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Computing Topological Indices of Some Types of Benzenoid Systems and Nanostars

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The PI and Szeged are two of most important topological indices defined in chemistry. In this paper, we compute the PI and Szeged indices of some important classes of benzenoid systems and nanostars. Some open questions are also included in the paper.

Key Words: Nanostar, PI index, Szeged index, benzenoid systems, Topological index.

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 were reported and its mathematical properties are well understood[1-4]. We encourage the reader to consult two survey articles by Dobrynin and co-authors[5,6] and references therein for a good information on the topic.

Khadikar and co-authors[7-10] defined a new topological index and named it Padmakar-Ivan index. 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 $PI(G) = \sum_{e\in G}[n_{eu}(e|G) + n_{ev}(e|G)]$, 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 is introduced by Ivan Gutman[11-13]. To define the Szeged index of a graph G, we assume 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 Szeged index of the graph G is defined as $Sz(G) = \sum_{e = uv\in E(G)} N_u(e|G)N_v(e|G)$.

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We now describe some notations which will be kept throughout. Benzenoid systems (graph representations of benzenoid hydrocarbons) are defined as finite connected plane graphs with no cut-vertices, in which all interior regions are mutually congruent regular hexagons. More details on this important class of molecular graphs can be found in the book of Gutman and Cyvin[14] and in the references cited therein.

In this paper we only consider connected graphs. Our notation is standard and mainly taken from work of previous authors[2,14-16].

PI and Szeged indices of some nanostars and benzenoid graphs

In this section we compute some topological indices of two types of nanostars and benzenoid graphs. To do this, we assume that $N(e) = |E| - (n_{eu}(e|G) + n_{ev}(e|G))$. Then $PI(G) = |E|^2 - S_{e\in E} N(e) \rightarrow PI(G) = |E|^2 - \Sigma_{e\in E} N(e)$. Therefore, for computing the PI index of G, it is enough to calculate N(e), for every $e \in E$.

PI and Szeged indices of $K^{n,n}$ Hexagonal system: Shiu *et al.*[17], the authors defined a new hexagonal system named jagged-rectangle. An $n \times m$ hexagonal jagged-rectangle whose shape forms a rectangle and the number of hexagonal cells in each chain alternate between n and n-1. Yousefi *et al.*[18] computed the PI and Szeged indices of two types of hexagonal jagged-rectangle, $I^{n,(n+1)/2}$ and $J^{n,n/2}$. We continue this program to compute the PI and Szeged indices of a $K^{n,n}$, $n \geq 2$, defined as $V(K^{n,m}) = \{(x,y) \mid 0 \leq x \leq 2n, 0 \leq y \leq 2m-1\} \cup \{(x,-1) \mid 0 \leq x \leq 2n-1\} \cup \{(x,2m) \mid 1 \leq x \leq 2n-1\}$.

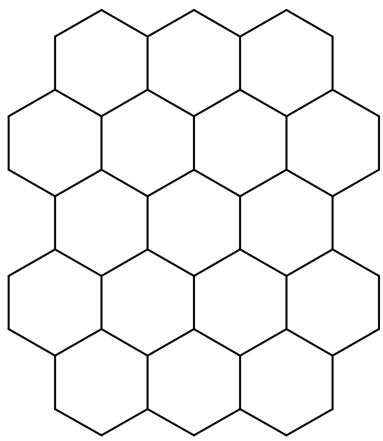

Fig. 1. The Graph $K^{4,2}$

One can see that $K^{n,n}$ has exactly $m = |E(K^{n,n})| = 2(n+1)(n-1) + 2n(2n+1) = 6n^2 + 2n - 2$ and also $v = |V(K^{n,n})| = n(2n+1)+(n+1)(2n-1) = 4n^2 + 2n - 1$. To compute PI index of this chemical graph, we consider two types of edges, vertical and oblique. At first, we assume that A is the set of all vertical edges of this graph and $e \in A$. If e is an edge of the 1s, 3rd, …, (n+1)th row of the graph then N(e) = n and also, N(e) = n+1, otherwise. Therefore, $S_{e\in A}N(e) = n\sum_{i=1}^{n}(n+1)^2 + (n+1)\sum_{i=1}^{n+1}n^2 = 2n^4 + 4n^3 + 2n^2$. There are two types of oblique edges, left and right. For the symmetry of the graph, it is enough to compute $S_{e\in B}N(e)$, where B is the set of all left oblique edges $K^{n,n}$. Then $PI(K^{n,n}) = |E|^2 - [2n^4 + 4n^3 + 2n^2 + 2\Sigma_{e\in B}N(e)]$. But

$$\sum_{e\in B}N(e) = 2\sum_{i=0}^{n-2}(3+2i)^2 + 4n^2 = 214/3n - 50 - 20n^2 + 8/3n^3,$$

and so $PI(K^{n,n}) = 34n^4 + 52/3n^3 - 2n^2 - 238/3n + 54$. We now compute the Szeged index of this graph. To do this, we assume that $a_i = (2n-1)(i+1) + i(2n+1)$, $b_i = (2n+1)i + i(2n-1)$ and $S_i = \sum_{k=1}^{i}(4k+1)$. Then we have:

$Sz(G) = \sum_{e=uv\in E(G)} Nu(e|G)N_v(e|G)$

$= \sum_{e=uv\in A} N_u(e|G)N_v(e|G) + 2\sum_{e=uv\in B} Nu(e|G)N_v(e|G)$

$$= \left(\sum_{i=0}^{n-1}na_i(v-a_i) + \sum_{i=1}^{n-1}(n+1)b_i(v-b)\right) + 2\sum_{i=0}^{n-2}[(2i+3)S_i(v-S_i)]$$

$$+ 2\left(n(S_{n-2}+4n)(v-S_{n-2}-4n) + n(S_{n-2}+8n)(v-S_{n-2}-8n\right)$$

$= 16/3n^6 - 32/5n^5 + 25/3n^4 + 9n^3 - 38/3n^2 - 48/5n$

PI and Szeged indices of $T^{b,a}$ Hexagonal system: A hexagonal trapezoid $T = T^{b,a}$ is a hexagonal system consisting a-b+1 rows of benzenoid chain in which every row has exactly one hexagon less than the immediate row, Fig. 2.

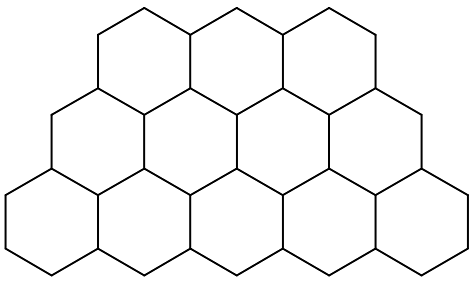

Fig. 2. The Graph $T^{3,5}$

In this section, the PI and Szeged indices of a hexagonal trapezoid $T = T^{b,a}$ is computed. It is easy to see that $|E(T)| = 3/2a^2 - 3/2b^2 + 5/2a - 1/2b$ and $v = |V(T)| = -b^2 + a^2 + 2a + 1$. Similar to our calculations as above, we consider two separate classes A and B of vertical and oblique edges, respectively. We have:

$$\sum_{e\in A} N(e) = \sum_{i=0}^{a-b} (b+i+1)^2$$

$= ab^2 – 2ab + 13/6a – 1/3b^3 – 1/2b^2 – 13/6b + 4/3a^3 - 2a^2b + 5/2a^2 + a^3b – 3a^2b^2 + 3ab^3 – b^4$,

$$\sum_{e\in A} N(e) = 2\sum_{i=0}^{a-b-1} (2+i)^2 + 2b(a-b+2)$$

$= 7/6b^2 – 23/6b + 35/6a – 4 + 13/6a^2 – 13/3ab + 1/3a^3 – a^2b + ab^2 – 1/3b^3$

Therefore, $PI(T) = |E(T)|^2 – \Sigma_{e\in A}N(e) – \Sigma_{e\in B}N(e) = 9/4a^4 – 9/2a^2b^2 + 41/6a^3 + 1/2a^2b + 9/4b^4 – 19/2b^2a + 13/6b^3 + 13/4a^2 + 3/2ab – 3/4b^2 – 13/3a + 1/3b – a$. To compute the Szeged index of this graph, assume that A is the set of all vertical edges of this graph and $e \in A$. If $e = uv$ is an edge of the ith row of the graph then $N_u(e|T)N_v(e|T) = (2b + 2i + 1)(v – 2b – 2i – 1)$ and so $\Sigma_{e=uv\in A} N_u(e|T)N_v(e|T) = 2/3a^5 + 4/3b^2a^3 + 13/6a^4 – 2b^3a^2 + 19/6a^3 – 9ab^3 – 2ab^4 + 7ba^2 – 5/2a^2b^2 + 13/6b^2a + 2ba^4 + 4/3a^2 + 13/3ba + 11/3ba^3 – 1/3a$. We now consider oblique edges of T. Using a similar calculation as above, we can see that

$$\sum_{e=i/v\in B} N_u(e|T)N_v(e|T) = 2\left(\sum_{i=0}^{a-b}[(2+i)S_i(v-S_i)] + (a-b+2)\sum_{i=1}^{a-b-1}[T_i(v-T_i)]\right),$$

in which $S_i = \sum_{k=0}^{i}(2k+3)$ and $T_i = S_{a-b} + 2i(a – b + 2)$. Now a tedious calculation shows that $Sz(T) = –36 + 108b – 84a – 391/3b^2 – 39b4a – 158/3a^2 + 183ab + 32/3b^5 + 166/3b^3a^2 + 673/6a^2b – 1205/6ab^2 + 109/3a^3b – 125a^2b^2 + 125ab^3 + 6a^4b + 5/3a^5 – 31/6a^3 + 563/6b^3 + 5a^4 – 124/3b^4 –104/3a^3b^2 + 1/6a^6 – 5/2a^4b^2 + 20/3a^3b^3 – 15/2a^2b^4 – 5/6b^6 + 4ab^5$.

PI Indices of two types of Nanostars: The subject of Nanostar is one of the main topics of Nanobiotechnology. In recent years, the Nanostar, a phenylacetylene dendrimer, has attracted attention due to its potential applications[19-23]. The Nanostar absorbs ultraviolet photons at its terminal groups and the energy transfers from the periphery to the core where it is collected with 99 % efficiency and then it is emitted in the visible range. This energy transfer process is in the order of picoseconds. Due to its localized excitations, the Nanostar was studied as the sum of separate units, which are 24 two-ring systems, 4 three-ring systems, 2 four-ring systems and a core. The aim of this section is computing the PI index of two types of Nanostars I and II, Figs. 3 and 4.

Suppose $G = G(n,k)$ is the graph of a Nanostar of type I. From Fig. 3, we can see that if e is an edge of a hexagon of G then $N(e) = 2$, otherwise $N(e) = 1$. We assume that A is the set of all hexagons, B is the set of all edges outside A, $a = |A|$ and $b = |B|$. We calculate that $a = 1 + 2n + 2^2(n–1) + 2^3(n–2) + \ldots + 2^{k+1}(n–k) + 2^{k+1}$ and $b = a–1+2^{k+2}$. Therefore, $\Sigma_{e\in A}N(e) = 12a$ and $\Sigma_{e\in B}N(e) = b$. Hence $PI(G) = |E(G)|^2 – \Sigma_{e\in A}N(e) – \Sigma_{e\in B}N(e) = 36a^2$

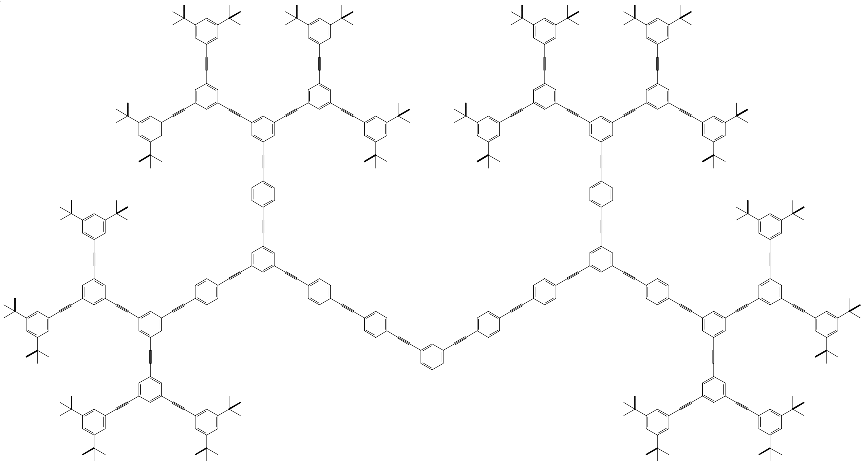

Fig. 3. A Nanostar of Type I, with n = 3 and k = 1

$+ b^2 + 12ab - 12a-b$. We now compute the PI index of the Nanostar H = H(n,k) of type II, Fig. 4. A similar argument as above, shows that if e is an edge of a hexagon of H then N(e) = 2, otherwise N(e) = 1. Suppose A, B, a and b are defined as above. Then $a = 1 + k(1+2 + 2^2 + \ldots + 2^n) = 1 + k(2^{n+1} - 1)$ and $b = a - 1$. Therefore, $\Sigma_{e\in A}N(e) = 12a$ and $\Sigma_{e\in B}N(e) = b$. Hence $PI(G) = |E(G)|^2 - \Sigma_{e\in A}N(e) - \Sigma_{e\in B}N(e) = 36a^2 + b^2 + 12ab - 12a-b$.

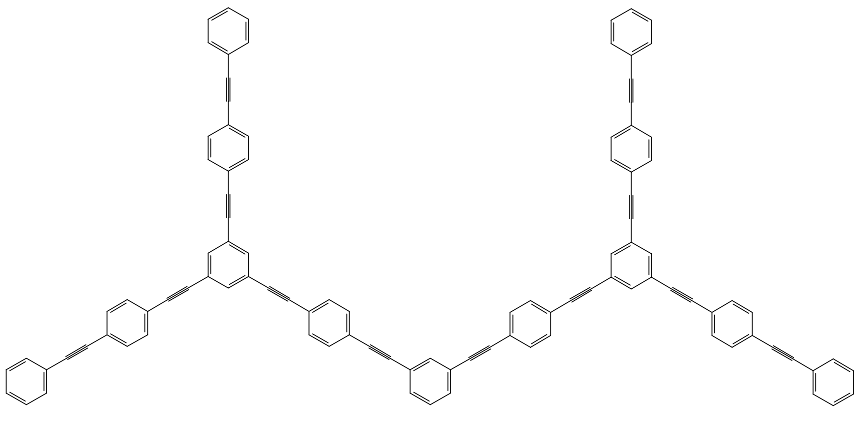

Fig. 4. A Nanostar of Type II, with n = 3 and k = 1

Conclusion

At the end, the two questions are arised: (1) Is there a simple closed formula for the Szeged indices of a Nanostar of types I and II? (2) Is it true that for every positive integer n, there exists a Nanostar T with this condition that PI(T) = n or Sz(T) = n?

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