On spectrum related topological descriptors of carbon nanocones

S. HAYAT[a,*], A. KHAN[b], F. YOUSAFZAI[b], M. IMRAN[a], M. U. REHMAN[c]
[a]*Department of Mathematics, School of Natural Sciences (SNS), National University of Sciences and Technology (NUST), Sector H-12, Islamabad, Pakistan*
[b]*School of Mathematical Sciences, University of Science and Technology of China (USTC), Hefei, Anhui, China*
[c]*Department of Mathematics, Karakoram International University, Gilgit-Baltistan, Pakistan*

The study of spectrum (i.e. multiset of eigenvalues) of graphs especially molecular graphs has found a considerable use in theoretical chemistry and computational nanoscience. There are various kinds of spectrum related topological indices such as, energy, Estrada index, Laplacian Estrada index, positive and negative inertia indices, nullity, signature etc., which play a key role in QSAR/QSPR studies. Energy and Estrada indices relate energies associated to the π-electron orbitals with the conjugated hydrocarbons and the degree of folding of proteins and some other long-chain biomolecules respectively. Whereas, inertia indices and nullity have found a significant use in the study of stability of chemical compounds. In this paper, inertia indices, nullity and signature of $CNC_3[n]$ and $CNC_5[n]$ nanocones are studied. Furthermore, we formulate a conjecture on these numerical parameters for general $CNC_{2k+1}[n]$ nanocones.

(Received April 30, 2015; accepted May 7, 2015)

Keywords: Inertia indices, Nullity, Signature, Carbon nanocones

1. Introduction

Carbon nanocones have been observed, since 1968 or even earlier [9], 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.

Carbon nanostructures have attracted considerable attention due to their potential use in many applications including energy storage, gas sensors, biosensors, nanoelectronic devices and chemical probes [14]. Carbon allotropes such as carbon nanocones and carbon nanotubes have been proposed as possible molecular gas storage devices. More recently, carbon nanocones have gained increased scientific interest due to their unique properties and promising uses in many novel applications such as energy and gas storage [22].

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 [7]. The notations used in this article are mainly taken from book [20].

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 [6, 21]. Nullity of a chemical graph is related to the stability of saturated hydrocarbons [4, 5]. For further study of these parameters in different perspectives for different chemical and nanostructures, see [1, 2, 3, 10, 11, 12, 13, 15, 16, 17, 18, 19].

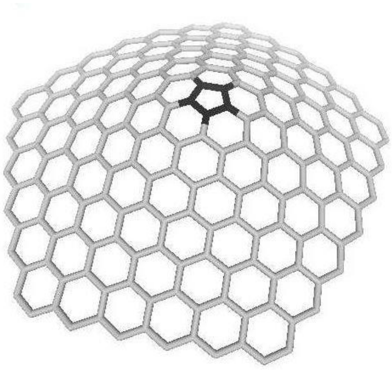

Fig. 1. A CNC_5 nanocone.

2. Results for $CNC_3[n]$ nanocone

In this section, we compute degree based topological indices of $CNC_3[n]$ nanocones. A $CNC_3[n]$ nanocones consists of a triangle 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 triangle, then we represent the graph of that nanocones as $CNC_3[n]$ 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 $CNC_3[2]$ nanocone is shown in Fig. 2.

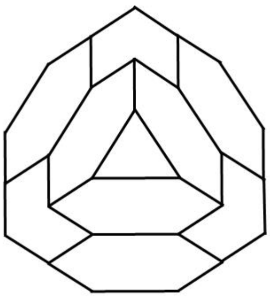

Fig. 2. Graph of $CNC_3[2]$ nanocone.

We denote T as the graph of $CNC_3[n]$ nanocone. The molecules of T are drawn in HyperChem [23] for each value of n, $1 \le n \le 11$. The adjacency matrices of these molecular graphs are constructed with the help of TopoCluj [8]. 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.

Table 1. The inertia indices, nullity and signature of $CNC_3[n]$ with $1 \le n \le 11$.

$\mathrm{T} = CNC_3[n]$	$p(\mathrm{T})$	$n(\mathrm{T})$	$\eta(\mathrm{T})$	$s(\mathrm{T})$
1	6	6	0	0
2	13	14	0	1
3	24	24	0	0
4	37	38	0	1
5	54	54	0	0
6	73	74	0	1
7	96	96	0	0
8	121	122	0	1
9	150	150	0	0
10	181	182	0	1
11	216	216	0	0

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 Fig. 3. The results are displayed in Table 2.

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

$\mathrm{T} = CNC_3[n]$	$p(\mathrm{T})$	$n(\mathrm{T})$	$\eta(\mathrm{T})$	$s(\mathrm{T})$
$n \equiv 1 \bmod (2)$	$\frac{3}{2}(n+1)^2$	$\frac{3}{2}(n+1)^2$	0	0
$n \equiv 0 \bmod (2)$ with $n > 0$	$\frac{3}{2}(n^2+2n)+1$	$\frac{3}{2}(n^2+2n)+2$	0	1

There are two important conclusions drawn about $CNC_3[n]$ nanocone.

For $\mathrm{T} = CNC_3[n]$, and $n \equiv 1 \bmod (2)$,

- $p(\mathrm{T}) = n(\mathrm{T})$
- $\eta(\mathrm{T}) = s(\mathrm{T}) = 0$

For $\mathrm{T} = CNC_3[n]$, and $n \equiv 0 \bmod (2)$, $n > 0$

- $| p(\mathrm{T}) - n(\mathrm{T}) | = 1$

- $\eta(\mathrm{T}) = 0$
- $s(\mathrm{T}) = 1$

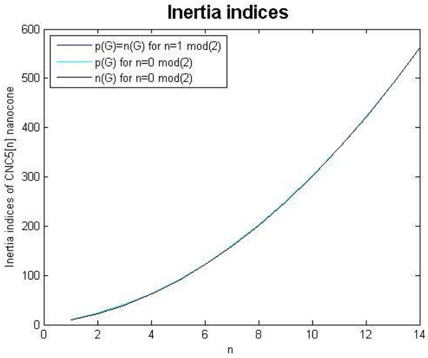

Fig. 3. Inertia of $CNC_3[n]$ nanocone.

3. Results for $CNC_5[n]$ nanocone

The vertex and edge cardinalities are $|V(CNC_5[n])| = 5(n+1)^2$ and $|E(CNC_5[n])| = \frac{15}{2}n^2 + \frac{25}{2}n + 5$. This family of nanocones are often called *one pentagonal* nanocones, and word pentagonal used for pentagon as its core and like other families of nanocones there are hexagonal layers on its conical surface (Fig. 4).

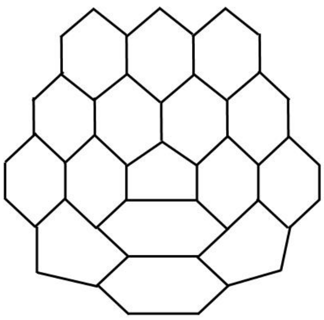

Fig. 4. Graph of one pentagonal nanocone $CNC_5[n]$ with $n = 2$.

We denote P as the graph of $CNC_5[n]$ nanocone. The molecules of P are drawn in HyperChem [23] for each value of n, $1 \le n \le 13$. The adjacency matrices of these molecular graphs are constructed with the help of TopoCluj [8]. 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 P for $1 \le n \le 13$. The obtained data is arranged in Table 3.

Table 3. The inertia indices, nullity and signature of $CNC_5[n]$ with $1 \le n \le 13$.

$\mathrm{P} = CNC_5[n]$	$p(\mathrm{P})$	$n(\mathrm{P})$	$\eta(\mathrm{P})$	$s(\mathrm{P})$
1	10	10	0	0
2	23	22	0	1
3	40	40	0	0
4	63	62	0	1
5	90	90	0	0
6	123	122	0	1
7	160	160	0	0
8	203	202	0	1
9	250	250	0	0
10	303	302	0	1
11	360	360	0	0
12	423	422	0	1
13	490	490	0	0

Using the data given by Table 3, a non-linear polynomial is fitted. The inertia of this nanocone is plotted using MATLAB as shown in Fig. 5. The results are displayed in Table 4.

Table 4. The quadratic curves fitted of the curves presented in Table 3.

$\mathrm{P} = CNC_5[n]$	$p(\mathrm{P})$	$n(\mathrm{P})$	$\eta(\mathrm{P})$	$s(\mathrm{P})$
$n \equiv 1 \bmod (2)$	$\frac{5}{2}(n+1)^2$	$\frac{5}{2}(n+1)^2$	0	0
$n \equiv 0 \bmod (2)$ with $n > 0$	$\frac{5}{2}n^2 + 5n + 3$	$\frac{5}{2}n^2 + 5n + 2$	0	1

There are two important conclusions drawn about $CNC_5[n]$ nanocone.

For $\mathsf{P} = CNC_5[n]$, and $n \equiv 1 \bmod (2)$, then

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

For $\mathsf{P} = CNC_5[n]$, and $n \equiv 0 \bmod (2)$, $n > 0$ then

- $|p(\mathsf{P}) - n(\mathsf{P})| = 1$
- $\eta(\mathsf{P}) = 0$
- $s(\mathsf{P}) = 1$

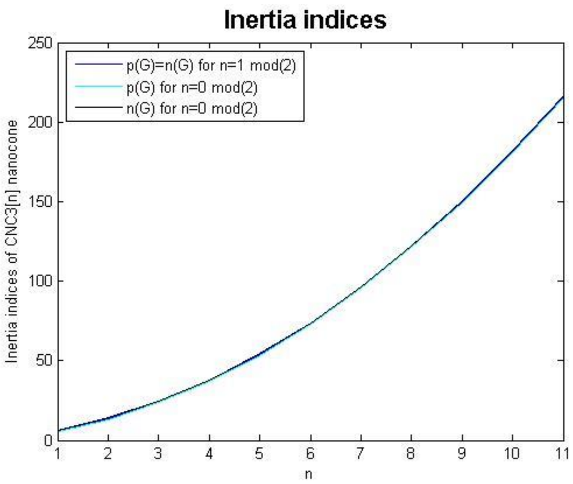

Fig. 5. Inertia of $CNC_5[n]$ *nanocone.*

4. Conjecture for $CNC_{2k+1}[n]$ nanocones

We have given the exact formulas to calculate the inertia indices and other parameters for $CNC_3[n]$ and $CNC_5[n]$ nanocones. We have given the data upto some fixed n for these two classes of nanocones. Now we formulate a conjecture to calculate of inertia indices and other related parameters for the whole family of nanocones having odd cycle as its core.

Conjecture 4.1 *Let* $G = CNC_{2k+1}[n]$, *then*

• For $n \equiv 1 \bmod (2)$,

$$p(G) = n(G) = \frac{k}{2}(n+1)^2$$
$$\eta(G) = s(G) = 0$$

• For $n \equiv 1 \bmod (4)$,

$$p(G) = \frac{k}{2}n^2 + k(n + \frac{1}{2}) + \frac{1}{2}$$
$$n(G) = \frac{k}{2}n^2 + k(n + \frac{1}{2}) - \frac{1}{2}$$
$$\eta(G) = 0$$
$$s(G) = 1$$

• For $n \equiv 3 \bmod (4)$,

$$p(G) = \frac{k}{2}n^2 + k(n + \frac{1}{2}) - \frac{1}{2}$$
$$n(G) = \frac{k}{2}n^2 + k(n + \frac{1}{2}) + \frac{1}{2}$$
$$\eta(G) = 0$$
$$s(G) = 1$$

5. Conclusion and general remarks

It is natural to ask for spectrum related parameters for fullerenes, nanotubes and nanocones. In this research, we have studied inertia, nullity and signature of $CNC_3[n]$ and $CNC_5[n]$ nanocones. 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.

Acknowledgements

[1] The first and fourth authors are partially supported by NUST Pakistan.
[2] The author is supported by Chinese Government Scholarship at USTC, China.
[3] The author is supported by CAS-TWAS President's Fellowship USTC, China.

References

[1] A. R. Ashrafi, Optoelectron. Adv. Mater. Rapid Comm. **4**(1), 48 (2010).
[2] A. R. Ashrafi, B. Bazigaran, M. Sadati, Optoelectron. Adv. Mater. Rapid Comm. **3**(10), 1080 (2009).
[3] A. R. Ashrafi, M. Faghani, S. M. Seyedaliakbar, Dig. J. Nanomater. Bios. **4**, 59 (2009).
[4] P. W. Atkins, J. de Paula, Physical Chemistry, eighthed., Oxford University Press, 2006.
[5] G. J. Chang, L. H. Huang, H. G. Yeh, Linear Algebra Appl. **436**(8), 4241 (2012).
[6] L. Collatz,U. Sinogowitz, Spektren endlicher Grafen, Abh. Math. Semin. Univ. Hambg., **21**(8), 63 (1957).
[7] D. Cvetkovic, M. Doob, H. Sachs, Spectra of Graphs-Theory and Application, third ed., Johann Ambrosius Barth Verlag, Heidelberg, Leipzig, 1995.
[8] M. V. Diudea, O. Ursu, Cs. L. Nagy, TOPOCLUJ, Babes-Bolyai University, Cluj 2002.
[9] J. Gillot, W. Bollmann, B. Lux, Carbon **6**, 381-7 (1968).

[10] S. Hayat, Sci. Int. **27**, 863 (2015).
[11] S. Hayat, M. Imran, Studia UBB Chemia, LIX, **4**, 113 (2014).
[12] S. Hayat, M. Imran, J. Comput. Theor. Nanosci. **12**, 70 (2015).
[13] S. Hayat, A. Khan, F. Yousafzai, M. Imran, Optoelectron. Adv. Mater. Rapid Comm. **9**, 478 (2015).
[14] S. Iijima, Nature, **354**, 56(1991).
[15] M. Imran, S. Hayat, M. K. Shafiq, Optoelectron. Adv. Mater. Rapid Comm. **8**, 9-10, 948 (2014).
[16] H. Ma, W. Yang, Sh. Li, Linear Algebra Appl. **438**, 331 (2013).
[17] M. A. Malik, R. Farooq, Optoelectron. Adv. Mater. Rapid Comm. **9**, 311 (2015).
[18] M. A. Malik, R. Farooq, Optoelectron. Adv. Mater. Rapid Comm. **9**, 415 (2015).
[19] G. R. Omidi, Graphs Combin. **25**, 111 (2009).
[20] N. Trinajstic, CRC Press, Boca Raton, FL, 1992.
[21] G. Yu, L. Feng, Q. Wang, Linear Algebra Appl. **438**, 2036 (2013).
[22] M. Yudasaka, S. Iijima, Crespi, V. H. Top. Appl. Phys., **111**, 629 (2008).
[23] HyperChem package Release 7.5 for Windows, Hypercube Inc., 1115 NW 4th Street, Gainesville, Florida 32601, USA 2002.

*Corresponding author: sakander@mail.ustc.edu.cn