Conjugated Chemical Trees with Extremal Energy

Xueliang Li, Huishu Lian

Center for Combinatorics and LPMC-TJKLC
Nankai University, Tianjin 300071, China
E-mail: lxl@nankai.edu.cn, lianhuishu@mail.nankai.edu.cn

(Received November 29, 2010)

Abstract

For a simple graph G, the energy $\mathcal{E}(G)$ of G is defined as the sum of the absolute values of all eigenvalues of its adjacency matrix. A conjugated tree is a tree that has a perfect matching. Denote by Φ_n the class of trees with n vertices which have perfect matchings, and by $\Omega_{n,d}$ the subclass of Φ_n whose vertex degrees do not exceed $d+1$. Let $\Delta(T)$ denote maximum degree of T. Zhang and Li determined the minimal energy tree F_n in Φ_n, and M_n in $\Omega_{n,2}$, respectively, where F_n is a tree obtained by adding a pendent edge to each vertex of the star $K_{1,(n/2-1)}$ and M_n by adding a pendent edge to each vertex of the path $P_{n/2}$. This paper is to solve the problem of determining minimal energy conjugated chemical trees, i. e., trees with perfect matchings whose vertex degrees do not exceed 4, or in the class $\Omega_{n,3}$. In fact, we obtain the minimal energy trees in $\Omega_{n,d}$ for any $d \geq 3$, a more general result. For maximal energy conjugated trees with given maximum degree Δ, it is easy to determine their structures, and we also present them here.

1 Introduction

In chemistry, the experimental heats from the formation of conjugated hydrocarbons are closely related to the total π-electron energy. The total π-electron energy $\mathcal{E}$, as calculated within the Hückel molecular orbital (HMO) model, is one of the most important and most studied chemical-graph-based quantum mechanical characteristics of conjugated molecules. And the calculation of the total energy of all π-electrons in conjugated hydrocarbons can be reduced to (within the framework of HMO approximation) [1] that of,

$$\mathcal{E} = \mathcal{E}(G) = \sum_{j=1}^{n} |\lambda_j|, \tag{1}$$

where G is the chemical graph representing the π-electron system, λ_j the eigenvalues, and n the number of vertices of G. Details of the theory of the HMO total π-electron energy can be found in appropriate textbooks, say [2][3]. In the 1970s, Ivan Gutman noticed that practically all results that until then were obtained for the HMO total π-electron energy, in particular those in the papers [4][5][6], tacitly assume the validity of Eq.(1), and in turn, are not restricted to the chemical graphs (whose vertex degrees are at most 3 or 4) encountered in the HMO theory, but for all graphs. This not only provided a stimulus for work on the mathematical theory of $\mathcal{E}(G)$ (as, for instance, in recent papers [7][8]), but also made it possible to apply $\mathcal{E}(G)$ in the study of the physico-chemical properties of saturated organic compounds and biopolymers [9].

Let G be a graph of order n and $A(G)$ its adjacency matrix. Let the characteristic polynomial $\phi(G,x)$ of G be

$$\phi(G,x) = \det(xI_n - A(G)) = \sum_{k=0}^{n} a_k x^{n-k},$$

and $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues. Then the energy of G is defined as $\mathcal{E}(G) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|$. For calculating the energy, Coulson [4] deduced the following formula

$$\mathcal{E}(G) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \left[n - \frac{\phi'(G,ix)}{\phi(G,ix)} \right] dx. \tag{2}$$

Moreover, Gutman and Polansky [1] converted Eq.(2) into an explicit formula as follows:

$$\mathcal{E}(G) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{1}{x^2} \log \left[\left(\sum_{k\geq 0} (-1)^k a_{2k} x^{2k} \right)^2 + \left(\sum_{k\geq 0} (-1)^k a_{2k+1} x^{2k+1} \right)^2 \right] dx.$$

Particularly, if G is a tree, then

$$\phi(G,x) = \sum_{k\geq 0} (-1)^k m(G,k) x^{n-2k},$$

and

$$\mathcal{E}(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \log \left[1 + \sum_{k \geq 1} m(G,k) x^{2k} \right] dx,$$

where $m(G,k)$ is the number of k-matchings of T.

From the above one can see that if T_1 and T_2 are two trees with the same number of vertices, it is clear that $\mathcal{E}(T_1) \leq \mathcal{E}(T_2)$ if $m(T_1,k) \leq m(T_2,k)$ for all $k = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$. So there exists a partial ordering $\preceq$ in the set of trees by comparing the number of k-matchings in each concerned tree, that is, for two trees T_1 and T_2 with n vertices, if $m(T_1,k) \leq m(T_2,k)$ holds for all $k \geq 0$, then we define $T_1 \preceq T_2$. Thus $T_1 \preceq T_2$ implies $\mathcal{E}(T_1) \leq \mathcal{E}(T_2)$.

A conjugated tree is a tree that has a perfect matching, and a chemical tree is a tree whose vertex degrees do not exceed 4. Conjugated chemical trees are known to be interested in chemical literature. In [10] Zhang and Li determined conjugated trees with minimal energy whose vertex degrees do not exceed 3. One natural question is what about the minimal energy conjugated trees whose vertex degrees do not exceed 4 ? or more generally, what about the minimal energy conjugated trees whose vertex degrees do not exceed a given number ? This paper is to solve this question. It turns out that the structures are not so simple as that in [10]. They heavily depend on the minimal energy structures given by Heuberger and Wagner in [11]. Details are given in next section. Another natural question is to determine maximal energy conjugated trees with given maximum degree, and this is easily done and presented in the last section.

2 Minimal energy conjugated trees

Given two positive integers n and d, denote by Φ_n the class of trees with n vertices which have perfect matchings and by $\Omega_{n,d}$ the subclass of Φ_n whose vertex degrees do not exceed $d+1$. Denote by $\mathcal{T}_{n,d}$ the class of trees with n vertices with maximum degree $\Delta \leq d+1$. Zhang and Li [10] determined the minimal energy tree F_n in Φ_n, and M_n in $\Omega_{n,2}$, respectively, where F_n is a tree obtained by adding a pendent edge to each vertex of the star $K_{1,(n/2-1)}$ and M_n by adding a pendent edge to each vertex of the path $P_{n/2}$. F_n and M_n are depicted in the Figure 1. In the following we will solve the problem of determining minimal energy conjugated chemical trees, i. e., trees in the class $\Omega_{n,3}$. In fact, we obtain the minimal energy trees in $\Omega_{n,d}$ for any $d \geq 3$, a more general result.

At first, we need some more notations. Let $E_{n,d}$ be a graph by adding a pendent edge

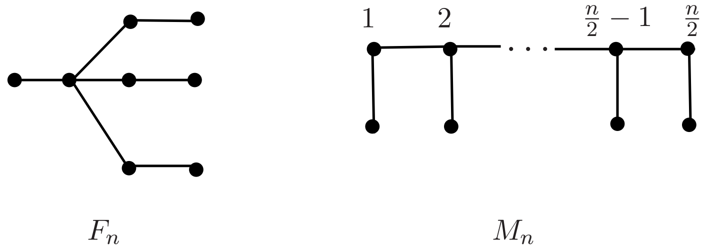

Figure 1: Trees with minimal energy in Φ_n and $\Omega_{n,2}$

to each vertex of $T^*_{\frac{n}{2},d-1}$, where the definition of $T^*_{n,d}$ will be given in Definition 2.1. In the following, we will use the notion of complete d-ary trees: the complete d-ary tree of height $h-1$ is denoted by CA_h, i. e., CA_1 is a single vertex and CA_h has d branches $CA_{h-1}, \ldots, CA_{h-1}$, as shown in Figure 2. It is convenient to set CA_0 to be the null graph.

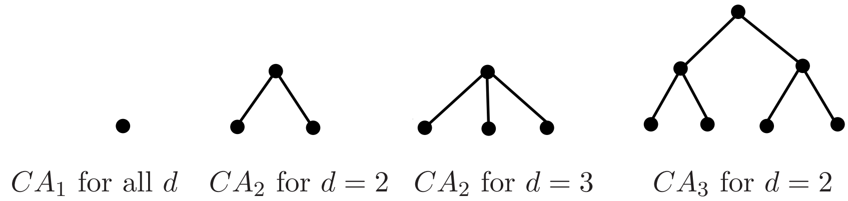

Figure 2: Some small complete d-ary trees

Then we define $T^*_{n,d}$ as follows. For more information about this special tree, one can see Heuberger and Wagner [11].

Definition 2.1. $T^*_{n,d}$ is the tree with n vertices that can be decomposed as in Figure 3

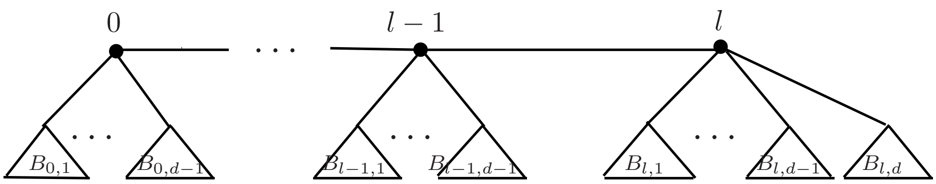

Figure 3: Tree $T^*_{n,d}$

with $B_{k,1}, \ldots, B_{k,d-1} \in \{CA_k, CA_{k+2}\}$ for $0 \le k < l$ and either $B_{l,1} \cong \cdots \cong B_{l,d} \cong CA_{l-1}$ or $B_{l,1} \cong \cdots \cong B_{l,d} \cong CA_l$ or $B_{l,1}, \ldots, B_{l,d} \in \{CA_l, CA_{l+1}, CA_{l+2}\}$, where at least two of $B_{l,1}, \ldots, B_{l,d}$ are equal to CA_{l+1}. This representation is unique, and one has the "digital expansion"

$$(d-1)n + 1 = \Sigma_{k=0}^{l} a_k d^k,$$

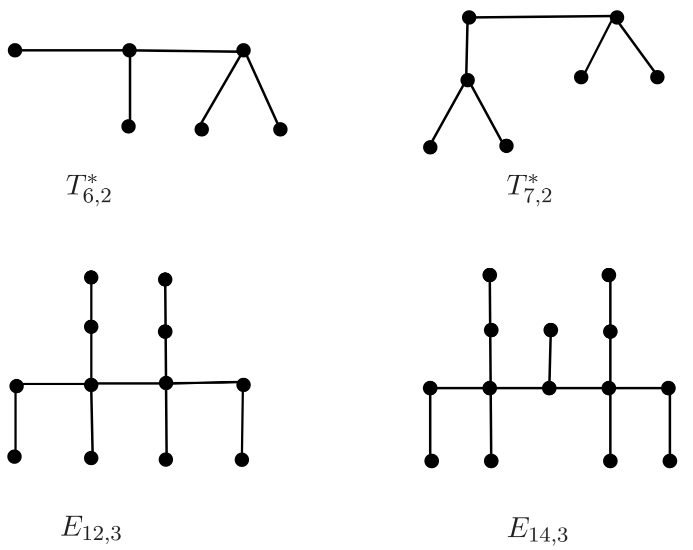

Figure 4: Some small trees for $T^*_{n,d}$ and $E_{n,d}$

where $a_k = (d-1)(1+(d+1)r_k)$ and $0 \le r_k \le d-1$ is the number of $B_{k,i}$ that are isomorphic to CA_{k+2} for $k < l$, and

- $a_l = 1$ if $B_{l,1} \cong \cdots \cong B_{l,d} \cong CA_{l-1}$
- $a_l = d$ if $B_{l,1} \cong \cdots \cong B_{l,d} \cong CA_l$
- or otherwise $a_l = d + (d-1)q_l + (d^2-1)r_l$ where $q_l \ge 2$ is the number of $B_{l,i}$ that are isomorphic to CA_{l+1} and r_l is the number of $B_{l,i}$ that are isomorphic to CA_{l+2}.

$\square$

For given n and d, $T^*_{n,d}$ is uniquely determined. Figure 4 depicts the structures of $T^*_{6,2}$ and $T^*_{7,2}$. At the same time, $E_{12,3}$ and $E_{14,3}$ are also shown, which are obtained by adding a pendent edge to each vertex of $T^*_{6,2}$ and $T^*_{7,2}$, respectively.

Denote by $M(T)$ a perfect matching of a tree $T = (V(T), E(T))$, and set $Q(T) = E(T) - M(T)$. Let $m = |M(T)|$. Denote by $\hat{T}$ the graph induced by $Q(T)$. We call $\hat{T}$ the capped graph of T and T the original graph of $\hat{T}$. For each k-matching Ω of T, it is partitioned into two parts: $\Omega = R \cup S$, where $S \subset M(T)$ and R is a matching in $\hat{T}$. On the other hand, for any i-matching R of $\hat{T}$, any set S of $k-i$ edges of $M(T)$ that are not incident with R forms a k-matching Ω of T with partition $\Omega = R \cup S$. From now on, when we say that a k-matching of T contains a certain i-matching of $\hat{T}$, it is in such sense, which is our fundamental principle of counting the matchings of T.

The following Lemmas 2.2, 2.4 and 2.5 are from Zhang and Li [10], which will be useful in the sequel.

Lemma 2.2. *Let T be a tree in a subclass of Φ_n. If for any i-matching R in $\hat{T}$, R is incident with $2i$ edges $M(T)$, or equivalently, $\hat{T}$ is connected, or $M(T)$ consists of pendent edges of T, and there is a bijection h from $Q(T)$ to $Q(T')$ for any tree T' in the same class, such that $h(R)$ is a matching in $\hat{T'}$ wherever R is a matching in $\hat{T}$, then T is minimal among this class.* □

Lemma 2.3. *Let $T \in \Omega_{n,d}$. If $\omega(\hat{T}) \geq 2$, then there is a tree $T' \in \Omega_{n,d}$ with a connected $\hat{T'}$ such that $T' \prec T$.*

Proof. In this case, $\hat{T}$ is the union of disjoint trees $\hat{T}_1, \hat{T}_2, \dots, \hat{T}_l$ with $\Delta(\hat{T}_i) \leq d$, $1 \leq i \leq l$, since $\Delta(T) \leq d + 1$. Each $\hat{T}_i$ contains at least two leaves. Concatenating one leaf of $\hat{T}_i$ with one of $\hat{T}_{i-1}$ and another with one of $\hat{T}_{i+1}$, we get a new graph $\hat{T'}$ with $\Delta(\hat{T'}) \leq d$ and $E(\hat{T'}) = E(\hat{T}) = \frac{n}{2} - 1$. Let T' be a graph obtained by adding a pendent edge to each vertex of $\hat{T'}$, thus $T' \in \Omega_{n,d}$. There is also a natural bijection h from $Q(T')$ to $Q(T)$ such that $h(R)$ is a matching in $\hat{T}$ for any matching R in $\hat{T'}$. And an i-matching R is incident with exactly $2i$ edges in $M(T')$, while $h(R)$ is incident with at most $2i$ edges in $M(T)$. For any $i \geq 0$, the number of k-matchings in T' that contain a certain i-matching R in $\hat{T'}$ is $\binom{m-2i}{k-i}$, since no two independent edges in $Q(T')$ are incident with a common edge in $M(T')$ and hence R is incident with exactly $2i$ edges in $M(T')$. And these cover all the k-matchings in T' as R goes over all matchings in $\hat{T'}$. In the same way, $h(R)$ determines at least $\binom{m-2i}{k-i}$ k-matchings in T, since $h(R)$ is incident with at most $2i$ edges in $M(T)$. Therefore,

$$m(T', k) = \sum_{i=0}^{k} m(\hat{T'}, i)\binom{m-2i}{k-i} \leq \sum_{i=0}^{k} m(\hat{T}, i)\binom{m-2i}{k-i} \leq m(T, k).$$

In addition, since $\hat{T}$ is disconnected, it has a 2-matching that cannot be the image of any 2-matching in $\hat{T'}$, then T has sharply more 2-matchings than T'. This implies $T' \prec T$. □

Define the polynomial for all positive values of x,

$$M(T, x) = \sum_{k} m(T, k)x^k,$$

where $m(T, k)$ denotes the number of matchings of T with cardinality k.

Lemma 2.4. *Let n and d be positive integers and $x > 0$, $T^*_{n,d}$ is the unique tree (up to isomorphism) in $\mathcal{T}_{n,d}$ that minimizes $M(T, x)$.* $\square$

About the minimal energy of trees in $\mathcal{T}_{n,d}$, one can see Heuberger and Wagner [11] and Lin et al. [12]. From the lemma above and the definition of the partial ordering $\preceq$, for any tree $T \in \mathcal{T}_{n,d}$ and nonnegative integer k, $m(T, k) \geq m(T^*_{n,d}, k)$, which is stated as a lemma below.

Lemma 2.5. *Let n and d be positive integers. For any tree $T \in \mathcal{T}_{n,d}$, $T \succeq T^*_{n,d}$, with equality holds if and only if $T \cong T^*_{n,d}$.* $\square$

The main result of this paper is the following theorem.

Theorem 2.6. *For any tree $T \in \Omega_{n,d}$, $\mathcal{E}(T) \geq \mathcal{E}(E_{n,d})$, with equality holds if and only if $T \cong E_{n,d}$.*

Proof. From the definition of $E_{n,d}$, we can get $\hat{E}_{n,d} \cong T^*_{\frac{n}{2},d-1}$ and any i-matching of $\hat{E}_{n,d}$ is incident with exactly $2i$ edges of $M(E_{n,d})$. Thus, the number of k-matchings in $E_{n,d}$ that contain a certain i-matching R of $\hat{E}_{n,d}$ is $\binom{m-2i}{k-i}$. Thus

$$m(E_{n,d}, k) = \sum_{i=0}^{k} m(\hat{E}_{n,d}, i)\binom{m-2i}{k-i}.$$

On the other hand, for any tree $T \in \Omega_{n,d}$, from Lemma 2.3, suppose $\hat{T}$ is connected, otherwise, there is a tree $T' \in \Omega_{n,d}$ such that $T' \prec T$. So $\hat{T}$ is a tree with $\frac{n}{2}$ vertices and the maximum degree $\Delta(\hat{T}) \leq d$ since $T \in \Omega_{n,d}$, i. e., $\hat{T} \in \mathcal{T}_{\frac{n}{2},d-1}$. From Lemma 2.5, for any nonnegative integer i, $m(\hat{T}, i) \geq m(\hat{E}_{n,d}, i)$. Moreover, any i-matching of $\hat{T}$ is also incident with exactly $2i$ edges of $M(T)$. Thus, the number of k-matchings in T that contain a certain i-matching of $\hat{T}$ is $\binom{m-2i}{k-i}$. Again, we get

$$m(T, k) = \sum_{i=0}^{k} m(\hat{T}, i)\binom{m-2i}{k-i}.$$

Since for any $i \geq 0$, $m(\hat{T}, i) \geq m(\hat{E}_{n,d}, i)$ and if $T \ncong E_{n,d}$, there exists an integer i_0 such that $m(\hat{T}, i_0) > m(\hat{E}_{n,d}, i_0)$. Consequently,

$$m(T, k) \geq m(E_{n,d}, k) \quad for\ k = 1, 2, \ldots, \frac{n}{2}\ ,$$

and there exists an integer k_0 such that $m(T, k_0) > m(E_{n,d}, k_0)$. So, if $T \ncong E_{n,d}$, $T \succ E_{n,d}$. $\square$

From our Theorem 2.6 we can get a result in [10] by Zhang and Li, as a corollary.

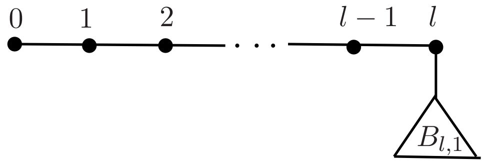

Figure 5: The tree $T^*_{\frac{n}{2},1}$

Corollary 2.7. *For any tree $T \in \Omega_{n,2}$, $\mathcal{E}(T) \geq \mathcal{E}(M_n)$, with equation holds if and only if $T \cong M_n$.*

Proof. From Theorem 2.6, the unique minimal energy tree in $\Omega_{n,2}$ is $E_{n,2}$, which is a tree obtained by adding a pendent edge to each vertex of $T^*_{\frac{n}{2},1}$. By Definition 2.1, $T^*_{\frac{n}{2},1}$ is depicted in Figure 5, where when n is even, $l = \frac{n}{2}$, $B_{l,1} \cong CA_{l-1} \cong P_{l-1}$; when n is odd, $l = \frac{n-1}{2}$, $B_{l,1} \cong CA_l \cong P_l$. Therefore, we have $T^*_{\frac{n}{2},1} \cong P_{\frac{n}{2}}$ and $E_{n,2} \cong M_n$. □

For minimal energy trees of maximum degree 4, things become not so easy as the above corollary. We still can give some structural descriptions.

Corollary 2.8. *For conjugated trees of maximum degree 4, $E_{n,3}$ is the unique tree with minimal energy, the structure of which is completely determined by $T^*_{\frac{n}{2},2}$.* □

In the following, we will make an algorithm to construct the structure of $T^*_{n,2}$ for different n, which is shown in Figure 6,

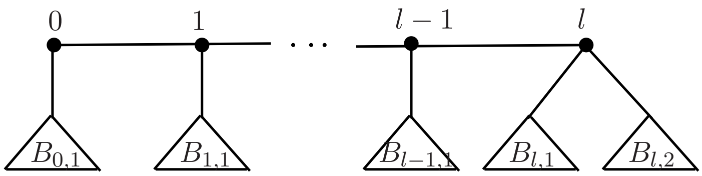

Figure 6: The tree $T^*_{n,2}$

where $B_{k,1} \in \{CA_k, CA_{k+2}\}$ for $0 \leq k < l$ and either $B_{l,1} \cong B_{l,2} \cong CA_{l-1}$ or $B_{l,1} \cong B_{l,2} \cong CA_l$ or $B_{l,1} \cong B_{l,2} \cong CA_{l+1}$, while CA_k is the complete 2-ary tree of height $k-1$. This representation is unique, and now its "digital expansion" can be written as

$$n + 1 = \Sigma_{k=0}^{l} a_k 2^k,$$

where $a_k = 1 + 3r_k$ and $r_k = 1$ if $B_{k,1} \cong CA_{k+2}$, otherwise $r_k = 0$ (i. e. if $B_{k,1} \cong CA_k$) for $k < l$, and

- $a_l = 1$ if $B_{l,1} \cong B_{l,2} \cong CA_{l-1}$;
- $a_l = 2$ if $B_{l,1} \cong B_{l,2} \cong CA_l$;
- $a_l = 4$ if $B_{l,1} \cong B_{l,2} \cong CA_{l+1}$.

For any given $n \geq 4$, we can determine the structure of $T^*_{n,2}$ by the following steps:

(1) If $n \equiv 0 \bmod 2$, then $a_0 = 1$, $B_{0,1} \cong CA_0$. Let $n_0 = n + 1 - a_0 = n + 1 - 1 = n$;
If $n \not\equiv 0 \bmod 2$, then $a_0 = 4$, $B_{0,1} \cong CA_2$. Let $n_0 = n + 1 - a_0 = n + 1 - 4 = n - 3$;

(2) If $n_0 = 2$, then $l = 1$ and $a_l = 1$. Now $B_{1,1} \cong B_{1,2} \cong CA_0$;
If $n_0 = 2^2$, then $l = 1$ and $a_l = 2$. Now $B_{1,1} \cong B_{1,2} \cong CA_1$;
If $n_0 = 2^3$, then $l = 1$ and $a_l = 4$. Now $B_{1,1} \cong B_{1,2} \cong CA_2$.
Otherwise, if $n_0 \not\equiv 0 \bmod 2^2$, then $a_1 = 1$ and $B_{1,1} \cong CA_1$. Let $n_1 = n_0 - 2^1$.
if $n_0 \equiv 0 \bmod 2^2$, then $a_1 = 4$ and $B_{1,1} \cong CA_3$. Let $n_1 = n_0 - 2^3$.

(3) If $n_1 = 2^2$, then $l = 2$ and $a_2 = 1$. Now $B_{2,1} \cong B_{2,2} \cong CA_1$;
If $n_1 = 2^3$, then $l = 2$ and $a_2 = 2$. Now $B_{2,1} \cong B_{2,2} \cong CA_2$;
If $n_1 = 2^4$, then $l = 2$ and $a_2 = 4$. Now $B_{2,1} \cong B_{2,2} \cong CA_3$.
Otherwise, if $n_1 \not\equiv 0 \bmod 2^3$, then $a_2 = 1$ and $B_{2,1} \cong CA_2$. Let $n_2 = n_1 - 2^2$.
if $n_1 \equiv 0 \bmod 2^3$, then $a_2 = 4$ and $B_{2,1} \cong CA_4$. Let $n_2 = n_1 - 2^4$.
$\vdots$

(k+1) If $n_{k-1} = 2^k$, then $l = k$ and $a_k = 1$. Now $B_{k,1} \cong B_{k,2} \cong CA_{k-1}$;
If $n_{k-1} = 2^{k+1}$, then $l = k$ and $a_k = 2$. Now $B_{k,1} \cong B_{k,2} \cong CA_k$;
If $n_{k-1} = 2^{k+2}$, then $l = k$ and $a_k = 4$. Now $B_{k,1} \cong B_{k,2} \cong CA_{k+1}$.
Otherwise, if $n_{k-1} \not\equiv 0 \bmod 2^{k+1}$, then $a_k = 1$ and $B_{k,1} \cong CA_k$. Let $n_k = n_{k-1} - 2^k$ and $k - 1 := k$.
if $n_{k-1} \equiv 0 \bmod 2^{k+1}$, then $a_k = 4$ and $B_{k,1} \cong CA_{k+2}$. Let $n_k = n_{k-1} - 2^{k+2}$ and $k - 1 := k$.
Continue step $(k + 1)$ until we obtain the final structure of the tree $T^*_{n,2}$.

An example for $n = 9$, i. e., $T^*_{9,2}$, is depicted in Figure 7.

(1) Sine $n \not\equiv 0 \bmod 2$, $a_0 = 4$, $B_{0,1} \cong CA_2$ and $n_0 = n - 3 = 6$;

(2) Sine $n_0 \not\equiv 0 \bmod 2^2$, $a_1 = 1$, $B_{1,1} \cong CA_1$ and $n_1 = n_0 - 2 = 4$;

(3) Sine $n_1 = 2^2$, $l = 2$, $a_2 = 1$ and $B_{2,1} \cong B_{2,1} \cong CA_1$.

Now for any even n, $T^*_{\frac{n}{2},2}$ can be determined by the procedure above, thus we can get $E_{n,3}$ just by adding a pendent edge to each vertex of $T^*_{\frac{n}{2},2}$. Figure 7 depicts trees $T^*_{9,2}$ and $E_{18,3}$.

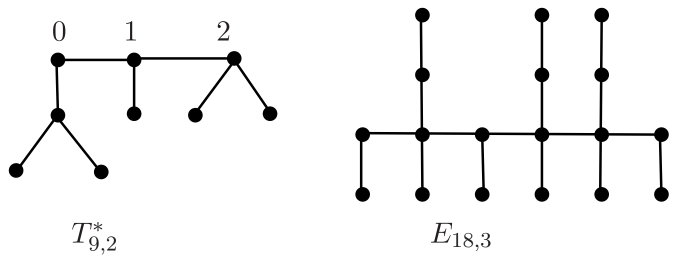

Figure 7: Trees $T^*_{9,2}$ and $E_{18,3}$

3 Maximal energy conjugated trees

In this section, we characterize the trees with maximal energy among all conjugated trees with n vertices and maximum degree $\Delta(T)$.

A vertex of a tree whose degree is 3 or greater will be called a branching vertex. A pendent vertex attached to a vertex of degree 2 will be called a 2-branch. Lin et al. [12] determined the trees with maximal energy among all trees with n vertices and maximum degree $\Delta(T)$. The result is stated in the following lemma.

Lemma 3.1. *Among trees of order n with maximum degree Δ, the maximal energy tree has exactly one branching vertex (of degree Δ) and as many as possible 2-branches.* □

For given n and Δ, the structure of the maximal energy tree in the lemma above is unique (up to isomorphism). We make a specific discussion according different n. Let T be the maximal energy tree among trees of order n with maximum degree Δ. Then $n \geq \Delta + 1$. Let v be the vertex with maximum degree. When $\Delta + 1 \leq n < 2\Delta$, the structure of T is depicted in Figure 8(a), where there are at least two pendent vertices adjacent to v and other branches of v are all 2-branches; When $n = 2\Delta$, there is exactly one pendent vertex adjacent to v and $\Delta - 1$ 2-branches, which is shown in Figure 8(b); When $n > 2\Delta$, the structure of T is depicted in Figure 8(c), where there are $\Delta - 1$ 2-branches and one path with length at least 2. It can be easily seen that if and only if n is

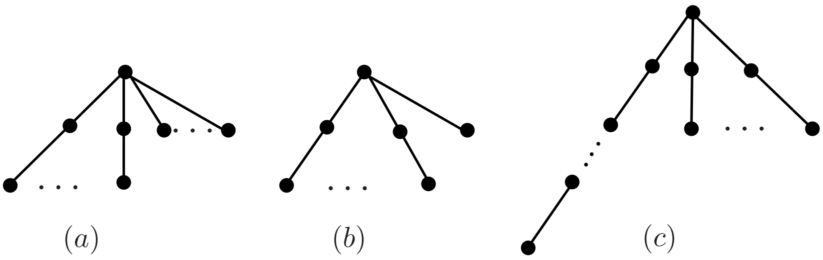

Figure 8: Maximal energy trees with given maximum degree

even and $n \geq 2\Delta$, the tree T has a perfect matching. Thus we can obtain the following result.

Theorem 3.2. *Among all conjugated trees of order n with maximum degree Δ, the maximal energy tree has exactly one branching vertex* (*of degree* Δ) *and as many as possible* 2*-branches.*

Proof. Let T be a conjugated tree with n vertices and maximum degree Δ with maximal energy. Then n is even and $n \geq 2\Delta$. By Lemma 3.1 and the discussion above, T is a starlike tree with a unique branching vertex of degree Δ and as many as possible 2-branches, whose structure is just the Figure 8(b) or (c). □

References

[1] I. Gutman, O.E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, 1986.

[2] C.A. Coulson, B. O'Leary, R.B. Mallion, *Hückel Theory for Organic Chemists*, Academic Press, London, 1978.

[3] M.J.S. Dewar, *The Molecular Orbital Theory of Organic Chemistry*, McGraw-Hill, New York, 1969.

[4] C.A. Coulson, On the calculation of the energy in unsaturated hydrocarbon molecules, *Proc. Cambridge Phil. Soc.* 36 (1940) 201–203.

[5] G.G. Hall, The bond orders of alternant hydrocarbon molecules, *Proc. Roy. Soc.* A 229 (1955) 251–259.

[6] B.J. McClelland, Properties of the latent roots of a matrix: The estimation of π-electron energies, *J. Chem. Phys.* 54 (1971) 640–643.

[7] I. Gutman, Hyperenergetic molecular graphs, *J. Serb. Chem. Soc.* 64 (1999), pp. 199–205.

[8] I. Gutman and Y. Hou, Bipartite unicyclic graphs with greatest energy. *MATCH–Commun. Math. Comput. Chem.* 43 (2001), pp. 17–28.

[9] M. Randić, M. Vračko, M. Novič, *in QSPR/QSAR Studies by Molecular Descriptors,* M. V. Diudea, Ed., Hova, Huntington, 2001, pp. 147–211.

[10] F. Zhang, H. Li, On acyclic conjugated molecules with minimal energies, *Discr. Appl. Math.* 92 (1999) 71–84.

[11] C. Heuberger, S. Wagner, Chemical trees minimizing energy and Hosoya index, *J. Math. Chem.* 46(2009) 214–230.

[12] W. Lin, X. Guo, H. Li, On the extremal energies of trees with a given maximum degree, *MATCH Commun. Math. Comput. Chem.* 54 (2005) 363–378.