The Edge Szeged Index of One–Pentagonal Carbon Nanocones

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Abstract
The edge Szeged index is a new molecular structure descriptor equal to the sum of products $m_u(e)m_v(e)$ over all edges $e = uv$ of the molecular graph G, where $m_u(e)$ is the number of edges which its distance to vertex u is smaller than the distance to vertex v, and $n_v(e)$ is defined analogously. In this paper, the edge Szeged index of one-pentagonal carbon nanocone $CNC_5[n]$ is computed for the first time.
Keywords: *Nanocone, edge Szeged index, molecular graph.*

1. INTRODUCTION

Carbon nanocones have originally been discovered by Ge and Sattler in 1994 [1]. These are constructed from a graphene sheet by removing a 60° wedge and joining the edges produces a cone with a single pentagonal defect at the apex, Fig.1 Removing additional wedges introduces more such defects reduces the opening angle. A cone with six pentagons has an opening angle of zero and is just a nanotube with one open end.

Topological indices are graph invariants and are used for Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies [2-5]. Many topological indices have been defined and several of them have found applications as means to model physical, chemical, pharmaceutical and other properties of molecules [6,7].

Now some algebraic definitions are recalled that will be used in the paper. Let G be a simple molecular graph without direct 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 which was introduced by Harold wiener [8].

The Szeged index is another topological index which was introduced by Ivan Gutman [9]. To define the Szeged index of a graph G, it was assumed that e = uv is an edge connecting the vertices u and v. Suppose $n_u(e)$ is the number of vertices of G lying closer to u and $n_v(e)$ is the number of vertices of G lying closer to v. Then the Szeged index of the molecular graph G is defined as $Sz(G) = \sum_{e=uv \in E(G)} n_u(e)n_v(e)$. Notice that vertices equidistance from u and v are not taken into account. Motivated by the success of the Szeged index, Khadikar proposed a seemingly similar molecular structure descriptor named PI index [10].

This index is defined as $PI(G) = \sum_{e=uv} [m_u(e) +$

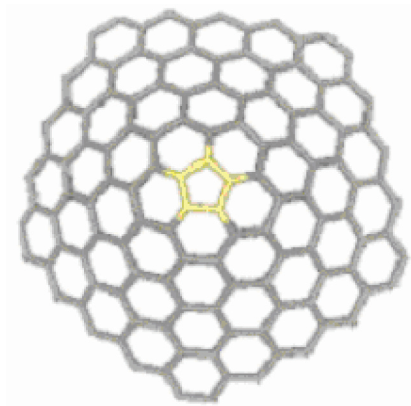

Figure 1: The Nanocone T = CNC_5 [4].

$m_v(e)$], where $m_u(e)$ is the number of edges of G which its distance to the vertex u is smaller than the distance to the vertex v and $m_v(e)$ is the number of edges of G which its distance to the vertex v is smaller than the distance to the vertex u. Note that edges equidistant to u and v are not counted. It was called such edges to be parallel to e = uv. For the theory and applications of the PI index see the papers [11-20] and the references are quoted therein.

The first author of this paper in a joint work continued this process to define an edge version of Szeged index [21]. This new index is defined as $Sz_e(G) = \sum_{e=uv} m_u(e)m_v(e)$, where $m_u(e)$ and $m_v(e)$ are defined as above. The aim of this paper is to continue this work to compute the edge Szeged index of a one-pentagonal carbon nanocone. Throughout this paper, our notation is standard and taken from the standard books of graph theory.

2. MAIN RESULTS

In this section, the edge Szeged index of the molecular graph S = CNC_5 [n] was computed. The number of edge parallel to a given edge e is denoted by N(e). this work was begun with computing the number of edges of S.

Lemma 1. $|E(S)| = (5/2)(3n^2 + 5n + 2)$.

Proof. Suppose λ_n denotes the number of edges in the boundary of S = CNC_5 [n]. Then $\lambda_n = \lambda_{n-1} + 10$ and so $\lambda_n = 5 + 10n$. On the other hand, there are 5n edges such that connect the boundary of CNC_5 [n] to the boundary of CNC_5 [n-1].

Thus $|E(CNC_5[n])| = \lambda_n + 5n + |E(CNC_5[n-1])| = 5 + 15n + |E(CNC_5[n-1])|$. Define $x_n = |E(CNC_5[n])|$ to find the recurrence equation $x_n = 5 + 15n + x_{n-1}$. But this is a linear recurrence relation and there are several well-known methods to solve such equations. Therefore, $x_n = |E(S)| = (5/2)(3n^2 + 5n + 2)$.

Two edges e = xy and f = uv of a graph G are side to be codistant[17] if and only if d(x,u) = d(y,v), d(x,v) = d(y,u) and |d(x,u) – d(x,v)| = 1. By Fig.1, every edge of central pentagonal is equidistant to n+1 edges of S = CNC_5 [n]. Suppose σ_1, σ_2, σ_3, σ_4 and σ_5 are edges of the central pentagon and $\overline{\sigma}_1, \overline{\sigma}_2, \overline{\sigma}_3, \overline{\sigma}_4$ and $\overline{\sigma}_5$ are their equidistant edges in the boundary of S, respectively. In the boundary of S, there are 2n edges between $\overline{\sigma}_i$ and $\overline{\sigma}_{i+1}$, $1 \le i \le 4$, as well as $\overline{\sigma}_5$ and $\overline{\sigma}_1$. These 2n edges in a fixed region is denoted with $e_1 = x_1x_2, e_2 = x_2x_3, \dots, e_{2n} = x_{2n}x_{2n+1}$. This property exists that $N(e_1) = N(e_{2n})$, $N(e_2) = N(e_{2n-1})$, …, $N(e_n) = N(e_{n+1})$ and so it is enough to compute $N(e_1), N(e_3), \dots, N(e_{2n-1})$.

Lemma 2. Suppose $\overline{\sigma}_i = a_ib_i$, $1 \le i \le 5$, then $N(\overline{\sigma}_i) = (3/2)n^2 + (5/2)n + 1$ and so $m_{a_i}(\overline{\sigma}_i) = m_{b_i}(\overline{\sigma}_i) = 3n^2 + 5n + 2$.

Proof. From the graph of S = CNC_5[n], Figure 2(a), it can be seen that there are n+1 edges

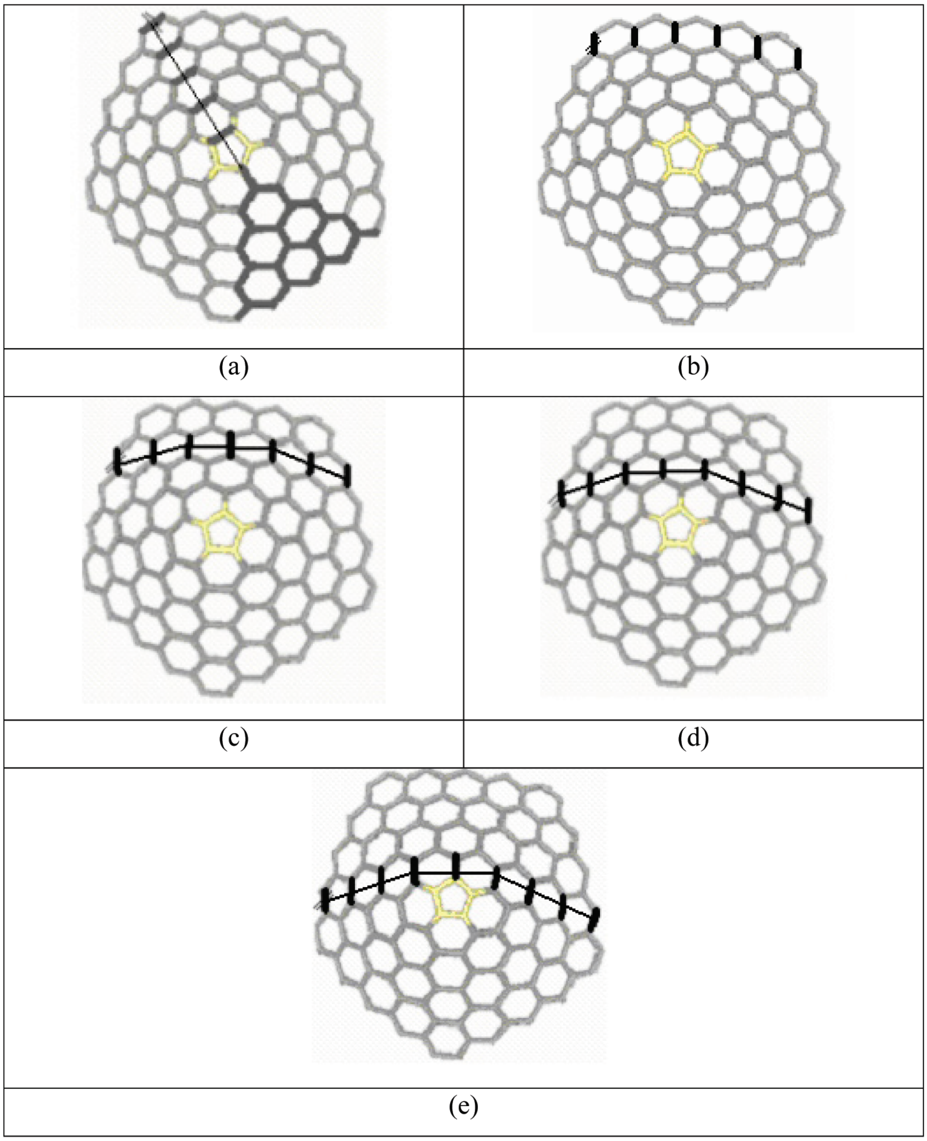

Figure 2: Five Cases of Parallel Edges with a Fixed Edge in CNC_5 [4].

which are codistant to $\overline{\sigma_i}$. On the other hand there are $3/2(n^2 + n)$ edges in the triangle region of S which are codistant to $\overline{\sigma_i}$. Therefore,

$$m_{a_i}(\overline{\sigma_i}) = m_{b_i}(\overline{\sigma_i}) = \frac{1}{2}\left(|E(S)| - \frac{3}{2}n^2 - \frac{5}{2}n - 1\right) = 3n^2 + 5n + 2$$

Lemma 3. $N(e_{2j-1}) = n+j+1$, $1 \leq j \leq n$.
Proof. It follows from the molecular graph of S = $CNC_5[n]$, Figure 2(b-d).

By orthogonal cut method of John, Khadikar and Singh [7], one can see that all of edges parallel to e_{2j-1} are codistant edges of e_{2j-1}, for $1 \leq j \leq n$.
The main results of this paper are as below:

Theorem 1. The edge Szeged index of a one pentagonal carbon nanocone is computed as follows:

$$S_e(S) = \frac{1215}{6}n^6 + \frac{5263}{6}n^5 + \frac{28595}{8}n^4 + \frac{28295}{8}n^3 + \frac{1045}{3}n^2 + \frac{1459}{2}n + 2$$

Proof. At first $m_{x_{2j-1}}(e_{2j-1})$ and $m_{x_{2j}}(e_{2j-1})$, $1 \leq j \leq n$ was computed.

By Lemma 3 and Figure 2, $m_{x_{2j}}(e_{2j-1})$ + $m_{x_{2j-1}}(e_{2j-1})$ + n + j + 1 = |E(S)|. So by Lemma 1, it is enough to compute $m_{x_{2j-1}}(e_{2j-1})$. On the other hand, by Figure 2, one can see $m_{x_1}(e_1) = 2n+2$, $m_{x_3}(e_3) = m_{x_1}(e_1) + (n+2) + (2n+4)$ and similarly for every j, 1≤ j ≤ n, and

$$m_{x_{2j+1}}(e_{2j-1}) = \frac{3}{2} j^2 + (3n + 3/2) j - (n-1).$$

$$m_{x_{2j+1}}(e_{2j-1}) = \frac{5}{2}(3n^2 + 5n + 2) - \frac{3}{2} j^2 - (3n + 5/2) j$$

Therefore,

$$Sz_e(S) = 5\sum_{j=1}^{n}(n+j+1)\left[\frac{3}{2}j^2 + (3n+3/2)j - n - 1\right]\left[|E(S)| - \frac{3}{2}j^2 + (3n+5/2)j\right]$$
$$+\frac{5}{4}(n+1)\left(|E(S)| - (n+1) - \frac{3}{2}(n^2+n)\right)^2$$
$$= \frac{1215}{6}n^6 + \frac{5263}{6}n^5 + \frac{28595}{8}n^4 + \frac{28295}{8}n^3 + \frac{1045}{3}n^2 + \frac{1459}{2}n + 2\ .$$

This completes all obtained theorem.

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