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Research Article

On the Extremal Modified Wiener Index of Molecular Graphs

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Abstract: In this article, we consider the relationship between modified Wiener index and some special parameters of molecular graph if parameter is a positive real number, and present the molecular graphs which minimize the modified Wiener index among all molecular graphs with given chromatic number and clique number and the molecular graphs which maximum the modified Wiener index among all molecular graphs with given clique number.
Keywords: Chemical graph theory, molecular graph, Wiener index, modified Wiener index, chromatic number, clique number

INTRODUCTION

The modified Wiener index, as an extension of Wiener index, is an important topological index in Chemistry. It is used for the structure of molecule. There is a very close relation between the physical, chemical characteristics of many compounds and the topological structure of that. The modified Wiener index is such a topological index and it has been widely used in Chemistry fields. Some conclusions for Wiener index and can refer to [1-3].

The molecular graphs considered in this paper are simple and connected. The vertex and edge sets of a molecular graph G are denoted by $V(G)$ and $E(G)$, respectively. The Wiener index is defined as the sum of distances between all unordered pair of vertices of a molecular graph G, i.e.,

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v),$$

where $d(u,v)$ is the distance between u and v in G.

The modified Wiener index is defined as

$$W_\lambda(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v)^\lambda,$$

where λ is some real number and $\lambda \neq 0$.

Several papers contributed to determine the modified Wiener index of special molecular graphs. Zhang and Zhou [4] determined the trees in $T_{n,p}$ (a class of trees with n vertices and p pendent vertices) with maximal and minimal λ-modified Wiener indices. Zhou [5] studied the modified Wiener index of thorn tree. Gutmanet. al., [6] determined the λ-modified Wiener indices for special classes of trees. Yang, H. Hua [7] investigated the mathematical property of modified Wiener index and computed the modified Wiener index for a type of dendrimernanostars. Gutman and Zerovnik [8] showed how the concept of the modified Wiener index can be extended to weighted molecular graphs. Lim [9] learned Mass-modified Wiener indices and the boiling points for lower chloroalkanes. Liu and Liu [10] identified the k-th smallest and k-th greatest modified Wiener indices for all k up to $\left\lfloor \frac{n}{2} \right\rfloor + 1$ among the class of trees of order n.

In this paper, we connect the modified Wiener index with some well-known molecular graph theoretic parameters, such as chromatic number and clique number. It is proved that among all molecular graphs with n vertices and chromatic

number *k*, the modified Wiener index with λ >0 is minimized by the molecular graph $T_{k,n}$, and among all molecular graphs with *n* vertices and clique number *k*, the modified Wiener index is minimized by the molecular graph $T_{k,n}$ and maximized by the molecular graph $K_k \cdot P_{n-k}$. Note that $T_{k,n}$ is complete *k*-partite molecular graph on *n* vertices in which each part has either $\lfloor n/k \rfloor$ or $\lceil n/k \rceil$ vertices. Let $\chi(G)$ and *c*(*G*) be the chromatic number and clique number of a molecular graph *G*, respectively.

MAIN RESULTS AND PROOFS

Theorem 1. Let *G* be a molecular graph on *n* vertices and with $\chi(G)$=*k*. Let *t*=$\lfloor n/k \rfloor$ and λ >0 be a real number. Then

$$W_\lambda(G) \geq 2^\lambda \binom{n}{2} - (2^\lambda - 1)[\binom{n-t}{2} + (k-1)\binom{t+1}{2}] \quad (1)$$

and the equality holds if and only if $G \cong T_{k,n}$.

Proof. Let *G** be a molecular graph with minimum modified Wiener index in all molecular graphs with *n* vertices and chromatic number *k*. Then the vertex set of *G** can be divided into *k* parts such that no edges joins two vertices from same part. Moreover, *G** includes all edges joining vertices in different parts. Otherwise, there exists two disconnect vertices *v* and *v*' which belong to different parts. Then the molecular graph *G**+*vv*' has chromatic number *k* and fewer modified Wiener index than *G**, which contradicts to the selection of *G**. Hence, *G** is a complete *k*-partite molecular graph $K_k(r_1, r_2, \cdots, r_k)$ with $r_1+r_2+\ldots+r_k=n$, where r_i is the number of vertex in *i*-th part ($1 \leq i \leq k$).

We now claim that $G^* \cong T_{k,n}$. Otherwise, the parts are not as equal as possible, suppose there are r_i vertices in the *i*-th part and $r_j \geq r_i + 2$ in the *j*-th part. Then by transferring one vertex from the *j*-th part to the *i*-th part, the modified Wiener index will decrease which contradicts to the selection of *G**.

Since $|E(T_{k,n})| = \binom{n-t}{2} + (k-1)\binom{t+1}{2}$. We have

$$W_\lambda(T_{k,n}) = [\binom{n-t}{2} + (k-1)\binom{t+1}{2}] + 2^\lambda(\binom{n}{2} - [\binom{n-t}{2} + (k-1)\binom{t+1}{2}])$$

$$= 2^\lambda \binom{n}{2} - (2^\lambda - 1)[\binom{n-t}{2} + (k-1)\binom{t+1}{2}].$$

The proof above implies that equality holds in (1) if and only if $G \cong T_{k,n}$. The Theorem thus follows. □

Our second result depends heavily on the following lemma.

Lemma 1. [11] Let *G* be a graph on *n* vertices. If *G* contains on K_{m+1}, then $|E(G)| \leq |E(T_{k,n})|$. Moreover, $|E(G)| = |E(T_{k,n})|$ only if $G \cong T_{k,n}$.

Since for *c*(*G*)=*n* or *n*-1, it is not hard to obtain the lower bound and upper bound on modified Wiener index. In following theorem, we only consider the molecular graph *G* on *n* vertices with clique number *c*(*G*)<*n*-1. Let $d(G,i)$ be the number of vertex pairs at distance*i*. Let $K_k \cdot P_{n-k}$ be the graph obtained from K_k and P_{n-k} by joining a vertex of K_k to one end vertex of P_{n-k}. The λ -distance of a vertex *v*, $d_G^\lambda(v)$, is the sum of λ –th power distances between *v* and all other vertices in molecular graph *G*, i.e.,

$$d_G^\lambda(v) = \sum_{u \in G-v} d(u,v)^\lambda .$$

Theorem 2. Let *G* be a molecular graph on *n* vertices with clique number *c*(*G*)=*k*<*n*-1. Let λ >0 be a real number. Then,

we have

$$2^{\lambda}\binom{n}{2}-(2^{\lambda}-1)[\binom{n-t}{2}+(k-1)\binom{t+1}{2}] \le W_{\lambda}(G) \le \binom{k}{2}+\sum_{i=1}^{n-k}(n-k-i+1)i^{\lambda}+(k-1)\sum_{i=2}^{n-k+1} i^{\lambda}$$

Where, $t=\lfloor n/k \rfloor$. Moreover, the lower bound is achieved if and only if $G \cong T_{k,n}$ and the upper bound is achieved if and only if $G \cong K_k \cdot P_{n-k}$.

Proof. Let G be a molecular graph on n vertices with clique number $c(G)=k<n-1$ and l be the diameter of G. Then, in terms of Lemma 1, we get

$$\begin{aligned} W_{\lambda}(G) &= |E(G)| + \sum_{i=2}^{l} i^{\lambda} d(G,i) \\ &\ge |E(G)| + 2^{\lambda}\sum_{i=2}^{l} d(G,i) \qquad (2) \\ &= |E(G)| + 2^{\lambda}[\binom{n}{2} - |E(G)|] \\ &= 2^{\lambda}\binom{n}{2} - (2^{\lambda}-1)|E(G)| \\ &\ge 2^{\lambda}\binom{n}{2} - (2^{\lambda}-1)|E(T_{k,n})| \qquad (3) \\ &= 2^{\lambda}\binom{n}{2} - (2^{\lambda}-1)(\binom{n-t}{2}+(k-1)\binom{t+1}{2}). \end{aligned}$$

It is fact that equality in both (2) and (3) will hold if and only if $G \cong T_{k,n}$. Note that the clique number of graph $T_{k,n}$ is k. Hence, we obtain

$$W_{\lambda}(G) \ge 2^{\lambda}\binom{n}{2} - (2^{\lambda}-1)(\binom{n-t}{2}+(k-1)\binom{t+1}{2}),$$

and the equality holds if and only if $G \cong T_{k,n}$.

In the following, we will prove the upper bound on modified Wiener index by induction on vertex number n.

Let G^* be a molecular graph with maximum modified Wiener index in all molecular graphs with n vertices and clique number $k<n-1$. Clearly, G^* has a pendent vertex, say u. Let v be the pendent vertex of $K_k \cdot P_{n-k}$. Then, we infer

$$W_{\lambda}(G^*) = W_{\lambda}(G^*-u) + d^{\lambda}_{G^*}(u),$$
$$W_{\lambda}(K_k \cdot P_{n-k}) = W_{\lambda}(K_k \cdot P_{n-k}-v) + d^{\lambda}_{K_k \cdot P_{n-k}}(v).$$

Obviously, G^*-u has $n-1$ vertices and with clique number k. In view of induction hypothesis, we deduce $W_{\lambda}(G^*-u) \le W_{\lambda}(K_k \cdot P_{n-k}-v)$. Since $d^{\lambda}_{G^*}(u) \le d^{\lambda}_{K_k \cdot P_{n-k}}(v)$ and the equality holds if and only if $G \cong K_k \cdot P_{n-k}$. We yield $W_{\lambda}(G^*) \le W_{\lambda}(K_k \cdot P_{n-k})$.

By straightforward calculation, we have

$$W_{\lambda}(K_k \cdot P_{n-k}) = \binom{k}{2}+\sum_{i=1}^{n-k}(n-k-i+1)i^{\lambda}+(k-1)\sum_{i=2}^{n-k+1} i^{\lambda}.$$

Thus,

$$W_{\lambda}(G) \le \binom{k}{2}+\sum_{i=1}^{n-k}(n-k-i+1)i^{\lambda}+(k-1)\sum_{i=2}^{n-k+1} i^{\lambda}.$$

and the proof above reveals that the equality holds if and only if $G \cong K_k \cdot P_{n-k}$. □

CONCLUSION AND DISCUSSIONS

The contributions of our paper are presenting the lower bound of modified Wiener index under fixed chromatic number if λ >0, and determining the upper bound and lower bound of modified Wiener index under fixed clique number when λ >0. Our results also present the sufficient and necessary condition for reaching the upper and lower bound.

The terminal Wiener index (TW) of a molecular graph is defined as the sum of distances between all pairs of pendent vertices of the graph:

$$TW(G) = \sum_{\{u,v\}\subseteq V(G), d(u)=d(v)=1} d(u,v).$$

As an extension of terminal Wiener index, the modified terminal Wiener index of a molecular graph is defined as

$$TW_\lambda(G) = \sum_{\{u,v\}\subseteq V(G), d(u)=d(v)=1} d(u,v)^\lambda,$$

where λ is a real number.

Hence, it is natural to ask some questions that what is the upper bound and lower bound of modified terminal Wiener index under fixed chromatic number and clique number, and what is the sufficient and necessary condition for reaching the upper and lower bound.

At last, by following the technologies presented in the above section, we get following conclusions on λ <0.

Theorem 3. Let *G* be a molecular graph on *n* vertices and with $\chi(G)$ =*k*. Let *t*=$\lfloor n/k \rfloor$ and λ <0 be a real number. Then

$$W_\lambda(G) \le 2^\lambda \binom{n}{2} - (2^\lambda - 1)\left[\binom{n-t}{2} + (k-1)\binom{t+1}{2}\right]$$

and the equality holds if and only if $G \cong T_{k,n}$.

Theorem 4. Let *G* be a molecular graph on *n* vertices with clique number *c*(*G*)=*k*<*n*-1. Let λ <0 be a real number. Then, we have

$$2^\lambda \binom{n}{2} - (2^\lambda - 1)\left[\binom{n-t}{2} + (k-1)\binom{t+1}{2}\right] \ge W_\lambda(G) \ge \binom{k}{2} + \sum_{i=1}^{n-k}(n-k-i+1)i^\lambda + (k-1)\sum_{i=2}^{n-k+1} i^\lambda$$

Where *t*=$\lfloor n/k \rfloor$. Moreover, the upper bound is achieved if and only if $G \cong T_{k,n}$ and the lower bound is achieved if and only if $G \cong K_k \cdot P_{n-k}$.

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