

The PI and edge Szeged indices of $CNC_3[n]$ and $CNC_4[n]$ carbon nanocones

ALI REZA ASHRAFI*, FARZANEH GHOLAMI-NEZHAAD

Institute of Nano Science and Nano Technology, University of Kashan, Kashan 87317-51167, I. R. Iran

Suppose $CNC_3[n]$ and $CNC_4[n]$ are carbon nanocone with a unique, triangle and square, respectively. These new nanomaterials introduced recently by Diudea. In this paper, the PI and edge Szeged indices of these nanocones are computed.

(Received February 19, 2010; accepted April 11, 2010)

Keywords: Carbon nanocone, PI index, Szeged index

1. Introduction

In the past years, nanostructures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications. One pentagonal carbon nanocones originally 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. If a 120° wedge is considered then a cone with a single square defect at the apex is obtained. The case of 240° wedge yields a single triangle defect at the apex, see [2] for details.

A topological index is a graphic invariant used in structure—property correlations. Between topological indices those are defined by distance function $d(-, -)$ is called distance based topological index. Here for arbitrary vertices x and y , the distance $d(x, y)$ is defined as the length of a minimal path connecting x and y . The Wiener index [3] is the first distance based topological index. It is defined as the sum of all distances between vertices of G . Diudea and his co-workers [4,5] computed the Wiener index of armchair and zig-zag polyhex nanotubes. After publishing these papers, one of us (ARA) began the problem of computing some other distance-based topological indices of nanostructures containing PI and edge Szeged [6-11].

The Padmakar-Ivan (PI) index was introduced by Padmakar Khadikar [12]. By the best of our knowledge, it is the first topological index related to distances between edges of the graph under consideration. To explain, we assume that G is a graph and $e = uv$ is an edge of G . Define $m_u(e)$ to be the number of edges of G lying closer to u than to v and $m_v(e)$ is the number of edges of G lying closer to v than to u . Edges equidistant from both of ends of the edge uv are not counted. It is defined as $PI(G) = \sum_{e=uv} [m_u(e) + m_v(e)]$. The edge Szeged index is a recently defined topological index [13]. It is an edge version of another topological index introduced by Ivan Gutman

[14]. The edge Szeged index of G is defined as $Sz_e(G) = \sum_{e=uv} [m_u(e) \cdot m_v(e)]$.

Suppose G is a graph, x is a vertex of G and $e = uv$, $f = ab$ are edges of G . Define $d(x, e) = \min\{d(x, u), d(x, v)\}$. The edge e is said to be parallel to f , write $e \parallel f$, if $d(a, e) = d(b, e)$. It is easy to see that the parallelism is reflexiv, but no symmetric or transitive. If G is bipartite then the parallelism well be symmetric. Throughout this paper our notation is standard and taken mainly from the standard book of graph theory.

2. Main results and discussion

In this section the PI and edge Szeged indices of carbon nanocones $S_3 = CNC_3[n]$ and $S_4 = CNC_4[n]$ were computed. In Figs. 1 and 2, you can see the pictures of these two nanocones which were drawn by Hyperchem software. The number of layers of the graph is n and the number of edges parallel to a given edge $e = uv$ is denoted by $N(e)$.

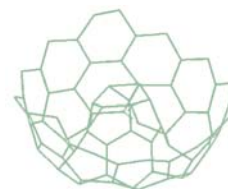


Fig. 1. The Carbon nanocone $CNC_3[4]$.

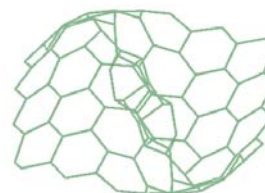


Fig. 2. The carbon nanocone $CNC_4[4]$.

Lemma 1. $|E(S_3)| = \frac{3}{2}(3n^2 + 5n + 2)$ and $|E(S_4)| = 6n^2 + 10n + 4$.

There are two types of edges in the molecular graphs of S_3 and S_4 : One type of edges is those that are parallel to every edge of central apex. Suppose α_i , $1 \leq i \leq 3$, is the edge of central apex in S_3 , and γ_i , $1 \leq i \leq 4$, denotes every edge of central apex in S_4 , and β_i are their equidistant edges in the boundary of S_p , $p = 3, 4$, respectively. In Fig. 3 and Fig. 4, the parallel edges of β_i are drawn by green color.

Lemma 2. Suppose $S_3 = CNC_3[n]$ and $\beta_i = a_i b_i$, $1 \leq i \leq 3$. Then $N(\beta_i) = (1/2)(3n^2 + 7n + 10)$ and so $m_{a_i}(\beta_i) = m_{b_i}(\beta_i) = (1/2)(3n^2 + 11n - 2)$.

Lemma 3. Suppose $S_4 = CNC_4[n]$ and $\beta_i = a_i b_i$, $1 \leq i \leq 4$. Then $N(\beta_i) = 2n + 2$ and $m_{a_i}(\beta_i) = m_{b_i}(\beta_i) = 3n^2 + 4n + 1$.

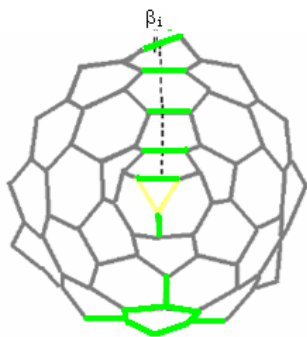


Fig. 3. The parallel edges in $CNC_3[4]$.

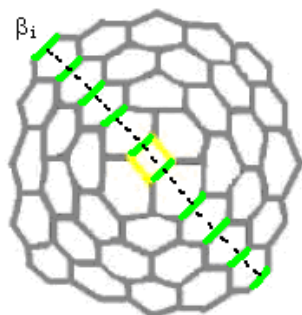


Fig. 4. The parallel edges in $CNC_4[4]$.

Another type of edges are $2n$ edges which are located between every β_i and β_{i+1} . We denote these $2n$ edges in a fixed region with $e_1 = x_1 x_2$, $e_2 = x_2 x_3$, ..., $e_{2n} = x_{2n} x_{2n+1}$. These are having this property 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 $N(e_{2j-1})$, for $1 \leq j \leq n$.

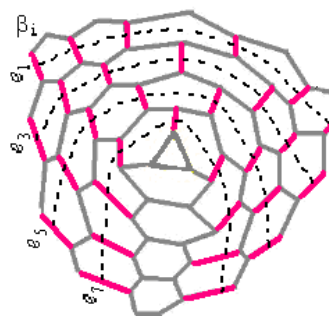


Fig. 5. The parallel edges to e_{2j-1} .

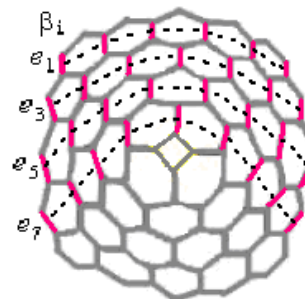


Fig. 6. The parallel edges to e_{2j-1} .

Lemma 4. In both of S_3 and S_4 , $N(e_{2j-1}) = n + j + 1$, $1 \leq j \leq n$. The parallel edges to every e_{2j-1} , were denoted by red color in Figs. 5 and 6.

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

Proof. By Figs. 5 and 6, one can see that the sequence $m_{x_{2j-1}}$ (in both of S_3 and S_4) is satisfied the recurrence relation $m_{x_{2j+1}}(e_{2j+1}) = m_{x_{2j-1}}(e_{2j-1}) + N(e_{2j-1}) + 2(n + j + 1)$ with $m_{x_1}(e_1) = 2n + 2$ as its initial value. By solving this relation the proof will be completed. On the other hand $m_{x_{2j-1}}(e_{2j-1}) + m_{x_{2j}}(e_{2j-1}) + N(e_{2j-1}) = |E(S_p)|$, so by substituting the obtained values, we can compute $m_{x_{2j}}(e_{2j-1})$ for every S_p .

Theorem 1. The edge Szeged index of $S_3 = CNC_3[n]$ is as follows:

$$Sz_e(S_3) = \frac{243}{16}n^6 + \frac{5619}{80}n^5 + \frac{2545}{16}n^4 + \frac{3349}{16}n^3 + \frac{299}{4}n^2 - \frac{551}{20}n + 3.$$

Proof. By substituting the values of pervious lemmas in edge Szeged formula and considering the number of choices of any β_i or e_{2j-1} , we have

$$\begin{aligned}
Sz_e(S_3) &= \sum_{e=uv \in E(S_3)} m_u(e) \cdot m_v(e) \\
&= \sum_{i=1}^3 [m_{a_i}(\beta_1) \cdot m_{b_i}(\beta_1) \cdot (n+1)] \\
&\quad + \sum_{i=1}^3 \left[\sum_{j=1}^n m_{x_{2j-1}}(e_{2j-1}) \cdot m_{x_{2j}}(e_{2j-1}) \cdot (n+j+1) \right] \\
&= 3 \left(\frac{1}{4} (3n^2 + 11n - 2) \cdot (n+1) \right) \\
&\quad + 3 \sum_{j=1}^n \left(\frac{3}{2} j^2 + (3n + \frac{3}{2})j - n - 1 \right) \\
&\quad \times \left(\frac{3}{2} (3n^2 + 5n + 2) - \frac{3}{2} j^2 - (3n + \frac{5}{2})j \right) \\
&= \frac{243}{16} n^6 + \frac{5619}{80} n^5 + \frac{2545}{16} n^4 + \frac{3349}{16} n^3 + \frac{299}{4} n^2 - \frac{551}{20} n + 3
\end{aligned}$$

This completes the proof.

Theorem 2. $PI(CNC_3[n]) = \frac{81}{4}n^4 + 56n^3 + \frac{303}{4}n^2 + 34n - 6$.

Proof. In Lemmas 1-5, we obtained the values of $m_{a_i}(\beta_1)$, $m_{b_i}(\beta_1)$, $m_{x_{2j-1}}(e_{2j-1})$ and $m_{x_{2j}}(e_{2j-1})$. Now by using the definition of the PI index we have:

$$\begin{aligned}
PI(S_3) &= \sum_{e=uv \in E} [m_u(e) + m_v(e)] = \sum_{e=uv \in E} [|E(S_3)| - N(e)] \\
&= 3(n+1)(m_{a_i}(\beta_1) + m_{b_i}(\beta_1)) \\
&\quad + 3 \sum_{j=1}^n (n+j+1) [|E(S_3)| - N(e_{2j-1})] \\
&= 3(n+1)(3n^2 + 11n - 2) + 3 \sum_{j=1}^n \left[\frac{1}{2} (9n^2 + 13n + 4) - j \right] \\
&= \frac{81}{4}n^4 + 56n^3 + \frac{303}{4}n^2 + 34n - 6.
\end{aligned}$$

This completes the proof.

Now we state the edge Szeged and PI indices of $S_4 = CNC_4$ without proof. The proofs of the following two theorems are like as S_3 .

Theorem 3. The edge Szeged index of $S_4 = CNC_4[n]$ is as follows:

$$Sz_e(S_4) = \frac{81}{2}n^6 + \frac{1919}{10}n^5 + \frac{2165}{6}n^4 + \frac{2027}{6}n^3 + \frac{488}{3}n^2 + \frac{574}{15}n + 4$$

Theorem 4. $PI(CNC_4[n]) = 36n^4 + \frac{332}{3}n^3 + 126n^2 + \frac{160}{3}n + 12$.

References

- [1] M. Ge, K. Sattler: Chem Phys Lett. **220** (1994), 192 (1994).
- [2] M. V. Diudea, Cs. L. Nagy: Periodic Nanostructures, Springer, Netherlands, 2007.
- [3] H. Wiener: J. Am. Chem. Soc. **69**, 17 (1947).
- [4] P. E. John, M. V. Diudea: Croat. Chem. Acta **77**, 127 (2004).
- [5] M. V. Diudea, M. Stefu, B. Pârv, P. E. John: Croat. Chem. Acta **77**, 111 (2004).
- [6] A. R. Ashrafi, H. Saati: J. Comput. Theor. Nanosci. **4**, 761 (2007).
- [7] A. R. Ashrafi, A. Loghman: MATCH Commun. Math. Comput. Chem. **55**, 447 (2006).
- [8] A. R. Ashrafi, A. Loghman: J. Comput. Theor. Nanosci. **3**, 378 (2006).
- [9] A. R. Ashrafi, F. Gholami-Nezhaad: Current Nanoscience **5**, 51 (2009).
- [10] M. V. Diudea, A. E. Vizitiu, F. Gholaminezhad, A. R. Ashrafi: MATCH Commun. Math. Comput. Chem. **60**, 945 (2008).
- [11] A. Iranmanesh, A. R. Ashrafi: J. Comput. Theor. Nanosci. **4**, 514 (2007).
- [12] P. V. Khadikar: Nat. Acad. Sci. Lett. **23**, 113 (2000).
- [13] I. Gutman, A. R. Ashrafi, Croat. Chem. Acta **81**, 263 (2008).
- [14] I. Gutman, Graph Theory Notes of New York **27**, 9 (1994).

*Corresponding author: ashrafi@kashanu.ac.ir