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Explicit Relation between the Wiener Index and the Schultz Index of Catacondensed Benzenoid Graphs

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The Wiener index (W) and the Schultz molecular topological index (MTI) are based on the distances between the vertices of chemical graphs. It is shown that $MTI(\mathrm{G}) = 5W(\mathrm{G}) - (12h^2 - 14h + 5)$ for an arbitrary catacondensed benzenoid graph G having h hexagons.

Key words: catacondensed, benzenoid, graphs, Schultz index, Wiener index

INTRODUCTION

The Wiener index was introduced in 1947 as a structural descriptor for characterization of alkanes.[1] The conventional generalization of W for an arbitrary molecular graph G is due to Hosoya.[2] According to his definition,

$$W(\mathrm{G}) = \frac{1}{2}\sum_{i=1}^{p}\sum_{j=1}^{p} D_{ij}$$

where D_{ij} is the element of the distance matrix[3] of G and p is the number of vertices in G. The entry D_{ij} is equal to the length of a shortest path between vertices i and j. Mathematical properties and chemical applications of the Wiener index are outlined in numerous works (see books[4–7] and selected reviews[8–13]).

The molecular topological index of a chemical graph G was put forward by Schultz[14] in 1989. It is defined as

$$MTI(\mathrm{G}) = \sum_{i=1}^{p}\sum_{j=1}^{p} v_i (A_{ij}+D_{ij})$$

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where v_i is the degree (valence) of vertex i in G and A_{ij} is the element of the adjacency matrix[5] of G. The entry A_{ij} is equal to unity if vertices i and j are adjacent and zero otherwise. The molecular topological index has found interesting chemical applications.[14–23] Mathematical properties of *MTI* are also described in several articles.[24–31]

It has been demonstrated that *MTI* and *W* are closely mutually related for certain classes of molecular graphs.[25–27] Klein *et al.* derived an explicit relation between *MTI* and *W* for trees.[25] Namely, if G is a tree with p vertices (*i.e.*, G is the molecular graph of an alkane), then

$$MTI(\mathrm{G}) = 4W(\mathrm{G}) + \sum_{i=1}^{p} (v_i)^2 - p(p-1)\,.$$

For an arbitrary graph G, the molecular topological index can be expressed as follows:[28]

$$MTI(\mathrm{G}) = \sum_{i=1}^{p} v_i D_i + \sum_{i=1}^{p} (v_i)^2 \qquad (1)$$

where $D_i = \sum_{j=1}^{p} D_{ij}$ is the sum of distances between vertex i and all other vertices of graph G.

In this paper, we establish a simple explicit relation between *MTI* and *W* for a catacondensed benzenoid graph.

BENZENOID GRAPHS

Benzenoid graphs are composed exclusively of hexagonal rings that are face bounded by six-membered cycles in the plane. Any two rings have either one common edge (and are then said to be adjacent) or have no common vertices. The characteristic graph of a given benzenoid graph consists of vertices corresponding to the rings of the graph; two vertices are adjacent if and only if the corresponding rings share an edge. A benzenoid graph is called *catacondensed* if its characteristic graph is a tree. The characteristic graph of a *hexagonal chain* is isomorphic to the path. The above defined graphs may contain non-planar molecular graphs corresponding to helicenic benzenoid hydrocarbons.[32] A benzenoid graph is called a *benzenoid system* if it can be embedded into a regular hexagonal lattice in the plane. Examples of benzenoid graphs are shown in Figure 1. The vertices of a benzenoid graph are either of degree two or of degree three. An *internal* vertex of a graph belongs to three hexagonal rings. A benzenoid graph G with h rings has $p = 4h + 2 - n_i$ vertices, where n_i is the number of internal vertices in G. Let L_h denote the linear polyacene with h rings (see Figure 1).

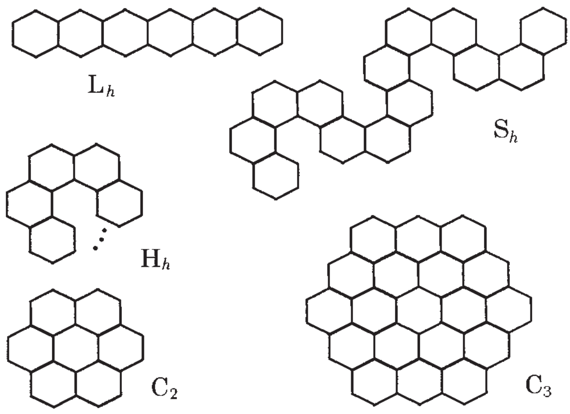

Figure 1. Benzenoid graphs with extremal Wiener index.

FORMULA FOR THE SCHULTZ INDEX

For benzenoid graphs, Gutman and Klavžar offer a simplified formula (1).[29] If G is a benzenoid graph, then

$$MTI(\mathrm{G}) = 4W(\mathrm{G}) + \frac{13p + 5n_i - 30}{2} + \sum_{\substack{i \\ v_i = 3}} D_i \ . \tag{2}$$

The following relation shows that the molecular topological index may be presented in terms of the Wiener index and the number of rings of the corresponding benzenoid graph.

PROPOSITION 1. Let G be an arbitrary catacondensed benzenoid graph having h rings. Then,

$$MTI(\mathrm{G}) = 5W(\mathrm{G}) - (12h^2 - 14h + 5)\ .$$

The obtained formula immediately leads to the recently published result: the discrimination power of *MTI* and *W* is the same for catacondensed benzenoid graphs.[31]

For every benzenoid graph G, the Wiener index may be decomposed into two parts: $2W(\mathrm{G}) = W_2(\mathrm{G}) + W_3(\mathrm{G})$, where $W_2(\mathrm{G}) = \sum_{i, v_i = 2} D_i$ and $W_3(\mathrm{G}) = \sum_{i, v_i = 3} D_i$. The proof of Proposition 1 is based on the following decomposition of the distance sums $W_2(\mathrm{G})$ and $W_3(\mathrm{G})$.[31]

PROPOSITION 2. Let G be an arbitrary catacondensed benzenoid graph having h rings. Then, $W_2(\mathrm{G}) = W_2(\mathrm{L}_h) - \Delta$ and $W_3(\mathrm{G}) = W_3(\mathrm{L}_h) - \Delta$, where $\Delta = \Delta(\mathrm{G}) > 0$.

It is not difficult to see that the following expressions hold for the linear polyacene L_h:

$$W_2(\mathrm{L}_h) = \frac{2}{3}(8h^3 + 36h^2 + 31h + 6) \text{ and } W_3(\mathrm{L}_h) = \frac{2}{3}(8h^3 - 5h - 3)\,.$$

Using Proposition 2, $W_2(\mathrm{G}) - W_3(\mathrm{G}) = W_2(\mathrm{L}_h) - W_3(\mathrm{L}_h) = 6(4h^2 + 4h + 1)$. Therefore, $W(\mathrm{G}) = (W_2(\mathrm{G}) + W_3(\mathrm{G}))/2 = W_3(\mathrm{G}) + 3(4h^2 + 4h + 1)$. Since a catacondensed benzenoid graph has no internal vertices, Proposition 1 follows from the last equalities and equation (2).

BOUNDS FOR THE SCHULTZ INDEX

There are several estimates of MTI in terms of the Wiener index W for benzenoid graphs.[28,29] The best bounds for a benzenoid system G are as follows[29]

$$4W + \lambda_1 W^{2/3} + \lambda_2 W^{1/3} - 15 < MTI < 6W + \lambda_3 W^{2/5} - \lambda_4 W^{1/6}$$

where $\lambda_1 = 4.4...$, $\lambda_2 = 1.04...$, $\lambda_3 = 14.76...$ and $\lambda_4 = 17.73...$.

The linear polyacene L_h has the maximum Wiener index among all benzenoid graphs,[33] $W(\mathrm{L}_h) = \frac{1}{3}(16h^3 + 36h^2 + 26h + 3)$. Using Proposition 1, we can write $MTI(\mathrm{G}) \le MTI(\mathrm{L}_h) = 5W(\mathrm{L}_h) - (12h^2 - 14h + 5)$. This implies a general upper bound for the molecular topological index in terms of the number of rings of benzenoid graphs.

COROLLARY 1. Let G be an arbitrary benzenoid graph having h rings. Then,

$$MTI(\mathrm{G}) \le \frac{4}{3}h(20h^2 + 36h + 43)$$

where the equality sign holds for the linear polyacene L_h.

The lower bound of MTI will be presented for hexagonal chains. The helicene H_h has the minimum W among all isomeric hexagonal chains G (see Figure 1): $MTI(\mathrm{G}) \ge MTI(\mathrm{H}_h) = 5W(\mathrm{H}_h) - (12h^2 - 14h + 5)$, where $W(\mathrm{H}_h) = \frac{1}{3}(8h^3 + 72h^2 - 26h + 27)$.[33]

COROLLARY 2. Let G be an arbitrary hexagonal chain having h rings. Then,

$$MTI(\mathrm{G}) \geq \frac{4}{3}\,(10h^3 + 81h^2 - 22h + 30)\,,$$

where the equality sign holds for the helicene H_h.

Consider now hexagonal chains belonging to benzenoid systems. The serpent-graph S_h shown in Figure 1 has the minimum W among these graphs.[34] Namely, $W(\mathrm{S}_h) = \frac{1}{9}\,(32h^3 + 168h^2 + \phi(h))$, where $\phi(h) = -6h + 49$ if $h = 1,4,7,...$; $\phi(h) = -54h + 161$ if $h = 2,5,8,...$; and $\phi(h) = -6h + 81$ if $h = 3,6,9,...$.

COROLLARY 3. Let G be an arbitrary hexagonal chain among benzenoid systems having h rings. Then,

$$MTI(\mathrm{G}) \geq \frac{4}{9}\,(40h^3 + 183h^2 + \psi(h))\,,$$

where $\psi(h) = 24h + 50$ if $h = 1,4,7,...$; $\psi(h) = -36h + 190$ if $h = 2,5,8,...$; and $\psi(h) = 24h + 90$ if $h = 3,6,9,...$. The equality sign holds for the serpent-graph S_h.

Graphs of coronene / circumcoronene series have the minimum W among all benzenoid systems[29] (see graphs C_2 and C_3 in Figure 1). However, Proposition 1 is not valid for the graphs of this series.

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SAŽETAK

Eksplicitna relacija između Wienerova i Schultzova indeksa za katakondenzirane benzenoidne grafove

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Wienerov (W) i Schultzov (MTI) indeks temelje se na udaljenostima između čvorova (kemijskih) grafova. Pokazano je da je $MTI(\mathrm{G}) = 5\ W(\mathrm{G}) - (12h^2 - 14h + 5)$ za proizvoljni katakondenzirani benzenoidni graf G s h šesteročlanih prstenova.