonup L_n \rightharpoonup C_n \rightharpoonup T, \quad (n \geq 11), \tag{57}$$
$$H_n \rightharpoonup Q'_n \rightharpoonup A_n \rightharpoonup I_n \rightharpoonup K_n \rightharpoonup B_n \rightharpoonup L_n \rightharpoonup J_n \rightharpoonup C_n \rightharpoonup T, \quad (n = 10), \tag{58}$$
$$H_n \rightharpoonup Q'_n \rightharpoonup A_n \rightharpoonup I_n \rightharpoonup K_n \rightharpoonup L_n \rightharpoonup B_n \rightharpoonup C_n \rightharpoonup T, \quad (n = 9), \tag{59}$$
$$H_n \rightharpoonup Q'_n \rightharpoonup A_n \rightharpoonup I_n \rightharpoonup L_n \rightharpoonup C_n \rightharpoonup T, \quad (n = 8), \tag{60}$$
$$H_n \rightharpoonup Q'_n \rightharpoonup A_n \rightharpoonup B_n \rightharpoonup M_n \rightharpoonup P_n, \quad (n = 7). \tag{61}$$

Proof As $n \geq 7$, it follows from $m(H_n, 2) = 2n - 7 < 3n - 13 = m(Q'_n, 2) < m(A_n, 2) = 3n - 12$, $m(H_n, 3) = m(Q'_n, 3) = m(A_n, 3) = n - 5$ and $m(H_n, k) = m(Q'_n, k) = m(A_n, k) = 0$ with $4 \leq k \leq n/2$ that $H_n \rightharpoonup Q'_n \rightharpoonup A_n$ in (57)–(61) holds. By Lemma 4, we have $A_n \rightharpoonup I_n$ in (57)–(60).

As $n \geq 7$, it follows from $m(I_n, 2) = 3n - 13 < 3n - 12 = m(B_n, 2)$, $m(I_n, 3) = 2n - 12 < 2n - 11 = m(B_n, 3)$ and $m(I_n, k) = m(B_n, k)$ with $4 \leq k \leq n/2$ that

$$I_n \rightharpoonup B_n, \quad (n \geq 7). \tag{62}$$

As $n \geq 8$, it follows from $m(K_n, 2) = 4n-21 < 4n-20 = m(L_n, 2) < 4n-19 = m(C_n, 2)$, $m(K_n, 3) = m(L_n, 3) = m(C_n, 3) = 2n-12$ and $m(K_n, k) = m(L_n, k) = m(C_n, k) = 0$ with $4 \leq k \leq n/2$ that

$$K_n \rightharpoonup L_n \rightharpoonup C_n, \quad (n \geq 8). \tag{63}$$

As $n \geq 11$, by (62), Lemma 5 and (63), we deduce $I_n \rightharpoonup B_n \rightharpoonup K_n \rightharpoonup L_n \rightharpoonup C_n$ in (57).

As $n = 10$ and $n = 9$, the calculation yields $I_n \rightharpoonup K_n \rightharpoonup B_n \rightharpoonup L_n \rightharpoonup J_n \rightharpoonup C_n$ in (58) and $I_n \rightharpoonup K_n \rightharpoonup L_n \rightharpoonup B_n \rightharpoonup C_n$ in (59), respectively.

As $n = 8$, by (63), we have $I_n \rightharpoonup L_n \rightharpoonup C_n$ in (60) since I_8 and K_8 are identical.

As $n = 7$, Lemma 3 and the calculation yield $A_n \rightharpoonup B_n \rightharpoonup M_n \rightharpoonup P_n$ in (61).

Next, we prove the last inequality $C_n \rightharpoonup T$ in (57)–(60).

Since $m(T_n^6(n-7, 0, 0, 0, 0), 2) = 4n - 18 > 4n - 19$ and $m(T_n^6(n-7, 0, 0, 0, 0), 3) = 3n - 17 > 2n - 12$ for $n \geq 8$, by Lemma 18, we have $C_n \rightharpoonup T_n^6(n-7, 0, 0, 0, 0)$ for $n \geq 7$. Therefore, by Lemma 3, we deduce $C_n \rightharpoonup T$ for $T \in \mathcal{T}_n^d$ with $d \geq 6$ and $n \geq 8$. By Lemma 8, we have $C_n \rightharpoonup T$ for $T \in \mathcal{T}_n^5$ with $n \geq 8$. Next, we prove $C_n \rightharpoonup T$ for $T \in \mathcal{T}_n^4$ with $n \geq 8$. Since $T \in \mathcal{T}_n^{\mathrm{B}}$, we have $1 \leq n_2 \leq n - 5$. Let $n_1 + n_3 = r$, then $0 \leq r \leq n - 6$. We consider six cases according to the values of r as follows.

Case (i) $r = 0$, namely $T = D_n^4(0; n - 5 - 2p, p; 0)$.

Since $T \neq H_n$, we have $1 \leq p \leq [(n-5)/2]$ with $n \geq 8$. Obviously, $M_n = D_n^4(0; n-7, 1; 0)$. By Lemma 17, we get $M_n \rightrightarrows T$. By Lemma 6, we deduce $C_n \rightharpoonup T$ in (57)–(60).

Case (ii) $r = 1$, namely $T = D_n^4(1; n - 6 - 2p, p; 0)$.

Since $T \neq I_n$, we have $1 \leq p \leq [(n-6)/2]$ with $n \geq 8$. By Lemma 17, we get $D_n^4(1; n-8, 1; 0) \rightrightarrows T$. Since $m(D_n^4(1; n-8, 1; 0), 2) = 4n - 19$ and $m(D_n^4(1; n-8, 1; 0), 3) = 5n - 33 > 2n - 12$ for $n \geq 8$, by Lemma 18, we have $C_n \rightharpoonup D_n^4(1; n-8, 1; 0)$ with $n \geq 8$. Therefore, $C_n \rightharpoonup T$ in (57)–(60) holds.

Case (iii) $r = 2$, namely $T = D_n^4(2 - n_3; n - 7 - 2p, p; n_3)$, where $0 \leq p \leq [(n-7)/2]$ and $n \geq 8$.

As $n \geq 11$, by Lemmas 16 and 17, we get $J_n \rightrightarrows T$. By Lemma 7, we deduce $C_n \rightharpoonup T$ in (57). As $n = 10, 9$, the calculation yields $C_n \rightharpoonup T$ in (58)–(59). As $n = 8$, there are only two trees Q_8' and L_8. Therefore, it is uncesessary to prove $C_n \rightharpoonup T$ in (60).

Case (iv) $3 \leq r \leq n - 8$, namely $T = D_n^4(r - n_3; n - 5 - r - 2p, p; n_3)$, where $0 \leq p \leq [(n-5-r)/2]$ and $n \geq 11$.

By Lemmas 16 and 17, we get $T_n^4(r, n-5-r, 0) \rightrightarrows T$. As $n = 11$, $C_n \rightharpoonup T$ in (57) holds from $r = 3$ and the calculation yields $C_n \rightharpoonup T_n^4(3, 3, 0)$. As $n \geq 12$, we have

$$m(T_n^4(r, n-5-r, 0), 2) = -r^2 + (n-5)r + (2n-7) \geq 5n - 31 \geq 4n - 19,$$
$$m(T_n^4(r, n-r-5, 0), 3) = (r+1)(n-5-r) \geq 3(n-7) > 2n - 12.$$

By Lemma 18, we have $C_n \rightharpoonup T_n^4(r, n-5-r, 0)$. Therefore, $C_n \rightharpoonup T$ in (57) holds for $n \geq 12$.

Case (v) $r = n - 7$, namely $T = T_n^4(n - 7 - n_3, 2, n_3)$ or $T = D_n^4(n - 7 - n_3; 0, 1; n_3)$.

Let $T = T_n^4(n-7-n_3, 2, n_3)$. Since $T \neq K_n$, we have $1 \leq n_3 \leq (n-7)/2$ with $n \geq 9$. As $n \geq 10$, by Lemma 16, we get $T_n^4(n-8, 2, 1) \rightrightarrows T$. Since $m(T_n^4(n-8, 2, 1), 2) = 5n - 29 \geq 4n - 19$ and $m(T_n^4(n-8, 2, 1), 3) = 4n - 28 > 2n - 12$ for $n \geq 10$, by Lemma 18, we obtain $C_n \rightharpoonup T_n^4(n-8, 2, 1)$ with $n \geq 10$. Therefore, $C_n \rightharpoonup T$ in (57)–(58) holds. As $n = 9$, $T = T_n^4(1, 2, 1)$ and the calculation yields $C_n \rightharpoonup T_n^4(1, 2, 1)$. Thus $C_n \rightharpoonup T$ in (59) holds.

Let $T = D_n^4(n - 7 - n_3; 0, 1; n_3)$ and $n \geq 8$. By Lemma 16, we have $D_n^4(n-7; 0, 1; 0) \rightrightarrows T$. Since $m(D_n^4(n-7; 0, 1; 0), 2) = 4n - 19$ and $m(D_n^4(n-7; 0, 1; 0), 3) = 3n - 17 > 2n - 12$ for $n \geq 8$, by Lemma 18, we obtain $C_n \rightharpoonup D_n^4(n-7; 0, 1; 0)$ with $n \geq 8$. Therefore, $C_n \rightharpoonup T$ in (57)–(60) holds.

Case (vi) $r = n - 6$, namely $T = T_n^4(n - 6 - n_3, 1, n_3)$.

Since $T \neq Q_n', L_n$, we have $2 \leq n_3 \leq (n-6)/2$ with $n \geq 10$. By Lemma 16, we get $T_n^4(n-8, 1, 2) \rightrightarrows T$. Since $m(T_n^4(n-8, 1, 2), 2) = 5n - 29 \geq 4n - 19$ and $m(T_n^4(n-8, 1, 2), 3) = 3n - 21 > 2n - 12$ for $n \geq 10$, by Lemma 18, we obtain $C_n \rightharpoonup T_n^4(n-8, 1, 2)$ with $n \geq 10$. Therefore, $C_n \rightharpoonup T$ in (57)–(58) holds. □

By Lemmas 9, 10, 14, and 19, we deduce the first 9 trees with minimal energies in $\mathcal{T}_n$ for $n \geq 46$ in Theorem 1.

Theorem 1 *Let $T \in \mathcal{T}_n$. We have $(\diamond) \rightharpoonup H_n \rightharpoonup T$ for $n \geq 46$.*

Proof By Lemma 9, we have $T_n^4(n-7,0,2) \rightharpoonup H_n$ as $n \geq 14$. By Lemmas 10 and 14, we get $H_n \rightharpoonup T$ for $T \in \mathcal{T}_n^{\mathrm{A}}$ with $n \geq 46$. By Lemma 19, we have $H_n \rightharpoonup T$ for $T \in \mathcal{T}_n^{\mathrm{B}}$ with $n \geq 7$. □

By the aforementioned lemmas and the calculation, we derive the first 12 and 11 trees in the increasing order according to their minimal energies within $\mathcal{T}_n$ for $7117598 \geq n \geq 26$ and $25 \geq n \geq 18$, respectively, as given in Theorem 2.

Theorem 2 *Let $T \in \mathcal{T}_n$, we have*

$$
\begin{aligned}
&(\diamondsuit) \rightharpoonup H_n \rightharpoonup T_n^3(n-8,4) \rightharpoonup T_n^4(n-8,0,3) \rightharpoonup Q_n' \\
&\quad \rightharpoonup T, \quad (7117598 \geq n \geq 59), && (64)\\
&(\diamondsuit) \rightharpoonup H_n \rightharpoonup T_n^3(n-8,4) \rightharpoonup T_n^4(n-8,0,3) \rightharpoonup T_n^3(n-9,5) \\
&\quad \rightharpoonup T, \quad (58 \geq n \geq 46), && (65)\\
&(\diamondsuit) \rightharpoonup T_n^3(n-8,4) \rightharpoonup H_n \rightharpoonup T_n^4(n-8,0,3) \rightharpoonup T_n^3(n-9,5) \\
&\quad \rightharpoonup T, \quad (45 \geq n \geq 40), && (66)\\
&(\diamondsuit) \rightharpoonup T_n^3(n-8,4) \rightharpoonup T_n^4(n-8,0,3) \rightharpoonup H_n \rightharpoonup T_n^3(n-9,5) \\
&\quad \rightharpoonup T, \quad (39 \geq n \geq 26), && (67)\\
&(\diamondsuit) \rightharpoonup T_n^3(n-8,4) \rightharpoonup T_n^4(n-8,0,3) \rightharpoonup T_n^3(n-9,5) \\
&\quad \rightharpoonup T, \quad (25 \geq n \geq 18). && (68)
\end{aligned}
$$

Proof By Lemmas 9, 10, 14, and 11, we have the first to the fourth inequalities in (64).

By Lemmas 9, 10 and 14, we have the first to the fourth inequalities in (65).

The calculation yields $H_n \rightharpoonup T_n^4(n-8,0,3)$ for $45 \geq n \geq 40$. By Lemmas 14 and 10, we have the first to the fourth inequalities in (66).

The calculation yields $T_n^4(n-8,0,3) \rightharpoonup H_n \rightharpoonup T_n^3(n-9,5)$ for $39 \geq n \geq 26$. By Lemma 14, we have the first to the fourth inequalities in (67).

By Lemma 14, we have the first to the third inequalities in (68).

Next, we prove the last inequalities in (64)–(68). By Lemmas 12 and 14, we deduce $Q_n' \rightharpoonup T$ in (64) for $T \in \mathcal{T}_n^{\mathrm{A}}$. By Lemma 19, we get $Q_n' \rightharpoonup T$ in (64) for $T \in \mathcal{T}_n^{\mathrm{B}}$. By Lemma 14, we have $T_n^3(n-9,5) \rightharpoonup T$ in (65)–(68) for $T \in \mathcal{T}_n^{\mathrm{A}}$. By Lemmas 12 and 19, we obtain $T_n^3(n-9,5) \rightharpoonup T$ in (65)–(67) for $T \in \mathcal{T}_n^{\mathrm{B}}$. The calculation yields $T_n^3(n-9,5) \rightharpoonup H_n$ for $25 \geq n \geq 18$. Therefore, by Lemma 19, we have $T_n^3(n-9,5) \rightharpoonup T$ in (68) for $T \in \mathcal{T}_n^{\mathrm{B}}$. □

It can be seen from Theorems 1 and 2 that the diameters of the trees with minimal energies obtained in $\mathcal{T}_n$ are less than 5 as $n \geq 18$. We conclude that the seventh-minimal tree in $\mathcal{T}_n$ is Q_n for $n \geq 18$. Theorem 2 shows that Q_n' is the twelfth-minimal tree in $\mathcal{T}_n$ for $7117598 \geq n \geq 59$ and Q_n' is not the seventh in $\mathcal{T}_n$ for $58 \geq n \geq 18$.

From Conjecture 2 and the proof for (64), we suggest Conjecture 3.

Conjecture 3 $(\diamondsuit) \rightharpoonup H_n \rightharpoonup T_n^3(n-8,4) \rightharpoonup T_n^4(n-8,0,3) \rightharpoonup Q_n' \rightharpoonup T$ *for* $n \geq 7117599$.

The calculation yields $T_n^4(n-11,0,6) \rightharpoonup H_n$ for $n = 17$, $T_n^4(n-10,0,5) \rightharpoonup H_n$ for $n = 16, 15$, $T_n^4(n-9,0,4) \rightharpoonup H_n$ for $n = 14, 13$, $T_n^4(n-8,0,3) \rightharpoonup H_n$ for $n = 12, 11$, $T_n^4(n-7,0,2) \rightharpoonup H_n$ for $n = 10, 9$, and $U_n \rightharpoonup H_n$ for $n = 8, 7$. In conclusion, the energies of the last trees in (46)–(54) and (41)–(42) are less than $E(H_n)$. Namely, the maximal energy for the trees in $\mathcal{T}_n^{\mathrm{A}}$ is less than the minimal energy for the trees in $\mathcal{T}_n^{\mathrm{B}}$. It should be noted that all the trees in $\mathcal{T}_n^{\mathrm{A}}$ for $n = 8$ and $n = 7$ are those in (41) and (42), respectively. Therefore, from Lemmas 15, 19 and the calculation, we have Theorem 3.

Theorem 3 *Let $T \in \mathcal{T}_n$. The increasing orders by their energies of the trees in $\mathcal{T}_n$ for $17 \geq n \geq 7$ are the inequalities obtained by connecting the last terms in* (46)–(54) *and* (41)–(42) *with the first terms in* (57)–(61).

Theorem 3 shows that the diameters of the trees with minimal energies obtained in $\mathcal{T}_n$ are less than 6 as $17 \geq n \geq 8$. It can be seen from Theorem 3 that the seventh-minimal tree is Q_n for $17 \geq n \geq 12$ and Q'_n is not the seventh one for $17 \geq n \geq 7$.

By Lemma 13, we can deduce the increasing orders in terms of their minimal energies for the trees in $\mathcal{T}_n^{\mathrm{A}}$ with $n \geq 18$. Furthermore, by Lemma 19 and the calculation, we can derive more than 12 trees for $7117598 \geq n \geq 26$ and more than 11 trees for $25 \geq n \geq 18$ in the increasing order in $\mathcal{T}_n$. However, the further series trees have no common ordering as $7117598 \geq n \geq 18$. We list the first 25 trees for $n = 58$ in (69) as an example. Let $T \in \mathcal{T}_{58}$. We have

$$\begin{aligned}(\perp) &\rightharpoonup H_n \rightharpoonup T_n^4(n-8,0,3) \rightharpoonup T_n^3(n-9,5) \rightharpoonup Q'_n \rightharpoonup A_n \\ &\rightharpoonup T_n^4(n-9,0,4) \rightharpoonup T_n^3(n-10,6) \rightharpoonup T_n^4(n-10,0,5) \rightharpoonup I_n \rightharpoonup B_n \\ &\rightharpoonup T_n^3(n-11,7) \rightharpoonup T_n^4(n-11,0,6) \rightharpoonup K_n \rightharpoonup L_n \rightharpoonup C_n \rightharpoonup T. \end{aligned} \tag{69}$$

Proof of (69) First, we prove

$$\begin{aligned}(\perp) &\rightharpoonup T_n^4(n-8,0,3) \rightharpoonup T_n^3(n-9,5) \rightharpoonup T_n^4(n-9,0,4) \rightharpoonup T_n^3(n-10,6) \\ &\rightharpoonup T_n^4(n-10,0,5) \rightharpoonup T_n^3(n-11,7) \rightharpoonup T_n^4(n-11,0,6) \rightharpoonup T_n^3(n-12,8) \\ &\rightharpoonup T \end{aligned} \tag{70}$$

for $T \in \mathcal{T}_n^{\mathrm{A}}$. As $n = 58$ and $2 \leq a \leq 6 < (n-11)/3$, by Lemma 13(i), we have the first to the eighth inequalities in (70). By the method similar to that for $T_n^3(n-9,5) \rightharpoonup T$ in (45) with $T \in \mathcal{T}_n^{\mathrm{A}}$, we deduce $T_n^3(n-12,8) \rightharpoonup T$ in (70) for $T \in \mathcal{T}_n^{\mathrm{A}}$.

As $n = 58$, the calculation yields $T_n^3(n-8,4) \rightharpoonup H_n \rightharpoonup T_n^4(n-8,0,3)$, $T_n^3(n-9,5) \rightharpoonup Q'_n \rightharpoonup A_n \rightharpoonup T_n^4(n-9,0,4)$, $T_n^4(n-10,0,5) \rightharpoonup I_n \rightharpoonup B_n \rightharpoonup T_n^3(n-11,7)$, $T_n^4(n-11,0,6) \rightharpoonup K_n$, and $C_n \rightharpoonup T_n^3(n-12,8)$. By comparing (70) with (57), we have the first to the fifteenth inequalities in (69). From (70) and $C_n \rightharpoonup T_n^3(n-12,8)$, we get $C_n \rightharpoonup T$ in (69) for $T \in \mathcal{T}_{58}^{\mathrm{A}}$. From (57), we have $C_n \rightharpoonup T$ in (69) for $T \in \mathcal{T}_{58}^{\mathrm{B}}$. □

4 Conclusions

Using the quasi-ordering relation and the theorem of zero points, we studied the ordering of the trees in terms of their minimal energies. We provided the preceding trees in the increasing order of their energies within the set of the trees with n vertices. In Theorem 1, we deduced the first 9 trees for $n \geq 46$. In Theorem 2, we deduced the first 12 and 11 trees for $7117598 \geq n \geq 26$ and $25 \geq n \geq 18$, respectively. In Theorem 3, we listed the first $n + 6$, 17, 15, and 12 trees for $17 \geq n \geq 11$, $n = 10$, $n = 9$ and $n = 8$, respectively, and derived all the 11 trees in the increasing order of their energies for $n = 7$. The numbers of the trees obtained exceed Gutman's [3] and Li and Li's results [7]. The further ordering for $n \geq 7117598$ is beyond the method presented here and a new approach should be devised in the future work.

The results obtained here are in agreement with a generally accepted idea that the energy of trees increases as the extent of branching decreases [19]. For the trees under consideration, the ones with smaller diameters have smaller energies. The maximal diameters of the trees with minimal energies obtained here are 4 for $n \geq 18$ and 5 for $17 \geq n \geq 8$, respectively.

Acknowledgments The work was partially supported by the National Natural Science Foundation of China under Grant No. 60773078 and the Shanghai Leading Academic Discipline Project under Project No. S30104.

References

1. D.M. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs Theory and Application* (Academic Press, New York, 1980)
2. I. Gutman, O.E. Polansky, *Mathematical Concepts in Organic Chemistry.* (Springer, Berlin, 1986)
3. I. Gutman, Acyclic systems with extremal Hückel π-electron energy. Theoret. Chim. Acta **45**, 79–87 (1977)
4. I. Gutman, F.J. Zhang, On the ordering of graphs with respect to their matching numbers. Discrete Appl. Math. **15**, 25–33 (1986)
5. F.J. Zhang, H. Li, On acyclic conjugated molecules with minimal energies. Discrete Appl. Math. **92**, 71–84 (1999)
6. H. Li, On minimal energy ordering of acyclic conjugated molecules. J. Math. Chem. **25**, 145–169 (1999)
7. N. Li, S. Li, On the extremal energies of trees. MATCH Commun. Math. Comput. Chem. **59**, 291–314 (2008)
8. J.M. Guo, On the minimal energy ordering of trees with perfect matchings. Discrete Appl. Math. **156**, 2598–2605 (2008)
9. W.H. Wang, Ordering of Hückel trees according to minimal energies. Linear Algebra Appl. **430**, 703–713 (2009)
10. Y.P. Hou, Unicyclic graphs with minimal energy. J. Math. Chem. **29**, 163–168 (2001)
11. Y.P. Hou, I. Gutman, C.W. Woo, Unicyclic graphs with maximal energy. Linear Algebra Appl. **356**, 27–36 (2002)
12. W.H. Wang, A. Chang, D.Q. Lu, Unicyclic graphs possessing Kekulé structures with minimal energy. J. Math. Chem. **42**, 311–320 (2007)
13. I. Gutman, B. Furtula, H. Hua, Bipartite unicyclic graphs with maximal, second-maximal and third-maximal energy. MATCH Commun. Math. Comput. Chem. **58**, 75–82 (2007)
14. Z. Liu, B. Zhou, Minimal energies of bipartite bicyclic graphs. MATCH Commun. Math. Comput. Chem. **59**, 381–396 (2008)
15. S. Li, X. Li, Z. Zhu, On tricyclic graphs with minimal energy. MATCH Commun. Math. Comput. Chem. **59**, 397–419 (2008)

16. B. Zhou, F. Li, On minimal energies of trees of a prescribed diameter. J. Math. Chem. **39**, 465–473 (2006)
17. I. Gutman, S. Radenkovic, N. Li, S. Li, Extremal energy trees. MATCH Commun. Math. Comput. Chem. **59**, 315–320 (2008)
18. W.G. Yan, L.Z. Ye, On the minimal energy of trees with a given diameter. Appl. Math. Lett. **18**, 1046–1052 (2005)
19. I. Gutman, Acyclic conjugated molecules, trees and their energies. J. Math. Chem. **1**, 123–143 (1987)