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On Ordering Chemical Trees by Energy[1]

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Abstract Three graph-transformations are introduced for maximizing the total number of matchings of a graph, by which chemical trees that have maximal energy and any prescribed maximum vertex-degree are characterized. Orderings of n-vertex chemical trees are presented according to their energy, some of which contain approximate n trees. Finally, acyclic graphs with maximal energy but without perfect matchings are also characterized.

1 Introduction

Let G be a graph of order n (n-vertex graph). Gutman defined in [1] the sum of the absolute values of all eigenvalues of graph G as its energy, written as $E(G)$, namely

$$E(G) = \sum_{k=1}^{n} |\lambda_k|,$$

where λ_k is the eigenvalue of graph G, or the eigenvalue of its adjacency matrix $A(G)$. This energy can be expressed in terms of Coulson function, for acyclic graphs the expression is reduced to

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

where $\lfloor n/2 \rfloor$ is the integer part of $n/2$ and $m(G,k)$ is the number of k-matchings, or set of independent edges of order k, of graph G. It is known that the experimental

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heats of formation of conjugated hydrocarbons have a close relationship with their total π-electron energy, and the calculation of the total π-electron energy of these conjugated hydrocarbons can be reduced (within the framework of the HMO approximation [2]) to the energy of the corresponding graph G.

Hosoya index of a graph G, written as $Z(G)$, is defined as the total number of its matchings [3], namely

$$Z(G) = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G,k) \tag{2}$$

As a chemical structure descriptor, Hosoya index plays an important role in the so-called inverse structure-property relationship problems, refer to [4] for example. From formulas (1) and (2) we see that if n-vertex trees G and H satisfy $m(G,k) \leq m(H,k)$ for every nonnegative integer k, then H has greater energy as well as Hosoya index than G. Results on various graphs with extremal energy or Hosoya index are obtained in many works, refer to [4-11] for example.

For maximizing the number of matchings, we introduce three graph-transformations and their properties in section two and five. In section three, these transformations help to characterize trees with any given maximum degree that have most k-matchings for every nonnegative integer k. An ordering of n-vertex molecular trees with maximum-degree three is presented in section four according to their energy, which contains as many as approximate n trees at the best case. Section five characterizes even-order trees with maximal energy but without perfect matching.

For graph-theoretical symbols and terminologies not defined here, we follow that of [13].

2 Graph transformations

Let G be a graph and w be one of its vertex. If w has degree $d(w) \geq 3$ and $G \backslash w$, the graph obtained by deleting vertex w from G, contains two path-components (components that are paths) $P_n = u_1u_2..u_n$ and $P_m = v_1v_2...v_m$ such that u_1 and v_1 is the unique neighbor of w in P_n and P_m respectively, then G is called transformable at vertex w and w is called a transformable vertex of G. Paths P_n and P_m are both called branches of G corresponding to vertex w. In this section we present two graph-transformations: DB-transformation and GSP-transformation, aiming to decrease the number of branches of the corresponding graph and increase the number of its i-matchings, where $i \geq 2$.

Definition 2.1 Let G be a graph and w be one of its transformable vertex. If P_m and P_n are two branches corresponding to w, delete the edge between P_m and w from G and then join by an edge one endpoint of P_m to the endpoint of P_n that has degree 1 in G. We call such process a *DB-transformation* at vertex w, meaning transformation for decreasing branches.

The following figure 1 shows an example of DB-transformation.

Figure 1. DB-transformation

Definition 2.2 GSP-transformation at vertex w: perform as many as possible DB-transformations at a transformable vertex w.

From the following example of GSP-transformation, we see that a generalized star (the graph obtained from a star by attaching a path to every 1-degree vertex of this star) of the original graph has been transformed into a path after it being performed a GSP-transformation (transformation of generalized star into path).

Figure 2. GSP-transformation

Lemma 2.3 Let G be a graph and w be one of its transformable vertex. If H is the graph obtained by performing a DB-transformation at w, then $m(G,k) \geq m(H,k)$ holds for every nonnegative integer k and the inequality strictly holds for some integer k.

To prove Lemma 2.3 we need to introduce another observation. Let G and T be two graphs of the same order. Graph G is called *m-smaller* than T, written as $G \preceq T$ or $T \succeq G$, if $m(G,k) \leq m(T,k)$ holds for every nonnegative integer k [7, 14].

Lemma 2.4 [15] Let P_n be a path of order $n = 4s + r$, $0 \leq r \leq 3$. Then

$$\begin{aligned} P_n &\succeq P_2 \cup P_{n-2} \succeq P_4 \cup P_{n-4} \succeq \cdots \succeq P_{2s} \cup P_{2s+r} \succeq P_{2s+1} \cup P_{2s+r-1} \\ &\succeq P_{2s-1} \cup P_{2s+r+1} \succeq \cdots \succeq P_3 \cup P_{n-3} \succeq P_1 \cup P_{n-1} \end{aligned}$$

Proof of Lemma 2.3. We shall prove this lemma by induction on the number n of branches corresponding to w. When $n = 2$, let $N(w) = \{u_1, u_2, ...u_s\}$ be the neighborhood of w, among which u_i is in branch B_i for $i = 1, 2$; let x be the other endpoint of B_2 (if any). Assume without loss of generality that after the DB-transformation performed at w, we get graph $H = G - wu_1 + u_1x$. Note that the k-matchings of G can be partitioned into two classes: those that contain some edge wu_i with $i \geq 3$ and those not. Since the component of $H - w - u_i$, $i \geq 3$, that contains vertices u_1 and u_2 is a path, but u_1 and u_2 are contained in different components of $G - w - u_i$, it follows from Lemma 2.4 that $m(B_1 \cup B_2, i) \leq m(B_1 \cup B_2 + u_1x, i)$ for every nonnegative integer i. And so $m(G - w - u_i, k) \leq m(H - w - u_i, k)$ holds for every nonnegative integer k. Let $S = \{wu_i | i = 3, 4, ..., s\}$. Then

$$\begin{aligned} m(G,k) &= \sum_{i=3}^{s} m(G - w - u_i, k-1) + m(G - S, k) \\ &\leq \sum_{i=3}^{s} m(H - w - u_i, k-1) + m(H - S, k) \\ &= m(H,k). \end{aligned} \tag{3}$$

We note here that $m(B_1 \cup B_2, 1) < m(B_1 \cup B_2 + u_1x, 1)$. The combination of this observation and formula (3) confirms the truth of Lemma 2.3 in the case when $n = 2$.

Now assume that $n \geq 3$ and B_i, $i = 1, ..., n$, are all the branches corresponding to w with u_i in B_i. By the induction assumption we have $m(G \setminus B_n, i) \leq m(H \setminus B_n, i)$ for every nonnegative integer i, where $G \setminus B_n$ denotes the graph obtained by deleting all the vertices of B_n from G. And so $m(G - wu_n, k) \leq m(H - wu_n, k)$ holds for every nonnegative integer k. On the other hand, recalling that $m(B_1 \cup B_2, i) \leq m(B_1 \cup B_2 + xu_1, i)$, we have $m(G - w - u_n, k-1) \leq m(H - w - u_n, k-1)$. Hence

$$\begin{aligned} m(G,k) &= m(G - wu_n, k) + m(G - w - u_n, k-1) \\ &\leq m(H - wu_n, k) + m(H - w - u_n, k-1) = m(H,k). \end{aligned}$$

Lemma 2.3 follows from the above formula and the observation that $m(B_1 \cup B_2, 1) < m(B_1 \cup B_2 + xu_1, 1)$. ■

As a direct observation we have the following result.

Theorem 2.5 If H is obtained by performing GSP-transformation at a vertex w of graph G, then $m(G,k) \leq m(H,k)$ holds for every nonnegative integer k and the inequality strictly holds for some integer k. ■

3 Extremal chemical trees with maximal energy and prescribed maximum valency

In this section we employ DB-transformation and GSP-transformation to determine extremal chemical trees with maximal energy and any given maximum valency (vertex degree). Let Ω_n^k denote the collective of n-vertex trees obtained by pasting one endpoint of k paths to a same isolated vertex respectively. Let ω_n^k stand for the tree of Ω_n^k such that when $n \geq 2k+2$ every path pasted but one is of order three; when $k+1 \leq n \leq 2k+1$, $n-k-1$ paths pasted are of order three and every other path (if any) is of order two. For clarity, we depict ω_n^k as follows.

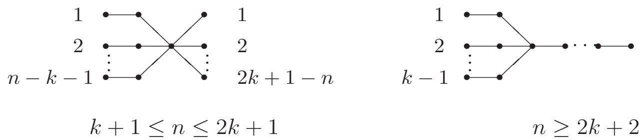

Figure 3. Tree ω_n^k

Lemma 3.1 Let T be an n-vertex tree of maximum degree k. Then there is a tree $G \in \Omega_n^k$ such that $m(T,i) \leq m(G,i)$ for every nonnegative integer i.

Proof If $T \notin \Omega_n^k$, then T contains a vertex w of degree at least three such that after performing a GSP-transformation at w one gets a new tree T_1 with $\Delta(T) = \Delta(T_1)$, where $\Delta(T)$ represents the maximum degree of T. By Theorem 2.5, for every nonnegative integer i we have $m(T,i) \leq m(T_1,i)$. The lemma follows from induction on the number of vertices that have degree at least three. ■

Theorem 3.2 Let T be an n-vertex tree of maximum degree k. Then $m(T,i) \leq m(\omega_n^k, i)$ for every nonnegative integer i.

Proof By Lemma 3.1, it suffices to show that $m(T,i) \leq m(\omega_n^k,i)$ holds for any tree $T \in \Omega_n^k$ and every nonnegative integer i. If $T \in \Omega_n^k$ but $T \neq \omega_n^k$, let w be the maximum-degree vertex, then T contains a branch P_s with $s \geq 3$ when $k+1 \leq n \leq 2k+1$, or T contains either a 1-vertex branch or at least two branches P_r and P_t with $r,t \geq 3$ when $n \geq 2k+2$.

Case 1. $k+1 \leq n \leq 2k+1$.

When $n = k+1$ or $k+2$, since $T \in \Omega_n^k$ it is obviously that $T = \omega_n^k$. And so, assume $n \geq k+3$ in what follows. Let u be the endpoint of the branch P_s that is not adjacent to w and v be the unique neighbor of u. Since vertex u is at distance at least three from w, it follows that $T-u \in \Omega_{n-1}^k$ and $T-u-v \in \Omega_{n-2}^k$. By induction on n we deduce that

$$m(T-u,i) \leq m(\omega_{n-1}^k, i) \tag{4}$$

Since $T-u-v$ contains a 1-vertex branch, performing a DB-transformation at w to delete one 1-vertex branch and increase the length of $P_s - u - v$, by induction on n we have

$$m(T-u-v, i-1) \leq m(\omega_{n-2}^{k-1}, i-1) \tag{5}$$

Combining this observation with formula (4), we have

$$\begin{aligned} m(T,i) &= m(T-u,i) + m(T-u-v, i-1) \\ &\leq m(\omega_{n-1}^k, i) + m(\omega_{n-2}^{k-1}, i-1) = m(\omega_n^k, i) \end{aligned} \tag{6}$$

Noticing that $T-u-v \neq \omega_{n-2}^{k-1}$, from Lemma 2.3 we deduce that the inequality in formula (5) strictly holds for some nonnegative integer $i-1$. Hence the inequality in formula (6) strictly holds for some nonnegative integer i and the theorem follows in this case.

Case 2. $n \geq 2k+2$.

If T contains at least two branches P_r and P_t of order at least three, let u be the vertex of P_r with degree 1 in T and v be its unique vertex, then either $T-u \neq \omega_{n-1}^k$ or $T-u-v \neq \omega_{n-2}^k$. By induction on n we have

$$\begin{aligned} m(T,i) &= m(T-u,i) + m(T-u-v, i-1) \\ &\leq m(\omega_{n-1}^k, i) + m(\omega_{n-2}^k, i-1) = m(\omega_n^k, i). \end{aligned}$$

If T contains only one branch of order at least three and at least one 1-vertex branch, defining u, v as before and considering that $n \geq 2k+2$ we conclude that $T-u \neq \omega_{n-1}^k$. And so, by induction assumption we deduce that

$$\begin{aligned} m(T,i) &= m(T-u,i) + m(T-u-v, i-1) \\ &\leq m(\omega_{n-1}^k, i) + m(\omega_{n-2}^k, i-1) = m(\omega_n^k, i) \end{aligned}$$

holds for every nonnegative integer and the inequality strictly holds for some integer i. Theorem 3.2 follows from the above discussion. $\blacksquare$

As a direct result we have

Corollary 3.3 Let T be an acyclic graph of order n and maximum degree k. Then $E(T) \leq E(\omega_n^k)$, with equality holding if and only if $T = \omega_n^k$. $\blacksquare$

Remark Let ${}^2T^2$ denote the tree obtained by pasting an endpoint of path P_{n-4} to the middle vertex of P_5 (refer to Figure 4). The authors obtain the following observation in [9], which is clearly a special case of corollary 3.3 when $k = 3$.

Proposition [9] Let T be an acyclic graph of order n and maximum degree 3. Then $E(T) \leq E({}^2T^2)$, with the equality holding if and only if $T = {}^2T^2$.

4 Ordering of molecular trees

According to Corollary 3.3, for any molecular tree T that has maximum-degree three there is a tree $T' \in \Omega_n^3$ with $E(T) \leq E(T')$. In this section, we consider the ordering of these molecular trees. Let r, s, t be three positive integers and ${}^rT_t^s$ be the tree obtained by pasting respectively an endpoint of $P_{r+1}, P_{s+1}, P_{t+1}$ to a same isolated vertex, refer to the following figure 4 for clarity.

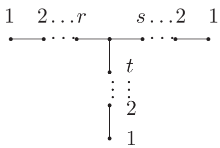

Figure 4. Tree ${}^rT_t^s$

Lemma 4.1 Let T be a tree in Ω_n^3 and r be the minimum order of its branches. If r is odd, let $n - r - 1 = 4k + s$ with $s \in \{0, 1, 2, 3\}$, then for every nonnegative integer i,

$$\begin{aligned} m({}^rT_{n-2r-2}^{r+1}, i) &\geq m({}^rT_{n-2r-4}^{r+3}, i) \geq m({}^rT_{n-2r-6}^{r+5}, i) \\ &\geq ... \geq m({}^rT_{2k+s}^{2k}, i) \qquad (7) \\ &\geq m({}^rT_{2k+s-1}^{2k+1}, i) \geq m({}^rT_{2k+s-3}^{2k+3}, i) \\ &\geq ... \geq m({}^rT_r^{n-2r-1}, i) \qquad (8) \end{aligned}$$

Proof Let w be the maximum-degree vertex and u be its neighbor in the component of $T-w$ that has order r. By Lemma 2.4, for every nonnegative integer l such that $r+2l+1 \leq 2k-2$ we have

$$m({}^{r}T^{r+2l+1}_{n-2r-2l-2}, i) =$$

$$m({}^{r}T^{r+2l+1}_{n-2r-2l-2} - wu, i) + m({}^{r}T^{r+2l+1}_{n-2r-2l-2} - w - u, i-1)$$

$$= m(P_r \cup P_{n-r}, i) + m(P_{r-1} \cup P_{r+2l+1} \cup P_{n-2r-2l-2}, i-1)$$

$$\geq m(P_r \cup P_{n-r}, i) + m(P_{r-1} \cup P_{r+2l+3} \cup P_{n-2r-2l-4}, i-1)$$

$$= m({}^{r}T^{r+2l+3}_{n-2r-2l-4}, i).$$

Formula (7) follows from above formula. Formula (8) follows from a similar reasoning, and so we leave its proof to the readers. ■

With similar technique employed in the proof of Lemma 4.1, one can prove with ease the following lemma. And so, we leave its proof to the readers.

Lemma 4.2 Let T be a tree in Ω_n^3 and r be the minimum order of its branches. If r is even, let $n-r-1 = 4k+s$ with $s \in \{0,1,2,3\}$, then for every nonnegative integer i

$$\begin{aligned} m({}^{r}T^{r}_{n-2r-1}, i) &\geq m({}^{r}T^{r+2}_{n-2r-3}, i) \geq m({}^{r}T^{r+4}_{n-2r-5}, i) \geq \ldots \geq m({}^{r}T^{2k}_{2k+s}, i) \\ &\geq m({}^{r}T^{2k+1}_{2k+s-1}, i) \geq m({}^{r}T^{2k+3}_{2k+s-3}, i) \geq \ldots \geq m({}^{r}T^{n-2r-2}_{r+1}, i). \end{aligned}$$

Theorem 4.3 Let T be a tree in Ω_n^3 and r be the minimum order of its branches, let $n-r-1 = 4k+s$ with $s \in \{0,1,2,3\}$.

(1) If r is odd then

$$\begin{aligned} E({}^{r}T^{r+1}_{n-2r-2}) &\geq E({}^{r}T^{r+3}_{n-2r-4}) \geq E({}^{r}T^{r+5}_{n-2r-6}) \geq \ldots \geq E({}^{r}T^{2k}_{2k+s}) \\ &\geq E({}^{r}T^{2k+1}_{2k+s-1}) \geq E({}^{r}T^{2k+3}_{2k+s-3}) \geq \ldots \geq E({}^{r}T^{n-2r-1}_{r}) \end{aligned}$$

(2) If r is even then

$$\begin{aligned} E({}^{r}T^{r}_{n-2r-1}) &\geq E({}^{r}T^{r+2}_{n-2r-3}) \geq E({}^{r}T^{r+4}_{n-2r-5}) \geq \ldots \geq E({}^{r}T^{2k}_{2k+s}) \\ &\geq E({}^{r}T^{2k+1}_{2k+s-1}) \geq E({}^{r}T^{2k+3}_{2k+s-3}) \geq \ldots \geq E({}^{r}T^{n-2r-2}_{r+1}). \end{aligned}$$

Proof This theorem follows directly from Lemma 4.1 and 4.2. ■

In next section we shall employ Theorem 4.3 and Lemma 2.3 to characterize even-order molecular trees with maximal energy but without perfect matching.

5 Trees with maximal energy but without perfect matching

To present the main result of this section, we need introduce another graph transformation and its property.

Definition 5.1 TTVOB-transformation: let w be a transformable vertex of graph G, B_1 and B_2 be two branches corresponding to w. If $B_1 = P_{2r+1}$ and $B_2 = P_{2s+1}$ with $r > s$, then substitute P_{2r-1} for B_1 and P_{2s+3} for B_2 in G, where r and s are two nonnegative integers. This process is called a *TTVOB-transformation* of graph G at vertex w.

If we perform a TTVOB-transformation on graph G, a 1-degree vertex and its neighbor of an odd-order branch are transferred to another odd-order branch corresponding to the same transformable vertex. So this process results in a transfer of two vertices from a longer odd-order branch to a shorter odd-order branch, for this reason this process is called a TTVOB-transformation (transformation of transfer of two vertices between odd-order branches).

Lemma 5.2 If G' is obtained by performing a TTVOB-transformation at a vertex w of graph G, then $m(G', k) \geq m(G, k)$. The equality holds for every nonnegative integer k if and only if $G' = G$.

Proof Assume that after the TTVOB-transformation, B_1 is replaced by path P_{2r-1} and B_2 is replaced by P_{2s+3}, where $r \geq s + 1$. Let u_i be the neighbor of vertex w in B_i, $i = 1, 2$, and $H = G \setminus (B_1 \cup B_2)$. Notice that the matchings of G' are partitioned in two classes: those that contain wu_1 or wu_2 and those not. Denote by n the order of graph G. From Lemma 2.4 we deduce that

$$\begin{aligned} m(G', k) &= \sum_{i=0}^{k} m(H, i) m(P_{2r-1} \cup P_{2s+3}, k - i) + \sum_{i=0}^{k-1} m(H \setminus w, i) \times \\ &\quad (m(P_{2r-2} \cup P_{2s+3}, k - i - 1) + m(P_{2r-1} \cup P_{2s+2}, k - i - 1)) \\ &\geq \sum_{i=0}^{k} m(H, i) m(P_{2r+1} \cup P_{2s+1}, k - i) + \sum_{i=0}^{k-1} m(H \setminus w, i) \times \\ &\quad (m(P_{2r} \cup P_{2s+1}, k - i - 1) + m(P_{2r+1} \cup P_{2s}, k - i - 1)) \\ &= m(G, k). \end{aligned}$$

It follows from above formula and Lemma 2.4 that $m(G', k) = m(G, k)$ holds if and only if

$$m(P_{2r-1} \cup P_{2s+3}, k-i) = m(P_{2r+1} \cup P_{2s+1}, k-i) \tag{9}$$

and

$$\begin{aligned} &m(P_{2r-2} \cup P_{2s+3}, k-i-1) + m(P_{2r-1} \cup P_{2s+2}, k-i-1) \\ &= m(P_{2r} \cup P_{2s+1}, k-i-1) + m(P_{2r+1} \cup P_{2s}, k-i-1) \end{aligned} \tag{10}$$

holds for every nonnegative integer $k-i$ and $k-i-1$. Since $m(P_n, k) = \binom{n-k}{k}$, it follows that

$$m(P_n \cup P_m, k) = \binom{n}{j}\binom{m}{k-j} \tag{11}$$

It is not difficult to see that for any given integer k and $m+n$, the value of the hand right side of formula (11) increases as the absolute value of $n-m$ decreases. This observation implies that (9) and (10) hold if and only if $P_{2r-1} \cup P_{2s+3} = P_{2r+1} \cup P_{2s+1}$, namely $G' = G$ as is desired. ■

It is known that P_n has maximal energy among n-vertex trees, which characterizes odd-order trees without perfect matching that have maximal-energy. In what follows we characterize even-order trees without perfect matching that have maximal energy.

Lemma 5.3 Let T be an n-vertex tree with $n = 6k + 2r \geq 4$, where k is a positive integer and $r \in \{0, 1, 2\}$. If T contains no perfect matching, then

(1) $m(T, i) \leq m({}^{2k-1}T^{2k-1}_{2k+1}, i)$ when $r = 0$;

(2) $m(T, i) \leq m({}^{2k+1}T^{2k+1}_{2k-1}, i)$ when $r = 1$;

(3) $m(T, i) \leq m({}^{2k+1}T^{2k+1}_{2k+1}, i)$ when $r = 2$.

In each case, the equality holds for every nonnegative integer i if and only if the corresponding two trees are isomorphic.

Proof Let w be the maximum-degree vertex of T. Since T is a non-conjugated tree of even-order, it follows that $d(w) \geq 3$. If T contains a transformable vertex $u \neq w$, one can perform a GSP-transformation at vertex u to obtain a new tree T_1 that contains no perfect matching. This transformation can be performed until we get a tree T' that contains unique vertex of degree at least three and contains no perfect matching. Now perform DB-transformations at w if necessary to obtain a tree $T^\star \in \Omega_n^3$ such that every branch corresponding to w has odd number of vertices.

If $T^\star$ contains a branch P_{2r+1} with $r \geq k+1$, then it contains a branch P_{2s+1} with $s \leq k-2$. Perform TTVOB-transformation at u to decrease the order of branch P_{2r+1}

and increase the order of branch P_{2s+1}, by Lemma 5.2 the resulted tree $T_1^\star$ satisfies $m(T^\star, i) \leq m(T_1^\star, i)$. This operation stops if and only if any two branches have order-difference at most two, and so the finally obtained tree is either ${}^{2k-1}T_{2k+1}^{2k-1}$ or ${}^{2k+1}T_{2k+1}^{2k+1}$ or ${}^{2k+1}T_{2k+1}^{2k+1}$. By Lemma 2.3, Theorem 2.5 and Lemma 5.2, the inequalities in item (1)-(3) follows and the equalities hold if and only if we never perform any DB-, GSP- or TTVOB-transformations. The lemma follows. ■

Theorem 5.4 Let T be a tree of order $6k+2s$, where $s \in \{0, 1, 2\}$ and k is a positive integer. If T contains no perfect matching, then

(1) $E(T) \leq E({}^{2k-1}T_{2k+1}^{2k-1})$ when $s = 0$;

(2) $E(T) \leq E({}^{2k+1}T_{2k-1}^{2k+1})$ when $s = 1$;

(3) $E(T) \leq E({}^{2k+1}T_{2k+1}^{2k+1})$ when $s = 2$.

In each case, the equality holds if and only if T is isomorphic to the corresponding tree.

Proof The theorem follows directly from Lemma 5.3. ■.

Remark Employ the graph transformations introduced here we also characterize a series of unicyclic and bicyclic graph with maximal energy that have some prescribed properties. Other graph transformations are also observed by the present author to characterize graph with minimal energy and Hosoya index, we shall introduction them in a subsequent article.

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