Wiener and Schultz Molecular Topological Indices of Graphs with Specified Cut Edges *

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Abstract

Let $G$ be a simple, undirected and connected graph. The Wiener index $W(G)$ of $G$ is defined to be the sum of distances between all pair of vertices of $G$, that is, $W(G) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d_G(i, j)$. The Schultz molecular topological index of $G$, denoted by $MTI(G)$, is defined to be the summation $\sum_{i=1}^{n} \sum_{j=1}^{n} d_G(i) (A_{ij} + d_G(i, j))$, where $n$ is the order of $G$, $d_G(i)$ is the degree of vertex $i$ in $G$, and $d_G(i, j)$ is the distance between vertices $i$ and $j$ and $A_{ij}$ is the $(i, j)$ - th entry of the adjacency matrix $A$ of $G$. Denote by $\mathcal{G}_{n,k}$ the set of graphs with $n$ vertices and $k$ cut edges. In this note, we determine resp. the minimal elements with respect to $W(G)$ and $MTI(G)$ among all elements $G$ in $\mathcal{G}_{n,k}(1 \leq k \leq n - 3)$.

1 Introduction

Given that $G$ is a simple, undirected and connected graph with $V(G)$ and $E(G)$ being the set of vertices and edges, respectively. For any two vertices $i$ and $j$ in $G$, we mean, by $d_G(i)$, the degree of vertex $i$, the number of edges incident with $i$ in $G$, while, by $d_G(i, j)$, the distance between $i$ and $j$ in $G$, the length of the shortest path connecting $i$ and $j$ in $G$.

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The Schultz molecular topological index, or simply denoted as $MTI$, of a (chemical) graph $G$ proposed by Schultz [1] in 1989 is defined as

$$MTI = MTI(G) = \sum_{i=1}^{n} \sum_{j=1}^{n} d_G(i) (A_{ij} + d_G(i, j)),$$

where $n$ is the order of $G$, the number of vertices in $G$, $d = (d_G(1), d_G(2), \ldots, d_G(n))$ is the degree sequence in $G$, and $A_{ij}$ is the $(i,j)$-th entry of the adjacency matrix $A$ of $G$.

Let $D_G(i) = \sum_{j=1}^{n} d_G(i, j)$ be the sum of distances between the vertex $i$ and all the remaining vertices in $G$. The Schultz molecular topological index can also be expressed via the following manner [3]:

$$MTI = MTI(G) = \sum_{i=1}^{n} d_G^2(i) + \sum_{i=1}^{n} d_G(i)D_G(i),$$

which can be further reduced to the following form:

$$MTI = MTI(G) = \sum_{i=1}^{n} d_G^2(i) + \sum_{i,j=1}^{n} (d_G(i) + d_G(j))d_G(i,j). \quad (1)$$

Another much–studied distance–based molecular topological index is the Wiener index $W(G)$, for this index see the recent survey [8,9], which is defined to be the sum of distances between all pair of vertices of $G$, that is,

$$W = W(G) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d_G(i, j).$$

It has been demonstrated that $MTI$ and $W$ are closely mutually related for certain amount of molecular graphs [2,3,5–9]. Moreover, it has been proved [5,7] that the Schultz molecular topological index has the same discriminating power with the Wiener index

$$MTI(G_1) = MTI(G_2) \quad \text{if and only if} \quad W(G_1) = W(G_2) \quad (2)$$

for arbitrary catacondensed benzenoid graphs. So it is both significant and interesting to study the Schultz molecular topological index for some given class of graphs, no matter whether they are molecular graphs or not.

Most recent research papers concerning on Schultz molecular topological index are mainly restricted to give formulas for computing the exact value of $MTI$ for some molecular graphs, see for instance [10–12]. In general, for any given graph $G$, its Schultz molecular topological index $MTI(G)$ is not always easily calculated. So it makes sense to determine the (upper and/or lower) bound(s) of $MTI(G)$ among a given class of graphs, or, to characterize the
graphs with extremal (maximal or/and minimal) Schultz molecular topological index among a certain class of graphs. Based on such a consideration, we shall determine resp. in this work that the graphs with minimal Schultz molecular topological index and Wiener index among all elements in \( G_{n,k} \), the set of graphs with \( n \) vertices and \( k \) cut edges.

2 Graph in \( G_{n,k} \) with minimal value of \( MTI(G) \) or \( W(G) \)

As usual, we begin with some notations and terminology. For any two graphs \( G_1 \) and \( G_2 \), if there exists a bridge \( uv \) between \( G_1 \) and \( G_2 \) such that \( u \in G_1 \) and \( v \in G_2 \), we denote this graph as \( G_1uvG_2 \). If there are a sequence of graphs \( G_1, G_2, \ldots, G_s(s \geq 2) \) with all graphs sharing one common (cut) vertex \( x \), then we denote this graph as \( G_1xG_2\cdots xG_s \).

Denote by \( G_{n,k} \) the set of graphs with \( n \) vertices and \( k \) cut edges. For a \( n \)-vertex connected graph \( G \) having no cycle, namely, a tree on \( n \) vertices, we know that \( G \) has exactly \( n - 1 \) cut edges and the tree with minimal \( MTI(G) \) can be easily determined by using Eq.(2), since star \( S_n \) has the minimum cardinality of \( W(G) \), which has been determined long time ago. For a connected graph \( G \) on \( n \) vertices having at least one cycle, the number of its cut edges is at most \( n - 3 \). So it will be always assumed in the subsequent part of this paper that \( G \) has \( k \) cut edges with \( 1 \leq k \leq n - 3 \).

![Operation A](image)

Fig. 1.

In the following, we shall introduce some lemmas which are crucial to the proofs of our main results. Let \( |V(G)| \) denote the number of vertices in \( G \), then we have

**Lemma 1.** Let \( G_1uvG_2 \) and \( G_1uG_2uK_2 \) be two graphs with \( |V(G_1)|, |V(G_2)| \geq 2 \), as shown in Fig.1. Then \( MTI(G_1uvG_2) > MTI(G_1uG_2uK_2) \).

**Proof.** Set \( G_1^* = G_1uvG_2, G_2^* = G_1uG_2uK_2 \). By Eq. (1), we obtain
\[ MTI(G_1uG_2uK_2) - MTI(G_1uvG_2) \]

\[ = (d_{G_1^*}(u) + d_{G_1^*}(v) - 1)^2 + d_{G_1^*}(u) - d_{G_1^*}(v) + \sum_{x \in G_1 - \{u\}} (1 + d_{G_1^*}(x))d_{G_2^*}(w, x) + \]

\[ \sum_{y \in G_2 - \{v\}} (1 + d_{G_2^*}(y))d_{G_2^*}(w, y) - \sum_{x \in G_1 - \{u\}} (d_{G_1^*}(v) + d_{G_1^*}(x))d_{G_1^*}(v, x) - \sum_{y \in G_2 - \{v\}} (d_{G_1^*}(u) + d_{G_1^*}(y))d_{G_1^*}(u, y) + (d_{G_2^*}(u) + d_{G_2^*}(w)) \times 1 - (d_{G_1^*}(u) + d_{G_1^*}(v)) \times 1 + \]

\[ \sum_{x \in G_1 - \{u\}} (d_{G_1^*}(u) + d_{G_1^*}(x))d_{G_1^*}(u, x) + \sum_{y \in G_2 - \{v\}} (d_{G_2^*}(v) + d_{G_2^*}(y))d_{G_2^*}(v, y) - \sum_{x \in G_1 - \{u\}} (d_{G_1^*}(v) + d_{G_1^*}(y))d_{G_1^*}(v, y) - \sum_{y \in G_2 - \{v\}} (d_{G_1^*}(u) + d_{G_1^*}(y))d_{G_1^*}(u, y) + \]

\[ \sum_{x \in G_1 - \{u\}} \sum_{y \in G_2 - \{v\}} (d_{G_1^*}(x) + d_{G_1^*}(y))d_{G_2^*}(x, y) - \sum_{x \in G_1 - \{u\}} \sum_{y \in G_2 - \{v\}} (d_{G_1^*}(x) + d_{G_1^*}(y))d_{G_1^*}(x, y) . \]

For \( x \in G_1 - \{u\}, y \in G_2 - \{v\} \), we clearly have \( d_{G_1^*}(x) = d_{G_1^*}(x), d_{G_2^*}(y) = d_{G_1^*}(y), d_{G_2^*}(u, x) = d_{G_1^*}(u, x), d_{G_2^*}(v, y) = d_{G_1^*}(v, y) \), and \( d_{G_2^*}(x, y) = d_{G_1^*}(x, y) - 1 \). Also, \( d_{G_2^*}(w, x) = d_{G_1^*}(v, x) \), \( d_{G_2^*}(w, y) = d_{G_1^*}(u, y) \).

So we have

\[ MTI(G_1uG_2uK_2) - MTI(G_1uvG_2) \]

\[ = 2(d_{G_1^*}(u) - 1)(d_{G_1^*}(v) - 1) + \sum_{x \in G_1 - \{u\}} (1 - d_{G_1^*}(v))d_{G_1^*}(v, x) + \]

\[ \sum_{y \in G_2 - \{v\}} (1 - d_{G_1^*}(u))d_{G_1^*}(u, y) + \sum_{x \in G_1 - \{u\}} (d_{G_1^*}(v) - 1)d_{G_1^*}(u, x) + \]

\[ \sum_{y \in G_2 - \{v\}} (d_{G_1^*}(u) - 1)d_{G_1^*}(v, y) - \sum_{x \in G_1 - \{u\}} \sum_{y \in G_2 - \{v\}} (d_{G_1^*}(x) + d_{G_1^*}(y))d_{G_1^*}(x, y) \leq 2(d_{G_1^*}(u) - 1)(d_{G_1^*}(v) - 1) + \sum_{x \in G_1 - \{u\}} (1 - d_{G_1^*}(v))d_{G_1^*}(u, x) + \]

\[ \sum_{y \in G_2 - \{v\}} (1 - d_{G_1^*}(u))d_{G_1^*}(v, y) + \sum_{x \in G_1 - \{u\}} (d_{G_1^*}(v) - 1)d_{G_1^*}(u, x) + \]

\[ \sum_{y \in G_2 - \{v\}} (d_{G_1^*}(u) - 1)d_{G_1^*}(v, y) - \sum_{x \in G_1 - \{u\}, y \in G_2 - \{v\}} (d_{G_1^*}(x) + d_{G_1^*}(y))d_{G_1^*}(x, y) = 2(d_{G_1^*}(u) - 1)(d_{G_1^*}(v) - 1) - \sum_{x \in G_1 - \{u\}} \sum_{y \in G_2 - \{v\}} (d_{G_1^*}(x) + d_{G_1^*}(y))d_{G_1^*}(x, y) . \]

Note that \( d_{G_1^*}(x, y) \geq 3 \), \( d_{G_1^*}(x) + d_{G_1^*}(y) \geq 2 \). So we have

\[ \sum_{x \in G_1 - \{u\}} \sum_{y \in G_2 - \{v\}} (d_{G_1^*}(x) + d_{G_1^*}(y))d_{G_1^*}(x, y) \geq 6 \sum_{x \in G_1 - \{u\}} 1 \sum_{y \in G_2 - \{v\}} 1 = 6(|V(G_1)| - 1)(|V(G_2)| - 1). \]
But \(2(d_{G_1}(u) - 1)(d_{G_1}(v) - 1) \leq 2(|V(G_1)| - 1)(|V(G_2)| - 1)\), which concludes the proof. 

Similar to Lemma 1, we can obtain:

**Lemma 2.** Let \(G_1 uv G_2\) and \(G_1 uG_2 uK_2\) be two graphs with \(|V(G_1)|, |V(G_2)| \geq 2\), as shown in Fig.1. Then \(W(G_1 uv G_2) > W(G_1 uG_2 uK_2)\).

**Lemma 3.** Let \(G_1^*, G_2^*\) and \(G_3^*\) be graphs with \(|V(G_0)| \geq 3\), as shown in Fig.2. Then \(MTI(G_1^*) > MTI(G_2^*)\) or \(MTI(G_1^*) > MTI(G_3^*)\).

**Proof.** Write \(G^*_0 = G_0 - \{u, v\}\). By Eq. (1), we obtain \(MTI(G_2^*) - MTI(G^*_0)\)

\[
= (d_{G_0}(u) + s + t)^2 + d_{G_0}^2(v) - (d_{G_0}(u) + s)^2 - (d_{G_0}(v) + t)^2 +
\]

\[
\sum_{w \in G^*_0} [(t + d_{G_0}(u) + s) + d_{G_0}(w)] d_{G_0}(u, w) - \sum_{w \in G^*_0} [(s + d_{G_0}(u)) + d_{G_0}(w)] d_{G_0}(u, w) +
\]

\[
\sum_{w \in G^*_0} (d_{G_0}(v) + d_{G_0}(w)) d_{G_0}(v, w) - \sum_{w \in G^*_0} [(d_{G_0}(v) + t) + d_{G_0}(w)] d_{G_0}(v, w) +
\]

\[
t[(s + d_{G_0}(u) + t + 1] \times 1 - t(d_{G_0}(u) + s + 1)(d_{G_0}(u, v) + 1) + s[(s + d_{G_0}(u) + t + 1] \times 1 -
\]

\[
s[(s + d_{G_0}(u)) + 1] \times 1 + s(d_{G_0}(v) + 1)(d_{G_0}(v, u) + 1) - s(d_{G_0}(v) + t + 1)(d_{G_0}(v, u) + 1) +
\]

\[
st(1 + 1) \times 2 - st(1 + 1)(2 + d_{G_0}(v, u)) + t \sum_{w \in G^*_0} (1 + d_{G_0}(w))(d_{G_0}(u, w) + 1) -
\]

\[
t \sum_{w \in G^*_0} (1 + d_{G_0}(w))(d_{G_0}(v, w) + 1) + t(d_{G_0}(v) + 1)(d_{G_0}(v, u) + 1) - t(d_{G_0}(v) + t + 1) \times 1
\]

\[
= t[\sum_{w \in G^*_0} (2 + d_{G_0}(w))(d_{G_0}(u, w) - d_{G_0}(v, w)) - (d_{G_0}(u) - d_{G_0}(v) + 3s)d_{G_0}(u, v) + 2s +
\]

\[
2d_{G_0}(u) - 2d_{G_0}(v)]).
\]
Similarly, we have

\[ MTI(G_3^{**}) - MTI(G_1^{**}) = s \left[ \sum_{w \in G_0^*} (2 + d_{G_0}(w))(d_{G_0}(v, w) - d_{G_0}(u, w)) - (d_{G_0}(v) - d_{G_0}(u) + 3t)d_{G_0}(u, v) + 2t + 2d_{G_0}(v) - 2d_{G_0}(u) \right]. \]

If \( MTI(G_1^{**}) > MTI(G_2^{**}) \), the proof is completed. Otherwise, we have

\[ \sum_{w \in G_0^*} (2 + d_{G_0}(w))(d_{G_0}(v, w) - d_{G_0}(u, w)) - (d_{G_0}(v) - d_{G_0}(u) + 3s)d_{G_0}(u, v) + 2s + 2d_{G_0}(u) - 2d_{G_0}(v) \geq 0, \]

that is,

\[ \sum_{w \in G_0^*} (2 + d_{G_0}(w))(d_{G_0}(v, w) - d_{G_0}(u, w)) \leq -(d_{G_0}(v) - d_{G_0}(u) + 3s)d_{G_0}(u, v) + 2s + 2d_{G_0}(u) - 2d_{G_0}(v). \]

So we get

\[ MTI(G_3^{**}) - MTI(G_1^{**}) \leq s[-(d_{G_0}(u) - d_{G_0}(v) + 3s)d_{G_0}(u, v) + 2s + 2d_{G_0}(u) - 2d_{G_0}(v) - (d_{G_0}(v) - d_{G_0}(u) + 3t)d_{G_0}(u, v) + 2t + 2d_{G_0}(v) - 2d_{G_0}(u)] \]

\[ = s[2(s + t) - 3(s + t)d_{G_0}(u, v)] < 0, \]

resulting in \( MTI(G_1^{**}) > MTI(G_3^{**}) \), which completes the proof. \( \blacksquare \)

By the same reasoning as used in Lemma 3, we can demonstrate:

**Lemma 4.** Let \( G_1^{**}, G_2^{**} \) and \( G_3^{**} \) be graphs with \( |V(G_0)| \geq 3 \), as shown in Fig.2. Then \( W(G_1^{**}) > W(G_2^{**}) \) or \( W(G_1^{**}) > W(G_3^{**}) \).

**Theorem 5.** Let \( G \) be a connected simple \((n, m)\)-graph, a graph with \( n \) vertices and \( m \) edges. Then \( MTI(G) \geq 4(n - 1)m \) with equality if and only if the diameter of \( G \) is no more than two.

**Proof.** Suppose that \( G \) is a graph of diameter at least two. By definition of \( MTI(G) \), we have

\[ MTI(G) = \sum_{i=1}^{n} d_G^2(i) + \sum_{i=1}^{n} d_G(i)D_G(i) \geq \sum_{i=1}^{n} d_G^2(i) + \sum_{i=1}^{n} d_G(i) [d_G(i) + 2(n - 1 - d_G(i))] = 4(n - 1)m. \]
It is not difficult to see that the equality holds in the above inequality if and only if the diameter of $G$ is exactly two.

When the diameter of $G$ is one, namely, $G \cong K_n$, we have $MTI(G) = 2n(n-1)^2 = 4(n-1)m$. Therefore, the proof of the present theorem is completed. 

![Graphs G9,4 and G10,4](image)

**Fig. 3. Examples of graphs $G_{n,k}$ with given values of $n$ and $k$**

We use $G_{n,k}$ to denote the graph by introducing $\frac{n-k-1}{2}$ independent edges to the star $S_n$ if $n - k - 1$ is even and by adding $\frac{n-k-2}{2}$ independent edges to the star $S_{n-1}$, and then inserting a vertex to one of the above newly added independent edges and connecting it to the center of star if $n - k - 1$ is odd. Then we have:

**Theorem 6.** Let $G \in G_{n,k}$ with $1 \leq k \leq n - 3$, then $MTI(G) \geq MTI(G_{n,k})$ with equality if and only if $G \cong G_{n,k}$.

**Proof.** Let $G_{\text{min}}$ be a graph in $G_{n,k}$ such that $MTI(G)$ assumes the minimum cardinality. Then all cut edges in $G_{\text{min}}$ must be pendent edges. Moreover, all pendent vertices in $G_{\text{min}}$ must be adjacent to one common vertex, say $v$. If $G_{\text{min}}$ is not the graph as claimed above, then by Lemmas 1 and/or 3, we must get a graph $G'$ from $G_{\text{min}}$ by using Operation $A$ or $B$ such that $MTI(G') < MTI(G_{\text{min}})$, a contradiction. Then we must have $G_{\text{min}} \cong HvS_{k+1}$, where $H$ is a $2$-edge-connected graph and $S_{k+1}$ is a star of $k + 1$ vertices. If there exists a vertex $u \in H - \{v\}$ such that $u$ is not adjacent to $v$, then the diameter of $G_{\text{min}}$ is greater than or equal to 3, which contradicts the minimality of $MTI(G_{\text{min}})$ by Theorem 5. So we have $d_{G_{\text{min}}}(v) = n - 1$. By Theorem 5, in order for $MTI(G)$ to achieve the minimum cardinality, we must guarantee that $m$, the number of edges in $G_{\text{min}}$, takes the value as small as possible. Therefore we must have $G_{\text{min}} \cong G_{n,k}$, and the proof is completed. 

Similar to Theorem 6, by means of Lemmas 2 and/or 4, we can prove with no difficulty that:
Theorem 7. Let $G \in \mathcal{G}_{n,k}$ with $1 \leq k \leq n - 3$, then $W(G) \geq W(K_{n-k}^k)$ with equality if and only if $G \cong K_{n-k}^k$, the graph obtained by attaching $k$ pendent edges to any one vertex of $K_{n-k}$, the complete graph on $n - k$ vertices.

Fig. 4. An example of graph $K_{n-k}^k$ with $n = 8$ and $k = 3$.

It may be interesting to investigate the graph with maximal $MTI(G)/W(G)$ among all elements $G$ in $\mathcal{G}_{n,k}$ for $1 \leq k \leq n - 3$. But, as far as the author can see, it seems much more difficult than the present work we did here.

References


