INERTIA, NULLITY AND SIGNATURE OF $CNC_4[n]$ NANOCONE[i]

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ABSTRACT. *Spectrum related topological indices play a vital role in theoretical chemistry and nanotechnology as well. Inertia indices, nullity and signature are studied for different chemical structure and nanostructures by considering their chemical graphs. They relate the stability of various organic compounds.In this paper, inertia indices, nullity and signature of* $CNC_4[n]$ nanocone are studied.

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1 INTRODUCTION

Carbon nanocones have been observed, since 1968 or even earlier [6], on the surface of naturally occurring graphite. Their bases are attached to the graphite and their height varies between 1 and 40 micrometers. Their walls are often curved and are less regular than those of the laboratory made nanocones.

Let G be an n-vertex molecular graph with vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$ and edge set $E(G)$. The vertices of G correspond to atoms and an edge between two vertices corresponds to the chemical bond between these vertices. The adjacency matrix $A(G)=[a_{ij}]_{n\times n}$ (usually denoted by A) of the graph G is defined as:

$$a_{ij}=\begin{cases}1 & v_iv_j\in E(G)\\ 0 & otherwise\end{cases}(\forall\, v_i,v_j\in V(G)).$$

The characteristic polynomial of G is a polynomial of degree n, defined as $\Phi(G,\lambda)=det(\lambda I_n-A)$, where I_n denotes the identity matrix of order n. The zeros of $\Phi(G,\lambda)$ are eigenvalues of A and multiset of eigenvalues of A is called the spectrum of A. The eigenvalues and spectrum of A are respectively called the eigenvalues and spectrum of the graph G. As G is a simple graph, the matrix A is real, symmetric with zero trace. Thus all eigenvalues of A are real and their sum is zero [4]. The notations used in this article are mainly taken from book [14].

The positive (resp., negative) inertia index of a graph G, denoted by $p(G)$ (resp., $n(G)$), is defined to be the number of positive (resp., negative) eigenvalues of its adjacency matrix. The signature of G, denoted by $s(G)$, is defined as the difference between positive and negative eigenvalues of G. The nullity of G, symbolized as $\eta(G)$, is defined as the multiplicity of eigenvalue zero in adjacency spectrum of G. Obviously, $p(G)+n(G)+\eta(G)=|V(G)|$. These parameters attract much attention of the researchers in the field of mathematical chemistry, theoretical and computational chemistry due to their direct applications in chemistry [3]. Nullity of a chemical graph is related to the stability of saturated hydrocarbons [2]. For further study of these parameters in different perspectives for different chemical and nanostructures, see [1, 7, 8, 9, 10, 11, 12, 13].

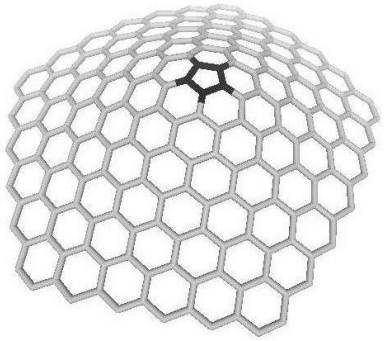

Figure 1: A type of pentagonal nanocone having a pentagon as its core.

2 RESULTS FOR $CNC_4[n]$ NANOCONE

In this section, we study certain spectrum based topological indices of $CNC_4[n]$ nanocones. A $CNC_4[n]$ nanocones consists of a square as its core and encompassing the layers of hexagons on its conical surface. If there are n layers of hexagons on the conical surface around square, then we represent the graph of that nanocones as $CNC_4[n]$ in which number n denotes the number of layers of hexagons and number in the subscript shows the sides of polygon which acts as the core of nanocones. The $CNC_4[2]$ nanocone is shown in Fig. 2.

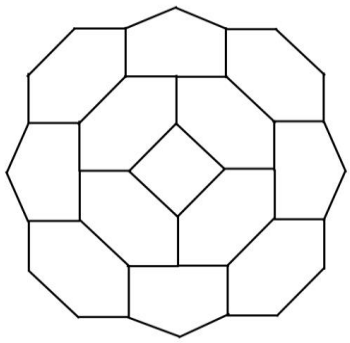

Figure 2: Graph of $CNC_4[2]$ nanocone.

Table 1: The inertia indices, nullity and signature of $CNC_4[n]$ with $1 \le n \le 11$.

$\mathsf{T} = CNC_3[n]$	$p(\mathsf{T})$	$n(\mathsf{T})$	$\eta(\mathsf{T})$	$s(\mathsf{T})$
1	8	8	0	0
2	18	18	0	0
3	32	32	0	0
4	50	50	0	0
5	72	72	0	0
6	98	98	0	0
7	128	128	0	0
8	162	162	0	0
9	200	200	0	0
10	242	243	0	0
11	288	288	0	0

Table 2: The quadratic curves fitted of the curves presented in Table 1.

$\mathsf{S} = CNC_4[n]$	$p(\mathsf{S})$	$n(\mathsf{S})$	$\eta(\mathsf{S})$	$s(\mathsf{S})$
$n \equiv 1 \bmod(2)$	$2(n+1)^2$	$2(n+1)^2$	0	0
$n \equiv 0 \bmod(2)$ with $n > 0$	$2(n^2+2n+1)$	$2(n^2+2n+1)$	0	0

We denote S as the graph of $CNC_4[n]$ nanocone. The molecules of S are drawn in HyperChem [15] for each value of n, $1 \le n \le 11$. The adjacency matrices of these molecular graphs are constructed with the help of TopoCluj [5]. Then the inertia indices, signature and nullity are calculated using MATLAB. By using "cftoolbox" of MATLAB, a quadratic polynomial is fitted to the exact values of inertia indices of T for $1 \le n \le 11$. The obtained data is arranged in Table 1.

Using the data given by Table 1, a non-linear polynomial is fitted. The inertia of this nanocone is plotted using MATLAB as shown in Figure 3. The results are displayed in Table 2.

There is an important conclusion drawn about $CNC_4[n]$ nanocone.

For $\mathsf{S} = CNC_4[n]$,

- $p(\mathsf{S}) = n(\mathsf{S})$
- $\eta(\mathsf{S}) = s(\mathsf{S}) = 0$

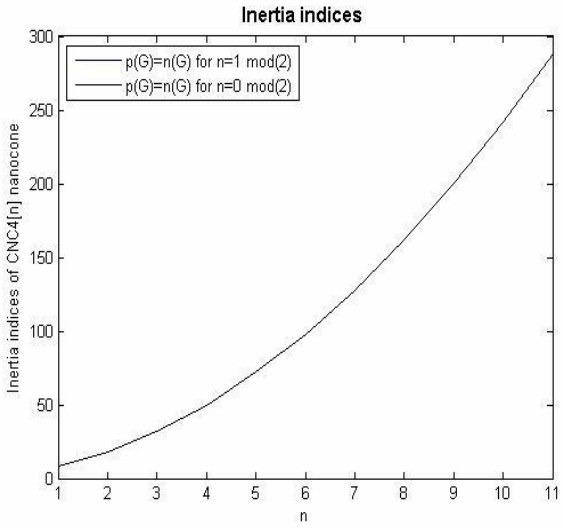

Figure 3: Inertia of $CNC_4[n]$ nanocone

3 CONCLUDING REMARKS

The study of spectrum based topological indices play an important role in QSPR/QSAR studies in which they relate the stability of different organic compounds especially carbon nanotubes and nanocones. In this paper, certain spectrum based topological indices of $CNC_4[n]$ nanocone are strong-minded. We used different software like Hyperchem to draw nanocones, TopoCluj to compute their adjacency matrices and MATLAB to compute its spectrum. These results theoretically provide a basis to study various physico-chemical properties like stability of these nanostructures.

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