

A Note on Connectivity and λ -Modified Wiener Index*

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Received 8 March 2015; Accepted 25 August 2015

ACADEMIC EDITOR: BO ZHOU

ABSTRACT In theoretical chemistry, λ -modified Wiener index is a graph invariant topological index to analyze the chemical properties of molecular structure. In this note, we determine the minimum λ -modified Wiener index of graph with fixed connectivity or edge-connectivity. Our results also present the sufficient and necessary condition for reaching the lower bound.

KEYWORDS Chemical graph theory • λ -modified Wiener index • connectivity • edge-connectivity

1. INTRODUCTION

Chemical compounds and drugs are often modeled as graphs where each vertex represents an atom of molecule and covalent bounds between atoms are represented by edges between the corresponding vertices. This graph derived from a chemical compounds is often called its molecular graph and can be different structures.

The λ -modified Wiener index, as an extension of Wiener index, is an important distance-based 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 λ -modified Wiener index is such a topological index and it has been widely used in chemistry fields. 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 notation and terminology used but undefined in this paper can be found in [1].

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 .

*Research supported partially by NSFC (No.11401519).

The λ -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 $\lambda \neq 0$. As numerical descriptors of the molecular structure obtained from the corresponding molecular graph, λ -modified Wiener index has found several applications in theoretical chemistry, especially in QSPR/QSAR study. For instance, λ -modified Wiener index is used to measure the stability of alkanes and the strain energy of cycloalkanes.

Several papers contributed to determine the Wiener index and modified Wiener index of special molecular graphs. Zhang and Zhou [2] 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. Liu and Liu [3] identified the k -th smallest and k -th greatest λ -modified Wiener indices for all k up to among the class of trees of order n . Yan et. al., [4] presented the molecular graphs which minimize the Hyper-Wiener index among all molecular graphs with given chromatic number and clique number and the molecular graphs which maximum the Hyper-Wiener index among all molecular graphs with given chromatic number and clique number. Dou et. al., [5] determined several characteristics concern the hyper-Wiener index of molecular graphs. More conclusions for Wiener index and related indices can refer to [6], [7], [8] and [9].

Connectivity is one of the basic concepts of graph theory: it asks for the minimum number of elements (vertices or edges) that need to be removed to disconnect the remaining vertices from each other. A cut, vertex cut, or separating set of a connected graph G is a set of vertices whose removal renders G disconnected. The connectivity or vertex connectivity (where G is not a complete graph) is the size of a minimal vertex cut. A graph is called k -connected or k -vertex-connected if its vertex connectivity is k or greater. The edge-connectivity is the size of a smallest edge cut. A graph is called k -edge-connected if its edge connectivity is k or greater.

In this paper, we determine the minimum λ -modified ($\lambda > 0$) Wiener index of molecular graph with fixed connectivity or edge-connectivity. And, the molecular graph reach the lower bound is presented. The tricks for proofing our main results follow from Gutman and Zhang [10].

2. MAIN RESULTS AND PROOFS

Let G be a connected molecular graph on n vertices. It is obvious that the λ -modified Wiener index is minimal for fixed λ if and only if $G = K_n$, in which case, $W_\lambda(G) = n(n-1)/2$. In what follows, we investigate when a molecular graph with a given vertex or edge-connectivity has minimum λ -modified Wiener index, and only consider the situation when $\lambda > 0$.

Theorem 1. Let G be a k -connected, n -vertex molecular graph, $1 \leq k \leq n - 2$, and $\lambda > 0$ be a real number. Then

$$W_\lambda(G) \geq \frac{n(n-1)}{2} + (2^\lambda - 1)(n - k - 1).$$

Equality holds if and only if $G \cong K_k \vee (K_1 \cup K_{n-k-1})$.

Proof. Let G_{\min} be the molecular graph that among all molecular graphs with n vertices and connectivity k has minimum λ -modified Wiener index. In terms of the connectivity of G_{\min} is k , there is a vertex-cut $X \subseteq V(G_{\min})$, which satisfies that $|X| = k$.

Let $G_1, G_2, \dots, G_\omega$ be the components of $G_{\min} - X$. Then each of the molecular sub-graphs $G_1, G_2, \dots, G_\omega$ must be complete. Otherwise, if one of them would not be complete, then by adding an edge between two nonadjacent vertices in this molecular sub-graph we would arrive at a molecular graph with the same number of vertices and same connectivity, but smaller λ -modified Wiener index (since two nonadjacent vertices become adjacent), a contradiction.

Next, we claim that $\omega=2$. Otherwise, if $\omega>2$, by adding an edge between a vertex from one component and a vertex from another component $G_1, G_2, \dots, G_\omega$, then the resulting molecular graph would still have connectivity k , but its λ -modified Wiener index would decrease (the distance between two vertices on the new edge decrease to 1), a contradiction. Therefore, $G_{\min} - X$ has two components G_1 and G_2 . By virtue of a similar discussion, we deduce that any vertex in G_1 and G_2 is adjacent to any vertex in X .

Denote the number of vertices of G_1 by n_1 and that of G_2 by n_2 . Then $n_1 + n_2 + k = n$ and by direct computation, we obtain

$$\begin{aligned} W_\lambda(G_{\min}) &= \frac{n_1(n_1-1)}{2} + \frac{n_2(n_2-1)}{2} + \frac{k(k-1)}{2} + k(n_1 + n_2) + 2^\lambda n_1 n_2 \\ &= \frac{n^2}{2} + (k - \frac{1}{2})n + \frac{k(k-1)}{2} + (2^\lambda - 1)n_1 n_2 \end{aligned}$$

which for fixed n and k is minimum for $n_1=1$ or $n_2=1$. This in turn means that $G_{\min} = K_k \vee (K_1 \cup K_{n-k-1})$. By directly calculating, we yield

$$W_\lambda(G_{\min}) = \frac{n(n-1)}{2} + (2^\lambda - 1)(n - k - 1).$$

Hence, we complete the proof. □

Our next result reveals that the edge-connectivity version for Theorem 1 is also established. Here, we don't consider the case of $k = n - 1$, since the only $(n - 1)$ -edge connected molecular graph is K_n .

Theorem 2. Let G be a k -edge connected, n -vertex molecular graph, $1 \leq k \leq n - 2$, and λ be a positive real number. Then

$$W_\lambda(G) \geq \frac{n(n-1)}{2} + (2^\lambda - 1)(n - k - 1).$$

Equality holds if and only if $G \cong K_k \vee (K_1 \cup K_{n-k-1})$.

Proof. Let now G_{\min} be the molecular graph that among all molecular graphs with n vertices and edge-connectivity k has minimum λ -modified Wiener index. Let X be an edge-cut of G_{\min} with $|V| = k$. Then $G_{\min} - X$ has two components, G_1 and G_2 . Both G_1 and G_2 must be complete molecular graphs. Let $|V(G_1)| = n_1$, $|V(G_2)| = n_2$, and $n_1 + n_2 = n$.

Denote the set of the end-vertices of the edges of X in G_1 by S , and that in G_2 by T . Let $|V(G_1) - S| = a_1$ and $|V(G_2) - T| = a_2$. There are

$$\frac{n_1(n_1-1)}{2} + \frac{n_2(n_2-1)}{2} + k = |E(G_{\min})|$$

pairs of vertices at distance 1, and $a_1 a_2$ pairs of vertices at distance of 3. All other vertex pairs, namely

$$\frac{n(n-1)}{2} - |E(G_{\min})| - a_1 a_2$$

are at distance 2. Therefore,

$$\begin{aligned} W_\lambda(G_{\min}) &= \left[\frac{n_1(n_1-1)}{2} + \frac{n_2(n_2-1)}{2} + k \right] + 3^\lambda a_1 a_2 \\ &\quad + 2^\lambda \left[\frac{n(n-1)}{2} - \left| \frac{n_1(n_1-1)}{2} + \frac{n_2(n_2-1)}{2} + k \right| - a_1 a_2 \right] \\ &= (2^\lambda - 1) \frac{n(n-1)}{2} - (2^\lambda - 1)k + (2^\lambda - 1)n_1 n_2 + (3^\lambda - 2^\lambda) a_1 a_2. \end{aligned}$$

which for fixed n and k is minimum for $n_1=1$, $a_1=0$ or $n_2=1$, $a_2=0$. This, as in the first theorem, implies $G_{\min} = K_k \vee (K_1 \cup K_{n-k-1})$. Hence,

$$W_\lambda(G) \geq \frac{n(n-1)}{2} + (2^\lambda - 1)(n - k - 1),$$

which completes the proof. \square

3. MORE RESULTS

Based on the tricks presented in above section, we get the following conclusions concern $\lambda < 0$.

Theorem 3. Let G be a k -connected, n -vertex molecular graph, $1 \leq k \leq n - 2$, and $\lambda < 0$ be a real number. Then

$$W_\lambda(G) \leq \frac{n(n-1)}{2} + (2^\lambda - 1)(n - k - 1).$$

Equality holds if and only if $G \cong K_k \vee (K_1 \cup K_{n-k-1})$.

Proof. Let G_{\max} be the molecular graph that among all molecular graphs with n vertices and connectivity k has maximum λ -modified Wiener index. In terms of the connectivity of G_{\max} is k , there is a vertex-cut $X \subseteq |V(G_{\max})|$, which satisfies that $|X| = k$.

Let $G_1, G_2, \dots, G_\omega$ be the components of $G_{\max} - X$. Then each of the molecular sub-graphs $G_1, G_2, \dots, G_\omega$ must be complete. Otherwise, if one of them would not be complete, then by adding an edge between two nonadjacent vertices in this molecular sub-graph we would arrive at a molecular graph with the same number of vertices and same connectivity, but larger λ -modified Wiener index (since $\lambda < 0$), a contradiction.

Next, we claim that $\omega = 2$. Otherwise, if $\omega > 2$, by adding an edge between a vertex from one component and a vertex from another component $G_1, G_2, \dots, G_\omega$, then the resulting molecular graph would still have connectivity k , but its λ -modified Wiener index would increase since $\lambda < 0$, a contradiction. Therefore, $G_{\max} - X$ has two components G_1 and G_2 . By virtue of a similar discussion, we deduce that any vertex in G_1 and G_2 is adjacent to any vertex in X .

Denote the number of vertices of G_1 by n_1 and that of G_2 by n_2 . Then $n_1 + n_2 + k = n$ and by direct computation, we obtain

$$\begin{aligned} W_\lambda(G_{\max}) &= \frac{n_1(n_1-1)}{2} + \frac{n_2(n_2-1)}{2} + \frac{k(k-1)}{2} + k(n_1 + n_2) + 2^\lambda n_1 n_2 \\ &= \frac{n^2}{2} + (k - \frac{1}{2})n + \frac{k(k-1)}{2} + (2^\lambda - 1)n_1 n_2 \end{aligned}$$

which for fixed n and k is maximum for $n_1 = 1$ or $n_2 = 1$ (since $\lambda < 0$). This in turn means that $G_{\max} = K_k \vee (K_1 \cup K_{n-k-1})$. By directly calculating, we yield

$$W_\lambda(G_{\max}) = \frac{n(n-1)}{2} + (2^\lambda - 1)(n - k - 1).$$

Hence, we complete the proof. □

Theorem 4. Let G be a k -edge connected, n -vertex molecular graph, $1 \leq k \leq n-2$, and λ be a negative real number. Then

$$W_\lambda(G) \leq \frac{n(n-1)}{2} + (2^\lambda - 1)(n - k - 1).$$

Equality holds if and only if $G \cong K_k \vee (K_1 \cup K_{n-k-1})$.

Proof. Let now G_{\max} be the molecular graph that among all molecular graphs with n vertices and edge-connectivity k has maximum λ -modified Wiener index. Let X be an edge-cut of G_{\max} with $|X| = k$. Then $G_{\max} - X$ has two components, G_1 and G_2 . Both G_1 and G_2 must be complete molecular graphs. Let $|V(G_1)| = n_1$, $|V(G_2)| = n_2$, and $n_1 + n_2 = n$.

Denote the set of the end-vertices of the edges of X in G_1 by S , and that in G_2 by T . Let $|V(G_1) - S| = a_1$ and $|V(G_2) - T| = a_2$. There are

$$\frac{n_1(n_1-1)}{2} + \frac{n_2(n_2-1)}{2} + k = |E(G_{\min})|$$

pairs of vertices at distance 1, and a_1a_2 pairs of vertices at distance of 3. All other vertex pairs, namely

$$\frac{n(n-1)}{2} - |E(G_{\min})| - a_1a_2$$

are at distance 2. Therefore,

$$\begin{aligned} W_\lambda(G_{\max}) &= \left[\frac{n_1(n_1-1)}{2} + \frac{n_2(n_2-1)}{2} + k \right] + 3^\lambda a_1a_2 \\ &\quad + 2^\lambda \left[\frac{n(n-1)}{2} - \left| \frac{n_1(n_1-1)}{2} + \frac{n_2(n_2-1)}{2} + k \right| - a_1a_2 \right] \\ &= (2^\lambda - 1) \frac{n(n-1)}{2} - (2^\lambda - 1)k + (2^\lambda - 1)n_1n_2 + (3^\lambda - 2^\lambda)a_1a_2. \end{aligned}$$

which for fixed n and k is maximum for $n_1 = 1$, $a_1 = 0$ or $n_2 = 1$, $a_2 = 0$ since $\lambda < 0$. This, as in the Theorem 3, implies $G_{\max} = K_k \vee (K_1 \cup K_{n-k-1})$. Hence,

$$W_\lambda(G) \leq \frac{n(n-1)}{2} + (2^\lambda - 1)(n - k - 1).$$

This completes our argument. □

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