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BOUNDS FOR THE SCHULTZ MOLECULAR TOPOLOGICAL INDEX

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Abstract

We present some lower and upper bounds for the Schultz molecular topological index (MTI) in terms of the graph invariants such as the number of vertices, the number of edges, minimum vertex degree, maximum vertex degree, and the Wiener index.

INTRODUCTION

Let G be a connected simple graph with n vertices. The adjacency matrix A of G is an $n \times n$ matrix (A_{ij}) such that $A_{ij} = 1$ if the vertices i and j are adjacent and 0 otherwise. The distance matrix D of G is an $n \times n$ matrix (D_{ij}) such that D_{ij} is just the distance between the vertices i and j. The degree v_i of the vertex i is the number of its first neighbors. The molecular topological index (MTI) of the graph G introduced by Schultz [1] in 1989 is defined as

$$MTI = MTI(G) = \sum_{i=1}^{n} [v(A+D)]_i$$

where $v = (v_1, v_2, \ldots, v_n)$ is the $1 \times n$ vector of the vertex degrees of G. Properties of MTI can be found in [2, 3, 4].

Setting $D_i = \sum\limits_{j=1}^{n} D_{ij}$. It is easy to see that MTI can be written as [4]

$$MTI = MTI(G) = \sum_{i=1}^{n} (v_i)^2 + \sum_{i=1}^{n} v_i D_i \,.$$

Recall that the Wiener index of a connected graph G can be written as [5] $W = W(G) = \frac{1}{2} \sum\limits_{i=1}^{n} D_i$ and that the first Zagreb index of G is defined as [6, 7] $M_1 = M_1(G) = \sum\limits_{i=1}^{n} (v_i)^2$. Thus

$$MTI(G) = M_1(G) + \sum_{i=1}^{n} v_i D_i \,.$$

BOUNDS FOR MTI

Let G be a connected simple graph with n vertices, minimum vertex degree δ and maximum vertex degree Δ. Klavžar and Gutman [4] noted that

$$\delta^2 n + 2\delta W(G) \leq MTI(G) \leq \Delta^2 n + 2\Delta W(G)$$

with equality (on both sides) if and only if G is regular. From this they derived the following simple bounds using the Wiener index:

$$2\delta W(G) < MTI(G) \leq 4\Delta W(G) \,.$$

In addition, the equality on the right–hand side holds if and only if G is a complete graph.

First we present a lower bound for MTI in terms of the number of vertices and the number of edges.

Theorem 1. *Let G be a connected simple 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 at most two.

Proof. Let n_k be the number of vertices of degree k in the graph G for every $1 \leq k \leq n-1$. Then

$$M_1 = \sum_{k=1}^{n-1} k^2 n_k \,.$$

Since $D_i \geq v_i + 2(n - v_i - 1) = 2n - v_i - 2$ for any vertex i, it follows that

$$\sum_{i=1}^{n} v_i D_i \geq \sum_{k=1}^{n-1} k n_k (2n - k - 2)\,.$$

Hence

$$MTI(G) \geq \sum_{k=1}^{n-1} k^2 n_k + \sum_{k=1}^{n-1} k n_k (2n - k - 2)\,.$$

Note that $\sum\limits_{k=1}^{n-1} k n_k = 2m$. We have

$$MTI(G) \geq (2n-2) \sum_{k=1}^{n-1} k n_k = 4(n-1)m\,.$$

From the arguments above, $MTI(G) = 4(n-1)m$ if and only if $D_i = v_i + 2(n - v_i - 1)$ for every vertex i, i.e., the diameter of G is at most two. $\square$

Corollary 2. *Let G be a connected simple graph with n vertices. Then*

$$MTI(G) \geq 4(n-1)^2$$

with equality if and only if G is a star.

Corollary 3. *Let G be a connected simple graph with n vertices.*

(1) *If G is a unicyclic graph, then*

$$MTI(G) \geq 4n(n-1)$$

with equality if and only if G is a quadrangle, a pentagon or a graph formed by attaching $n-3$ pendent edges to a vertex of a triangle.

(2) *If G is a bicyclic graph, then*

$$MTI(G) \geq 4(n-1)(n+1)$$

with equality if and only if G is one of the graphs in Figure 1.

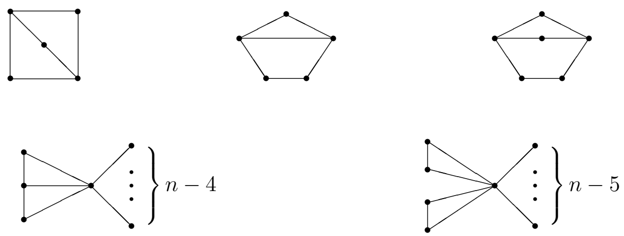

Figure 1. Bicyclic graphs of diameter 2.

The following result concerns the MTI of a graph and its complement.

Corollary 4. *Let G be a simple graph with $n \geq 4$ vertices, and $\overline{G}$ its complement. If both G and $\overline{G}$ are connected, then*

$$MTI(G) + MTI(\overline{G}) \geq 4(n-1)\binom{n}{2}$$

with equality if and only if the diameters of G and $\overline{G}$ are both two.

Proof. By the connectedness of G and $\overline{G}$, the diameters of G and $\overline{G}$ are both at least two. Let m and $\overline{m}$ be the number of edges of G and $\overline{G}$, respectively.

By Theorem 1,

$$MTI(G) \geq 4(n-1)m$$

with equality if and only the diameter of G is two. Similarly,

$$MTI(\overline{G}) \geq 4(n-1)\overline{m}$$

with equality if and only if the diameter of $\overline{G}$ is two.

It follows that

$$MTI(G) + MTI(\overline{G}) \geq 4(n-1)(m+\overline{m}) = 4(n-1)\binom{n}{2}$$

with equality if and only if the diameters of G and $\overline{G}$ are both two. $\square$

For any positive integer $n \geq 5$, let G be the graph formed by replacing a fixed vertex, say u of a pentagon by $n-4$ isolated vertices (and joining them to the two neighbors of u). Then the diameters of G and $\overline{G}$ are both two. Corollary 4 echoes the following result in [8, 9]: $W(G) + W(\overline{G}) \geq 3\binom{n}{2}$ and this bound is best possible for all $n \geq 5$.

Now we consider upper bounds for MTI.

Theorem 5. *Let G be a connected simple graph with n vertices, m edges and diameter D. Then*

$$MTI(G) \leq 2D(n-1)m - (D-2)M_1(G)$$

with equality if and only if the diameter of G is at most two.

Proof. Since $D_i \leq v_i + D(n - v_i - 1)$ for any vertex i, it follows that

$$MTI(G) \leq M_1(G) + \sum_{i=1}^{n} v_i\left[v_i + D(n - v_i - 1)\right] = 2D(n-1)m - (D-2)M_1(G)\,.$$

From the arguments above, $MTI(G) = 2D(n-1)m - (D-2)M_1(G)$ if and only if $D_i = v_i + D(n - v_i - 1)$ for every vertex i, i.e., the diameter of G is at most two. $\square$

Theorem 6. *Let G be a connected simple graph with n vertices and m edges, minimum vertex degree δ and maximum vertex degree Δ. Then*

$$MTI(G) \leq 2m(\delta + \Delta) - n\delta\Delta + 2\Delta W(G)$$

with equality if and only if G is regular.

Proof. From [10] or [11],

$$M_1 \leq 2m(\delta + \Delta) - n\delta\Delta$$

with equality if and only if G has only two types of degrees δ and Δ. Note also that

$$\sum_{i=1}^{n} v_i D_i \leq 2\Delta W(G)$$

with equality if and only if G is Δ-regular.

By combining the upper bounds for M_1 and $\sum_{i=1}^{n} v_i D_i$, the result follows. $\square$

Theorem 7. *Let G be a connected simple graph with n vertices and m edges. Then*

$$MTI(G) \leq m\left(\frac{2m}{n-1} + n - 2\right) + 2(n-1)W(G)$$

with equality if and only if G is a complete graph.

Proof. From [12]

$$M_1 \leq m\left(\frac{2m}{n-1} + n - 2\right)$$

with equality if and only if G is either a star or a complete graph.

Note also that

$$\sum_{i=1}^{n} v_i D_i \leq 2(n-1)W(G)$$

with equality if and only if G is a complete graph.

By the definition of MTI, the result holds. $\square$

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