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Computing PI and Szeged indices of multiple phenylenes and cyclic hexagonal–square chain consisting of mutually isomorphic hexagonal chains

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Abstract: PI and Szeged indices are two of the most important topological indices defined in chemistry. In this study, the PI and Szeged indices of linear [*n*]-phenylenes and a cyclic hexagonal-square chain consisting of *n* mutually isomorphic hexagonal chains were computed. The PI and Szeged indices of a multiple phenylene, which is the 2-dimensional case of a phenylenic nanotube and nanotorus, were determined.

Keywords: PI index, Szeged index, linear [*n*]-phenylenes, multiple phenylenes nanotube.

INTRODUCTION

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by $V(G)$ and $E(G)$, respectively. A topological index of a graph G is a numeric quantity related to G. The oldest topological index is the Wiener index. Numerous of its chemical applications have been reported and its mathematical properties are well understood.[1–4]

Khadikar and co-authors[5–9] defined a new topological index and named it the Padmakar–Ivan index. Here Padmakar comes from Padmakar Khadikar, and Ivan from Ivan Gutman. They abbreviated this new topological index as PI. This newly proposed topological index does not coincide with the Wiener index for acyclic molecules. It is defined as $PI(G) = \Sigma_{e\in G}[n_{eu}(e|G) + n_{ev}(e|G)]$, where $n_u(e|G)$ is the number of edges of G lying closer to u than to v and $n_v(e|G)$ is the number of edges of G lying closer to v than to u.

The Szeged index is another topological index which was introduced by Ivan Gutman.[10–13] To define the Szeged index of a graph G, it is assumed that $e = uv$ is an edge connecting the vertices u and v. Suppose $N_u(e|G)$ is the number of vertices of G lying closer to u and $N_v(e|G)$ is the number of vertices of G lying closer to v. Edges equidistance from u and v are not taken into account. Then the

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Szeged index of the graph G is defined as: $Sz(G) = \sum_{e = uv \in E(G)} N_u(e|G)N_v(e|G)$, see also Ref. 14.

The PI and Szeged indices of some hexagonal graphs containing nanotubes and nanotorus have been computed.[15–19] In this study, this work is continued with the computation of the PI and Szeged indices of some other important classes of chemical graphs. The notation is standard and mainly taken from the literature.[20,21]

RESULTS AND DISCUSSION

PI index of multiple phenylenes and cyclic hexagonal–square chains

In this section, the PI index of linear [n]-phenylenes, multiple phenylenes and a cyclic hexagonal–square chain consisting of n mutually isomorphic hexagonal chains are computed.[22,23] To do this, suppose that G is a graph, $e = uv \in E(G)$ and $N(e) = |E| - [n_{eu}(e|G) + n_{ev}(e|G)]$. Then $PI(G) = |E|^2 - \Sigma_{e \in E} N(e)$. Therefore, for computing the PI index of G, it is sufficient to calculate $N(e)$ for every $e \in E$.

Consider the molecular graph of a linear [n]-phenylene, Fig. 1. Then $|E(T)| = 6h + 2(h–1) = 8h – 2$ and, hence, $PI(T) = 64h^2 – 32h + 4 – \Sigma_{e \in E} N(e)$. To calculate $N(e)$, three cases are considered, *i.e.*, that e is vertical, horizontal or oblique. If e is horizontal or oblique, then $N(e) = 2$ and for vertical edges, one has $N(e) = 2h$. Thus, $PI(T) = 60h^2 – 44h + 8$.

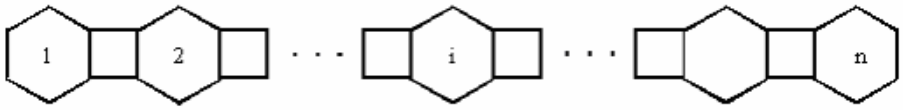

Fig. 1. The molecular graph of a linear [n]-phenylene.

Suppose $X_{m,n}$ is the chemical graph of a multiple phenylene, Fig. 2. Applying our method for computing $PI(X_{m,n})$, suppose $\alpha = \text{Min}\{m,n\}$. It is clear that $|E(X_{m,n})| = 2m(3n–1)$ and, hence, one obtains:

$$\sum_{e \in E(X_{m,n})} N(e) = \sum_{e \text{ is horizontal}} N(e) + \sum_{e \text{ is oblique}} N(e) + \sum_{e \text{ is vertical}} N(e) =$$

$$= 2\left\{ \sum_{i=0}^{\alpha-2} 2(2+2i)^2 + 4\alpha^2(|m-n|+1) \right\} + 4m^2(n-1) + 4n^2m = \frac{8}{3}\alpha + 8\alpha^2 + \frac{16}{3}\alpha^3 +$$

$$+ 16\alpha^2|m-n| + 4m^2n - 4m^2 + 4n^2m$$

Therefore, $PI(X_{m,n}) = 36m^2n^2 – 28m^2n + 8m^2 – 8/3\alpha – 8\alpha^2 – 16/3\alpha^3 – 16\alpha^2|m–n| – 4n^2m$.

Let $C_{m,n}$ denote the molecular graph of a cyclic hexagonal-square chain consisting of n mutually isomorphic hexagonal chains H_1, H_2,…, H_n, cyclically concatenated by circuits α_i of length 4, in which the H_is are chains containing m hexagons, Fig. 3. Some exact formulas for the algebraic structure count (ASC) of the linear [n]-phenylene, Fig. 1, the multiple phenylenes, Fig. 2 and the molecu-

lar graph of $C_{m,n}$, Fig. 3 were computed.[20,21] At the end of this section, PI($C_{m,n}$) is computed.

Obviously, $|E(C_{m,n})| = n(5m+3)$. Hence, one obtains:

$$\mathrm{PI}(C_{m,n}) = n^2(5m+3)^2 - \sum_{e\in E(C_{m,n})} N(e) = n^2(5m+3)^2 - \sum_{e \text{ is horizontal}} N(e) +$$

$$+ \sum_{e \text{ is oblique}} N(e) + \sum_{e \text{ is vertical}} N(e) = 25m^2n^2 + 9n^2 + 30mn^2 - 33n - nm^2 - 66mn.$$

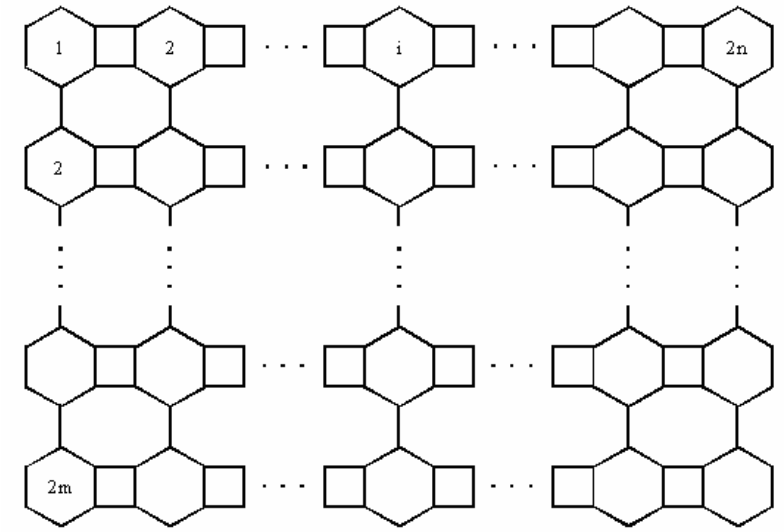

Fig. 2. The molecular graph of a multiple phenylene.

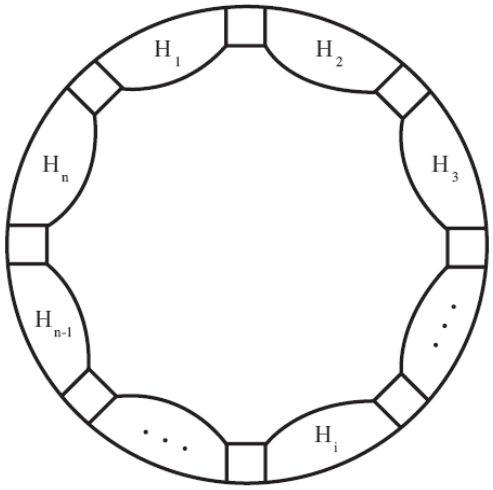

Fig. 3. The molecular graph of a cyclic hexagonal-square chain $C_{m,n}$.

Szeged index of multiple phenylenes and cyclic hexagonal-square chains

In the literature, there is a paper by Diudea in which the Szeged index is tested in QSPR.[24] In this paper, the use of the Szeged index and several other

distance-based indices on the correlation with the boiling points of 45 cycloalkanes were examined. Moreover, Khadikar *et al*.[25] described various applications of the Szeged index for modeling physicochemical properties, as well as the physiological activities of organic compounds acting as drugs or possessing pharmacological activity. The authors of this paper reviewed 175 papers published on the subject of the Szeged index. This shows that the subject of the Szeged index is growing more and more in chemistry, physics and also biology.

In this section, the Szeged index of the linear [n]-phenylene $X_{1,n}$, the multiple phenylene $X_{m,n}$ and $C_{m,n}$ were computed. First it should be noticed that $v_1 = |V(X_{1,n})| = 6n$, $v_2 = |V(X_{m,n})| = 6mn$ and $v_3 = |V(C_{m,n})| = 4mn+2n$. The Szeged index of $X_{1,n}$ was first calculated. To do this, it was assumed that A, B and C to be the set of all vertical, oblique and horizontal edges, respectively. Then one obtains:

$$\mathrm{Sz}(X_{1,n}) = \sum_{e\in E} N_u(e)N_v(e) = \sum_{e\in A} N_u(e)N_v(e) + \sum_{e\in B} N_u(e)N_v(e) + \sum_{e\in C} N_u(e)N_v(e) =$$

$$= \sum_{i=0}^{n-1} 2\{(3+6i)(6n-6i-3)\} + 18n^3 + \sum_{i=1}^{n-1}(12i) = 30n^3 + 6n^2$$

Then the Szeged index of a multiple phenylene $X_{m,n}$ was calculated. Similarly,

$$\mathrm{Sz}(X_{m,n}) = \sum_{e\in E} N_u(e)N_v(e) = \sum_{e\in A} N_u(e)N_v(e) + \sum_{e\in B} N_u(e)N_v(e) + \sum_{e\in C} N_u(e)N_v(e) =$$

$$= \sum_{i=1}^{n-1} \{(6mi)(6nm-6mi)(2m)\} + \sum_{i=1}^{2m-1}\{(3ni)(6nm-6ni)(2n)\} + \sum_{e\in B} N_u(e)N_v(e).$$

To compute the last summation, it was supposed that $U = \sum_{e\in B} N_u(e)N_v(e)$ and two separate cases were considered, as follows:

Case 1: $m \neq n$. In this case one obtains:

$$U = \sum_{i=1}^{|m-n|-1}\{(2\beta)(S_\beta + (6\beta-3)i))(6mn - S_\beta - (6\beta-3)i\},$$

where $S_i = 3+9+15+\ldots+(6i-3)$ and $\beta = \min(m,n)$. Hence, the Szeged index of $X_{m,n}$ is equal to $9\beta^2nm-18n+9mn\beta+18mn\beta^3+3/2\beta^2-15/2\beta^4-9\beta^5-3\beta^6+72n^2+72n^3m-$ $-36mn^2+36mn^4-72n^4-36n^3-18n^5$.

Case 2: $m = n$. In this case one has $U = 2n(S_n+6n-3)(6nm-S_n-6n+3)$ and hence the Szeged index of $X_{m,n}$ is equal to $6n^6+27n^5+3/2n^4-72n^3+147/2n^2-18n$.

In the end of this section, the Szeged index of $C_{m,n}$ is computed. Obviously, $v_3 = |V(C_{m,n})| = 2n(2m+1)$. If A, B and C are set as before, then

$$\mathrm{Sz}(C_{m,n}) = \sum_{e\in E} N_u(e)N_v(e) = \sum_{e\in A} N_u(e)N_v(e) + \sum_{e\in B} N_u(e)N_v(e) +$$

$$\sum_{e\in C} N_u(e)N_v(e) = n(m+1)(2m+1)(v_3)(2m-1) + 2n(v_3/2)(v_3/2) +$$

$$+ 4mn(v_3/2)(v_3/2) = 16m^2n^2 + 8m^3n^2 - 4nm^2 + 10mn^2 - 5mn + 2n^2 - n +$$

$$+ 24m^2n^3 + 16m^3n^3 + 12mn^3 + 2n^3.$$

И З В О Д

ИЗРАЧУНАВАЊЕ PI И SZEGED ИНДЕКСА ВИШЕСТРУКИХ ФЕНИЛЕНА И ЦИКЛИЧНОГ ХЕКСАГОНАЛНО–КВАДРАТНОГ ЛАНЦА САЧИЊЕНОГ ОД МЕЂУСОБНО ИЗОМОРФНИХ ХЕКСАГОНАЛНИХ ЛАНАЦА

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PI и Szeged индекси су два најважнија тополошка индекса дефинисана у хемији. У овом раду су израчунати PI и Szeged индекси линеарних [*n*]-фенилена и цикличног хексагонално–квадратног ланца сачињеног од *n* међусобно изоморфних хексагоналних ланаца. Одређени су PI и Szeged индекси вишеструког фенилена, као дводимензионог облика фениленских наноцеви и нанопрстена.

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