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BOUNDS FOR SCHULTZ INDEX OF PENTACHAINS

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The Wiener index (W) and the Schultz molecular topological index (MTI) are based on the distances between the vertices of molecular graphs. In this paper, we find the bounds of Schultz index for pentachains by the terms of Wiener index.

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1. Introduction

Topological indices are real numbers on graph parameters (vertex degree, distance between vertices, etc.) which have been defined during studies on molecular graphs in chemistry. The Wiener index was introduced by Wiener for characterization of alkanes in 1947[1]. The wiener index of molecular graph G defined as follows[2]: $W(G) = \frac{1}{2}\sum_{i=1}^{p}\sum_{j=1}^{p} D_{ij}$ where D_{ij} is the element of the distance matrix of G and p is the number of vertices in G. The mathematical properties and chemical applications of Wiener index are outlined in [3, 4, 5].

The molecular topological index of a molecular graph G was introduced by Schultz in 1989[6] and we call Schultz index, abbreviated MTI. It is defined as: $MTI(G) = \sum_{i=1}^{p}\sum_{j=1}^{p} d_i (A_{ij} + D_{ij})$ where d_i is the degree of vertex v_i in G and A_{ij} is the element of the adjacency matrix of G. The interesting chemical applications are found for Schultz index[7, 8]. It has been demonstrated that MTI and W are mutually related for certain classes of molecular graphs[9, 10].The explicit relation between MTI and W for trees is defined by Kelvin[9]. If G is a tree with p vertices, then:

$$MTI(G) = 4W(G) + \sum_{i=1}^{p}(d_i)^2 - p(p-1) \tag{1}$$

For an arbitrary graph G, Schultz index can be expressed as follows[11]:

$$MTI(G) = \sum_{i=1}^{p} d_i D_i + \sum_{i=1}^{p}(d_i)^2 \tag{2}$$

Where $D_i = \sum_{j=1}^{p} D_{ij}$.

In this paper, we establish a simple relation between MTI and W for a pentachains.

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2. Pentachains

Pentachains are chains that composed exclusively of pentagonal rings. Any tow rings have either one common edge or have no common vertices.If they have one common edge then said to be adjacent. A pentachain with h rings has $p = 3h + 2$ such that $h + 4$ vertices have 2 degree and $2h - 2$ vertices have 3 degree. Examples of pentachains are shown in Figure 1.

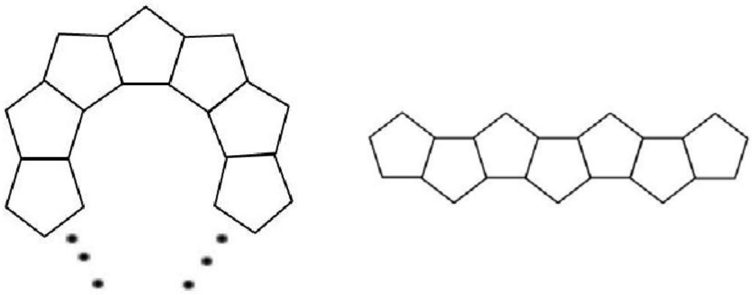

Fig. 1: H_h, L_h

We can represent these pentachains as represented in Figure 2 which we see L_h:

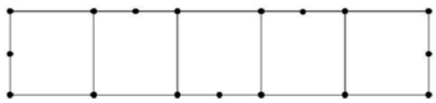

Fig. 2: L_h

3. Wiener index of L_h and H_h

If G has h rings. the first $h-1$ rings are named S_1 and the last $h-1$ rings are named S_2. Then, $(S_1 \bigcap S_2)$ is common in $h-2$ ring. We compute the Wiener index of G with h ring:

$$
\begin{aligned}
2W_h &= \sum_{v,w \in V(L_h)} d(v,w) \\
&= \sum_{v,w \in V(S_1)} d(v,w) + \sum_{v,w \in V(S_2)} d(v,w) + \sum_{v,w \in V(S_1 \cap S_2)} d(v,w) \\
&\qquad + \sum_{\substack{v \in V(S_1) \backslash V(S_2) \\ w \in V(S_2) \backslash V(S_1)}} d(v,w) \\
&= 4W_{h-1} - 2W_{h-2} + 2 \sum_{\substack{v \in V(S_1) \backslash V(S_2) \\ w \in V(S_2) \backslash V(S_1)}} d(v,w) \qquad (3)
\end{aligned}
$$

By the figure of L_h, we have:

$$\sum_{\substack{v\in V(S_1)\backslash V(S_2)\\ w\in V(S_2)\backslash V(S_1)}} d(v,w)=\begin{cases}\dfrac{27h-5}{2} & ,h \ \ is \ \ odd\\ \dfrac{27h-4}{2} & ,h \ \ is \ \ even\end{cases} \qquad (4)$$

Therefore, we have for $h\geq 3$:

$$2W_h = 4W_{h-1}-2W_{h-2}+\begin{cases}\dfrac{27h-5}{2} & ,h \ \ be \ \ odd\\ \dfrac{27h-4}{2} & ,h \ \ be \ \ even\end{cases} \qquad (5)$$

Then, for $h\geq 1$:

$$\begin{cases}2W_{h+2}-4W_{h+1}+2W_h = 27h+49 & ,h \ \ be \ \ odd\\ 2W_{h+2}-4W_{h+1}+2W_h = 27h+50 & ,h \ \ be \ \ even\end{cases} \qquad (6)$$

We have tow recessive equations with first values, $W_1=15$, $W_2=55$, $W_3=133$ and $W_4=262$. Then:

Theorem 3.1 *The Wiener index of linear pentachains, L_h with h rings is:*

$$W_h=\begin{cases}\dfrac{1}{4}(9h^3+22h^2+31h-2) & ,h \ \ be \ \ odd\\ \dfrac{1}{4}(9h^3+23h^2+24h+8) & ,h \ \ be \ \ even\end{cases} \qquad (7)$$

The Wiener index of H_h had computed in [12]:

Theorem 3.2 *The Wiener index of H_h is equal to:*

$$W(H_h)=9\binom{n}{3}+48\binom{n}{2}+78n+55 \qquad (8)$$

Where $n=h-2$.

4. Bounds for the schultz index

The degree of vertices are 2 or 3 in this graph. Therefore if we write the Schultz index of G to respect the degree of vertices, we have:

$$MTI(G)=\sum_{i=1}^{p}d_i^2+\sum_{\substack{i\\ d_i=2}}2D_i+\sum_{\substack{i\\ d_i=3}}3D_i=4W(G)+\sum_{i=1}^{2h-2}D_i+4\left(\frac{p+10}{3}\right)+9\left(\frac{2p-10}{3}\right)$$

Then:

$$MTI(G) = 4W(G) + \sum_{i=1}^{2h-2} D_i + \left(\frac{22p-50}{3}\right) \quad (9)$$

If degree of p_i is 3 and G has at least 4 rings, then G has 3 vertices with distance 1, at least 4 vertices with distance 2 and at least 6 vertices with distance 3 or more than 3. Hence, if p_i one vertex of degree 3 and $P \geq 14$, then, D_i is not less from $2p$. Then: $\sum_{i=1}^{2h-2} D_i \geq (2h-2)(2p)$. And:

$$MTI(G) \geq 4W(G) + (\frac{2p-10}{3})2p + (\frac{22p-50}{3}) = 4W + \frac{4p^2+2p-50}{3} \quad (10)$$

Lemma 4.1 *The linear pentachain* L_h *has the maximum Wiener index and the pentachain* H_h *has the minimum Wiener index among all pentachain graphs.*

Proof. If G is the pentachain graph and v, w are in $V(G)$. The $d(v,w)$ is maximum, if the number of pentagonal which tow edges of them counted for computation of $d(v,w)$. This is concluded easily from the Figure 2.

In the L_h has the maximum number and H_h has the minimum number of these pentachains among the pemtachains. Therefor the result conclude.

By above Lemma:

I) the lower bound for MTI is:

i) h is odd:

$$W(G) = \frac{1}{4}(9h^3 + 22h^2 + 31h - 2) = \frac{1}{36}(3p^3 + 4p^2 + 41p - 140)$$

For $p \geq 14$, $p^3 > \frac{20}{9}(4p2 + 41p - 140)$. Then:

$$W(G) < \frac{1}{36}(3p^3 + \frac{9p^3}{20}) = \frac{1}{36}(\frac{69p^3}{20}) \quad (11)$$

Therefor:

$$p > (\frac{720}{69}W)^{\frac{1}{3}} \quad (12)$$

ii) h is even:

$$W(G) = \frac{1}{4}(9h^3 + 23h^2 + 24h + 8) = \frac{1}{36}(3p^3 + 5p^2 + 16p - 4)$$

For $p \geq 14$, $p^3 > \frac{20}{9}(5p^2 + 16p - 4)$. Then:

$$p > (\frac{720}{69}W)^{\frac{1}{3}} \quad (13)$$

Therefore, the lower bound for MTI by (4.2) is:

$$MTI(G) > 4W + \frac{4}{3}(\frac{720}{69}W)^{\frac{2}{3}} + \frac{2}{3}(\frac{720}{69}W)^{\frac{1}{3}} - \frac{50}{3} \quad (14)$$

II) The upper bound for MTI is:

$$W(H_h) = \frac{1}{2}(3h^3 + 21h^2 - 6h + 14) = \frac{1}{18}(p^3 + 15p^2 - 90p + 238)$$

For $p \geq 14$, $W(H_h) > \frac{1}{18} p(p^2 + 15p - 90)$. The function $p^2 + 15p - 90$ has the minimum quantity in $p = \frac{15}{2}$. Then, for $p \geq 14$, the minimum quantity of this function is 316. Therefor:

$$W(G) > \frac{316}{18} p \Rightarrow p < \frac{18}{316} W \tag{15}$$

We have: $\sum_{i=1}^{2h-2} D_i < \sum_{i=1}^{p} D_i$. Therefor, by (4.1):

$$MTI(G) < 4W + 2W + (\frac{22p - 50}{3}) < 6W + \frac{22}{3}(\frac{18}{316})W - \frac{50}{3} \tag{16}$$

Then:

Theorem 4.2 *The bounds for Schultz index of pentachains are:*

$$\frac{50}{3} + \lambda_1 W^{\frac{1}{3}} + \lambda_2 W^{\frac{2}{3}} + 4W < MTI < \lambda_3 W - \frac{50}{3} \tag{17}$$

Where $\lambda_1 = -\frac{8}{3}(\frac{720}{69})^{\frac{1}{3}}, \lambda_2 = 2(\frac{720}{69})^{\frac{2}{3}} and \lambda_3 = 6 + \frac{22}{3}(\frac{18}{316})$.

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