

# Computing the Schultz molecular topological index of some graphs

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In this paper we compute the molecular topological index (MTI) for a cycle and complete graphs, and also we obtain the spanning tree with the smallest molecular topological index in a complete graph.

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## 1. Introduction

Molecular descriptors have found a wide application in QSPR/QSAR studies [4]. Among them, topological indices have a prominent place. One of them is Molecular Topological Index and denoted by MTI. It was introduced by Schultz in 1989. The molecular topological index of the graph  $G$  is defined by [1, 3, 2]:

$$MTI = \sum_{j=1}^n e_j,$$

where  $e_j$  ( $j=1, \dots, n$ ) are the elements of row matrix  $v(A+D)$ , ( i.e.,  $v(A+D) = (e_1, \dots, e_n)$ ),  $A = (a_{ij})$  and  $D = (d_{ij})$  are the adjacency and distance matrix respectively, and  $v$  is the vector of all the vertex valencies of graph  $G$ .

The distance matrix  $D$  is constructed for any graph on  $n$  vertices by setting up an  $n \times n$  matrix. Each entry  $d_{ij}$  is equal to the minimum number of edges in the graph connecting vertex  $i$  to vertex  $j$ . For chemical research on MTI see [5-10].

## 2. Main results and discussion

**Theorem 1.** Consider the complete graph  $K_n$ . The molecular topological index of  $K_n$  is computed as follow:

$$MTI(K_n) = 2n(n-1)^2$$

**Proof.** we know that the degree of all the vertices in a complete graph of order  $n$  is  $n-1$ , so we have  $v = (n-1, \dots, n-1)$ .

Since there exist an edge between each two vertices of a complete graph, we have  $A + D = 2A$ . Now we can write:  
 $v(A+D) = 2(n-1)(1, \dots, 1)A = 2(n-1)(n-1, \dots, n-1) = 2(n-1)^2(1, \dots, 1) = (e_1, \dots, e_n)$

and then

$$MTI(K_n) = \sum_{j=1}^n e_j = 2n(n-1)^2.$$

**Theorem 2.** Suppose  $C_n$  is a cycle of length  $n$  then

$$MTI(C_n) = \begin{cases} \frac{1}{2}n^3 + 4n & \text{if } n \text{ is even,} \\ 2n(2 + \left\lceil \frac{n}{2} \right\rceil + \left( \left\lceil \frac{n}{2} \right\rceil \right)^2) & \text{if } n \text{ is odd.} \end{cases}$$

**Proof.** The degree of each vertices of  $C_n$  is 2. So  $v = (2, \dots, 2)$ . Also it is easy to show that the sum of all components of each row of matrix  $D$  are equals. Suppose that  $n$  is even. We can see that the elements of the first row in matrix  $D$  are as follow

$$d_{11} = 0, d_{12} = 1, \dots, d_{1, 1+\frac{n}{2}} = \frac{n}{2}, d_{1, 2+\frac{n}{2}} = \frac{n}{2} - 1, \dots, d_{1n} = 1,$$

and sum of the components of the first row is  $(2 \sum_{j=1}^{\frac{n}{2}-1} j) + \frac{n}{2}$ . So we can write

$$\begin{aligned} v(A+D) &= 2(1, \dots, 1)(A+D) = 2(2 \sum_{j=1}^{\frac{n}{2}-1} j + \frac{n}{2} + 2, \dots, 2 \sum_{j=1}^{\frac{n}{2}-1} j + \frac{n}{2} + 2) \\ &= 4(\sum_{j=1}^{\frac{n}{2}-1} j, \dots, \sum_{j=1}^{\frac{n}{2}-1} j) + (n, \dots, n) + (4, \dots, 4) \end{aligned}$$

Let  $e = (1, \dots, 1)$ , then it is easy to see that  
 $v(A+D) = \frac{n^2+8}{2}e$ .

$$\text{So } e_j = \frac{n^2+8}{2} \text{ and } MTI(C_n) = \sum_{j=1}^n \frac{n^2+8}{2} = 4n + \frac{n^3}{2}.$$

Now suppose that  $n$  is odd, then

$$\begin{aligned}
 v(A+D) &= 2(1, \dots, 1)(A+D) = 2\left(2 \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} j + 2, \dots, \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} j + 2\right) \\
 &= 4\left(\sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} j, \dots, \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} j\right) + (4, \dots, 4) \\
 &= 2\left(2 + \left\lfloor \frac{n}{2} \right\rfloor + \left(\left\lfloor \frac{n}{2} \right\rfloor\right)^2\right)e.
 \end{aligned}$$

So  $e_j = 2\left(2 + \left\lfloor \frac{n}{2} \right\rfloor + \left(\left\lfloor \frac{n}{2} \right\rfloor\right)^2\right)$  and  $MTI(C_n) = \sum_{j=1}^n e_j = 2n\left(2 + \left\lfloor \frac{n}{2} \right\rfloor + \left(\left\lfloor \frac{n}{2} \right\rfloor\right)^2\right).$

## 2. The spanning tree with the smallest MTI

**Theorem 3.** let  $K_n$  be a complete graph and  $T_1, \dots, T_m$  be all of the spanning trees of  $K_n$ . Then

$$MTI(T_i) \geq 4(n-1)^2 \quad \text{for } i = 1, \dots, m,$$

and equality holds if and only if  $T_i$  be a spanning tree with a vertex of degree  $n-1$  and  $n-1$  vertices of degree 1, i.e.  $T_i$  be a star graph.

**Proof.** Suppose  $T_i$  is a star graph. Without loss of generality, let  $v = (n-1, 1, \dots, 1)$ . It is clear that the elements of adjacency matrix of  $T_i$  are as follow

$$\begin{cases} a_{il} = a_{li} = 1 & i \neq l, \\ a_{ij} = 0 & \text{otherwise.} \end{cases}$$

Since all of the vertices are joined to the center of  $T_i$ , so the distance between each non-center vertex of  $T_i$  and center is 1, and the distance between each two non-center vertices is 2, thus we have

$$C = A + D = \begin{bmatrix} 0 & 2 & \dots & 2 \\ 2 & 0 & \dots & 2 \\ \vdots & & \ddots & \vdots \\ 2 & 2 & \dots & 2 & 0 \end{bmatrix}$$

So  $c_{ij} = 2$  for  $j \neq i$ .

In this graph  $e_j$  can compute as follow

$$e_j = vC_j = (n-1, 1, \dots, 1) \begin{bmatrix} 2 \\ \vdots \\ 2 \\ 0 \\ 2 \\ \vdots \\ 2 \end{bmatrix} = \begin{cases} 2n-2 & i = j, \\ 4n-6 & i \neq j, \end{cases}$$

where  $C_j$  is the  $j^{th}$  column of matrix  $C$ . So

$$vC = v(A+D) = (4n-6, \dots, 4n-6, 2n-2, 4n-6, \dots, 4n-6).$$

Thus

$$MTI(T_i) = 2n-2 + (n-1)(4n-6) = 4(n-1)^2.$$

Now we show that for the others spanning trees

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

In general, for any spanning tree we have  $c_{ij} \geq 2$  for  $j \neq i$ . Since the total sum of vertex degrees is equal to twice the number of edges, we have

$$e_j = vC_j = (v_1, \dots, v_n) \begin{bmatrix} c_{1j} \\ \vdots \\ 0 \\ \vdots \\ c_{nj} \end{bmatrix} \geq 2 \sum_{\substack{i=1 \\ i \neq j}}^n v_i \geq 2(2n-2) - 2v_j.$$

So we can say

$$MTI(T_n) = \sum_{j=1}^n e_j \geq 2n(2n-2) - 2 \sum_{j=1}^n v_j = 4n(n-1) - 4(n-1) = 4(n-1)^2.$$

Now the proof is complete.

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