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Extremal values of matching energies of one class of graphs

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ABSTRACT

In 1978, Gutman proposed the concept of graph energy, defined as the sum of the absolute values of eigenvalues of the adjacency matrix of a molecular graph, which is related to the energy of π-electrons in conjugated hydrocarbons. Recently, Gutman and Wagner proposed the concept of matching energy and pointed out that the chemical applications of matching energy go back to the 1970s. In this paper, we study the extremal values of the matching energy and characterize the graphs with minimal matching energy among all tricyclic graphs with a given diameter. Our methods can help to find more extremal values for other classes of molecular networks and the results suggest the structures with extremal energies.

1. Introduction

In theoretical chemistry and biology, molecular structure descriptors are used for modeling physico-chemical, toxicologic, pharmacologic, biological and other properties of chemical compounds. These descriptors are mainly divided into three types: degree-based indices, distance-based indices and spectrum-based indices. Degree-based indices [52] contain (general) Randić index [44,45], (general) zeroth order Randić index [31,32], and so on [20,25,49,51,53,54,59]. Distance-based indices [56] include the Balaban index [13], Wiener indices [39,50] and so forth [1,2,42]. Various of graph energies [33,47], HOMO-LUMO index [46] belong to spectrum-based indices. Actually, there are also some topological indices defined based on both degrees and distances [18], such as graph entropies [7,12,17].

In this paper, all graphs under our consideration are finite, connected, undirected and simple. For more notation and terminology that will be used in the sequel, we refer to [3]. Let G be a graph with order n and $A(G)$ be its adjacency matrix. The characteristic polynomial of G, denoted by $\phi(G)$, is defined as

$$\phi(G) = \det(xI - A(G)) = \sum_{i=0}^{n} a_i(G)x^{n-i},$$

where I is the identity matrix of order n. The roots of the equation $\phi(G) = 0$, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, are the eigenvalues of $A(G)$. The energy of G, denoted by $E(G)$, is defined as the sum of the absolute values of the eigenvalues of $A(G)$, that is,

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

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The concept of the energy of simple undirected graphs was introduced by Gutman in [23] and now is well-studied. For more results about graph energy, we refer the readers to some recent papers [21,34–36,48] and the book [47]. There are various generalizations of graph energy [27], such as Randić energy [4,15,16], Laplacian energy [14], incidence energy [5,6], etc.

Let G be a graph with n vertices and m edges. Denote by $m_k(G)$ the number of k-matchings (= the number of selections of k independent edges = the number of k-element independent edge sets) of G. Specifically, $m_1(G) = m,\ m_2(G) = \binom{m}{2} - \sum_{i=1}^{n}\binom{d_i}{2}$ and $m_k(G) = 0$ for $k > \lfloor \frac{n}{2} \rfloor$ or $k < 0$, where d_i is the degree of the ith vertex. It is both consistent and convenient to define $m_0(G) = 1$. The matching polynomial of the graph G is defined as

$$\alpha(G) = \alpha(G, \mu) = \sum_{k\geq 0}(-1)^k m_k(G)\mu^{n-2k}. \tag{1}$$

Recently, Gutman and Wagner [30] defined the matching energy of a graph G based on the zeros of its matching polynomial [19,24].

Definition 1. Let G be a simple graph with order n, and $\mu_1, \mu_2, \ldots, \mu_n$ be the zeros of its matching polynomial. Then,

$$ME(G) = \sum_{i=1}^{n} |\mu_i|. \tag{2}$$

Moreover, Gutman and Wagner [30] pointed out that the matching energy is a quantity of relevance for chemical applications. They arrived at the simple relation:

$$TRE(G) = E(G) - ME(G),$$

where TRE(G) is the so-called "topological resonance energy" of G. About the chemical applications of matching energy, for more details see [28,29].

For the coefficients $a_i(G)$ of $\phi(G)$, let $b_i(G) = |a_i(G)|, i = 0, 1, \ldots, n$. Note that $b_0(G) = 1,\ b_1(G) = 0$ and $b_2(G)$ is the number of edges of G. For convenience, let $b_i(G) = 0$ if $i < 0$. In [22], we have

$$E(G) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dx}{x^2}\ln\left[\left(\sum_{j=0}^{\lfloor \frac{n}{2}\rfloor} b_{2j}(G)x^{2j}\right)^2 + \left(\sum_{j=0}^{\lfloor \frac{n}{2}\rfloor} b_{2j+1}(G)x^{2j+1}\right)^2\right]. \tag{3}$$

Thus $E(G)$ is a monotonically increasing function of $b_i(G), i = 0, 1, \ldots, n$.

Similar to Eq. (3), the matching energy also has a beautiful formula as follows [30]. Eq. (4) could be considered as the definition of matching energy, in which case Eq. (2) would become a theorem.

Theorem 1. *Let G be a simple graph of order n, and $m_k(G)$ be the number of its k-matchings, $k = 0, 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$. The matching energy of G is given by*

$$ME = ME(G) = \frac{2}{\pi}\int_0^{\infty}\frac{1}{x^2}\ln\left[\sum_{k\geq 0} m_k(G)x^{2k}\right]dx. \tag{4}$$

By Eq. (4) and the monotony of the logarithmic function, we can define a quasi-order "$\succeq$" as follows: If G and H are two graphs, then

$$G \succeq H \Longleftrightarrow m_k(G) \geq m_k(H) \text{ for all } k.$$

If $G \succeq H$ and there exists some k such that $m_k(G) > m_k(H)$, then we write $G \succ H$. Clearly, $G \succeq H \Rightarrow ME(G) \geq ME(H)$, $G \succ H \Rightarrow ME(G) > ME(H)$. And if $G \succeq H$ and $H \succeq G$, the graphs G and H are said to be m-equivalent, denote it by $G \sim H$.

Based on the quasi-order, there are some more extremal results on matching energy of graphs [8–11,38,41,43]. For instance, in [30], the authors gave some elementary results on the matching energy. Ji et al. [38] characterized the graphs with the extremal matching energy among all bicyclic graphs, while Chen and Shi [8] proved the same extremal results for tricyclic graphs. In [55], the authors determined the extremal graphs from $\mathcal{G}_{n,m}$ with $n \leq m \leq 2n - 4$ minimizing the matching energy; they also determined the minimal matching energy of graphs from $\mathcal{G}_{n,m}$ with a given matching number β for $m = n - 1 + t$ and $1 \leq t \leq \beta - 1$, where $\mathcal{G}_{n,m}$ denotes the set of connected graphs of order n and with m edges.

Chen et al. [9] characterized the graphs with minimal ME among all unicyclic and bicyclic graphs with a given diameter d. In this paper, we characterize the graphs with minimal ME among all tricyclic graphs with a given diameter d.

2. Methods

The following lemma gives two fundamental identities for the number of k-matchings of a graph (see [19,24]).

Lemma 1. *Let G be a simple graph, $e = uv$ be an edge of G, and $N(u) = \{v_1(= v), v_2, \ldots, v_j\}$ be the set of all neighbors of u in G. Then we have*

$$m_k(G) = m_k(G - uv) + m_{k-1}(G - u - v), \tag{5}$$