# Computational results on inertia indices, signature and nullity of $C_4C_8(R)$ nanotube

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A molecular/chemical graph is hydrogen depleted chemical structure in which vertices denote atoms and edges denote the bonds. Topological descriptors are the numerical indices based on the topology of the atoms and their bonds (chemical conformation, quaternary structure). They correlate various physico-chemical properties like boiling point, enthalpy of formation, enthalpy of vaporization, Kovat's constant etc., of various chemical compounds. Carbon nanotubes, a type of fullerene, have potential in fields such as nanotechnology, electronics, optics, materials science and architecture. The numerical parameters like inertia indices, signature and nullity attract much attention due to their diverse application in chemistry e.g., nullity of a molecular graph is related to the stability of saturated hydrocarbons.In this paper, inertia indices, signature and nullity of $TUC_4C_8(R)[2m-1,2n-1]$ nanotube are strong-minded. We conclude that the positive and negative inertia indices are equal for this nanotube and signature and nullity for this nanotube remain zero.

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*Keywords:* Inertia indices, Signature, Nullity, Nanotubes

## 1. Introduction

A fullerene is a carbon molecule in the shape of a hollow sphere, ellipsoid, tube, etc. Those whose shape resemble a sphere are called buckyballs and those which are in the form of a tube are called buckytubes or nanotubes. The structure of a nanotube is similar to a graphite sheet. Carbon nanotubes appear in different forms with respect to their length, thickness, number of layers and the types of the rings which cover the walls of the nanotubes.

Carbon nanotubes have exhibited unusual properties in experimental sciences. They have noteworthy applications in nanotechnology, optics, material sciences and electronics. The intrinsic mechanical properties of carbon nanotubes and their electrical and thermal conductivity makes them incomparable with other materials. With such a huge industrial applications, carbon nanotubes have attracted many researchers to investigate more and not yet discovered properties of these nano-materials.

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 atoms. 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 [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, theoretical and computational chemistry due to their direct application in chemistry [6, 16]. Nullity of a chemical graph is related to the stability of saturated hydrocarbons [4, 5]. For further study of these parameters in different perspectives, see [1, 2, 3, 8, 9, 10, 11, 12, 13].

Let $L$ denote the 2 -dimensional lattice of a $TUC_4C_8(R)[2m-1,2n-1]$ nanotube. Fig. 1 shows a $TUC_4C_8(R)[m,n]$ nanotube with $m=3$ and $n=6$.

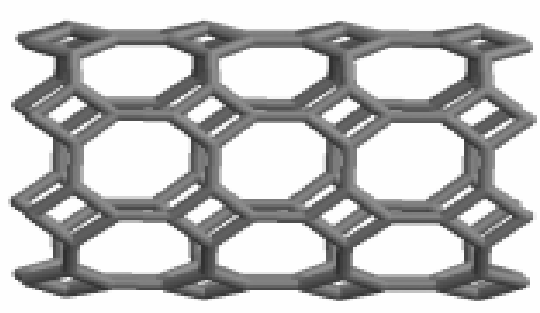

*Fig. 1. The* $TUC_4C_8(R)[m,n]$ *nanotube with* $m=3$ *and* $n=6$.

It is composed of $2n-1$ layers ($n\geq 1$) of heptagons (see Fig. 2) in each row and $2m-1$ layers ($n\geq 1$) of heptagons in each column. In this paper, we estimate the inertia indices, signature and nullity of the graph $L$.

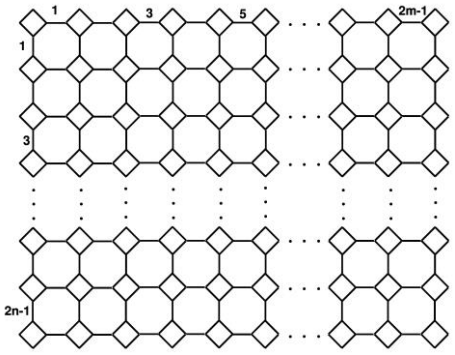


*Fig. 2. The graph of a* 2 *-dimensional lattice of* $TUC_4C_8(R)[2m-1,2n-1]$ *nanotube.*

## 2. Computational results

In this section, we explain the computational procedure to calculate the inertia indices, signature and nullity of the graph $L$.

The molecules of $L$ are drawn in HyperChem [17] for each value of $m$ and $n$, $1\leq m,n\leq 8$. The adjacency matrices of these molecular graphs are constructed with the help of TopoCluj [15]. Then the inertia indices, signature and nullity are calculated using MATLAB. By using "cftoolbox" of MATLAB, a linear polynomial is fitted to the exact values of inertia indices of $L$ for $1\leq m\leq 8$ and a fixed value of $n$. The obtained data is arranged in Table 1.

*Table 1. The linear curves fitted to the Inertia indices, signature and nullity of* $TUC_4C_8(R)[2m-1,2n-1]$. *For each curve, we have a fixed value of* $n$ *and* $1\leq m\leq 8$.

| $L$ | $p(L)$ | $n(L)$ | $s(L)$ | $\eta(L)$ |
|---|---|---|---|---|
| $[m,1]$ | $4m+4$ | $4m+4$ | 0 | 0 |
| $[m,3]$ | $8m+8$ | $8m+8$ | 0 | 0 |
| $[m,5]$ | $12m+12$ | $12m+12$ | 0 | 0 |
| $[m,7]$ | $16m+16$ | $16m+16$ | 0 | 0 |
| $[m,9]$ | $20m+20$ | $20m+20$ | 0 | 0 |
| $[m,11]$ | $24m+24$ | $24m+24$ | 0 | 0 |
| $[m,13]$ | $28m+28$ | $28m+28$ | 0 | 0 |
| $[m,15]$ | $32m+32$ | $32m+32$ | 0 | 0 |

Using the data given by Table 1, a non-linear polynomial is fitted. Since the positive and negative inertia indices for this nanotube are equal, so we name them as inertia of this nanotube. The inertia of this nanotube is plotted using MATLAB as shown in Fig. 3. The results are displayed in Table 2.

*Table 2. The non-linear curves fitted of the curves presented in Table 1.*

| $L$ | $p(L)$ | $n(L)$ | $s(L)$ | $\eta(L)$ |
|---|---|---|---|---|
| | $2(mn+m+n+1)$ | $2(mn+m+n+1)$ | 0 | 0 |

There are two important facts which we formulate after this study.

Let $G=TUC_4C_8(R)[2m-1,2n-1]$, then

- $p(G)=n(G)$
- $s(G)=\eta(G)=0$

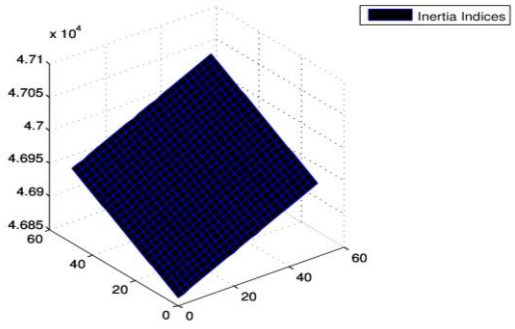


*Fig. 3. Inertia of* $C_4C_8(R)[2m-1,2n-1]$ *nanotube.*

## 3. Conclusion and general remarks

Since the order of a molecular graph grows very large when its dimension is increased, it is very hard to obtain data and perform calculations on it. This makes it important to study the computational and statistical methods and apply them to analyze the general behavior of data. This makes it possible to estimate the desired values of the data without going through the necessary calculations. These parameters have been discussed for different classes of graphs, we study these parameters of nanotube for the first time. We used different softwares like HyperChem, TopoCluj and MATLAB to study these parameters for this family of molecular graph. The important fact which we study that the signature and nullity for this nanotube will remain zero. These results are of much importance because they help us to study many chemical properties of these chemical compound.

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## Appendix

### 4. Appendix for the referee

The data given in Table 3 to Table 10 shows the exact values of inertia, signature and nullity of $\mathsf{L}$, $1 \le m,n \le 8$.

*Table 3. Inertia, signature and nullity of* $\mathsf{L}$.

| $[m,n]$ | $p(\mathsf{L})$ | $n(\mathsf{L})$ | $s(\mathsf{L})$ | $\eta(\mathsf{L})$ |
|---|---|---|---|---|
| [1,1] | 8 | 8 | 0 | 0 |
| [1,3] | 16 | 16 | 0 | 0 |
| [1,5] | 24 | 24 | 0 | 0 |
| [1,7] | 32 | 32 | 0 | 0 |
| [1,9] | 40 | 40 | 0 | 0 |
| [1,11] | 48 | 48 | 0 | 0 |
| [1,13] | 56 | 56 | 0 | 0 |
| [1,15] | 64 | 64 | 0 | 0 |

*Table 4. Inertia, signature and nullity of* $\mathsf{L}$.

| $[m,n]$ | $p(\mathsf{L})$ | $n(\mathsf{L})$ | $s(\mathsf{L})$ | $\eta(\mathsf{L})$ |
|---|---|---|---|---|
| [3,1] | 16 | 16 | 0 | 0 |
| [3,3] | 32 | 32 | 0 | 0 |
| [3,5] | 48 | 48 | 0 | 0 |
| [3,7] | 64 | 64 | 0 | 0 |
| [3,9] | 80 | 80 | 0 | 0 |
| [3,11] | 96 | 96 | 0 | 0 |
| [3,13] | 112 | 112 | 0 | 0 |
| [3,15] | 128 | 128 | 0 | 0 |

*Table 5. Inertia, signature and nullity of* $\mathsf{L}$.

| $[m,n]$ | $p(\mathsf{L})$ | $n(\mathsf{L})$ | $s(\mathsf{L})$ | $\eta(\mathsf{L})$ |
|---|---|---|---|---|
| [5,1] | 24 | 24 | 0 | 0 |
| [5,3] | 48 | 48 | 0 | 0 |
| [5,5] | 72 | 72 | 0 | 0 |
| [5,7] | 96 | 96 | 0 | 0 |
| [5,9] | 120 | 120 | 0 | 0 |
| [5,11] | 144 | 144 | 0 | 0 |
| [5,13] | 168 | 168 | 0 | 0 |
| [5,15] | 192 | 192 | 0 | 0 |

*Table 6. Inertia, signature and nullity of* $\mathsf{L}$.

| $[m,n]$ | $p(\mathsf{L})$ | $n(\mathsf{L})$ | $s(\mathsf{L})$ | $\eta(\mathsf{L})$ |
|---|---|---|---|---|
| [7,1] | 32 | 32 | 0 | 0 |
| [7,3] | 64 | 64 | 0 | 0 |
| [7,5] | 96 | 96 | 0 | 0 |
| [7,7] | 128 | 128 | 0 | 0 |
| [7,9] | 160 | 160 | 0 | 0 |
| [7,11] | 192 | 192 | 0 | 0 |
| [7,13] | 224 | 224 | 0 | 0 |
| [7,15] | 256 | 256 | 0 | 0 |

*Table 7. Inertia, signature and nullity of* $\mathsf{L}$.

| $[m,n]$ | $p(\mathsf{L})$ | $n(\mathsf{L})$ | $s(\mathsf{L})$ | $\eta(\mathsf{L})$ |
|---|---|---|---|---|
| [9,1] | 40 | 40 | 0 | 0 |
| [9,3] | 80 | 80 | 0 | 0 |
| [9,5] | 120 | 120 | 0 | 0 |
| [9,7] | 160 | 160 | 0 | 0 |
| [9,9] | 200 | 200 | 0 | 0 |
| [9,11] | 240 | 240 | 0 | 0 |
| [9,13] | 280 | 280 | 0 | 0 |
| [9,15] | 320 | 320 | 0 | 0 |

*Table 8. Inertia, signature and nullity of* $\mathsf{L}$.

| $[m,n]$ | $p(\mathsf{L})$ | $n(\mathsf{L})$ | $s(\mathsf{L})$ | $\eta(\mathsf{L})$ |
|---|---|---|---|---|
| [11,1] | 48 | 48 | 0 | 0 |
| [11,3] | 96 | 96 | 0 | 0 |
| [11,5] | 144 | 144 | 0 | 0 |
| [11,7] | 192 | 192 | 0 | 0 |
| [11,9] | 240 | 240 | 0 | 0 |
| [11,11] | 288 | 288 | 0 | 0 |
| [11,13] | 336 | 336 | 0 | 0 |
| [11,15] | 384 | 384 | 0 | 0 |

*Table 9. Inertia, signature and nullity of* $\mathsf{L}$.

| $[m,n]$ | $p(\mathsf{L})$ | $n(\mathsf{L})$ | $s(\mathsf{L})$ | $\eta(\mathsf{L})$ |
|---|---|---|---|---|
| [13,1] | 56 | 56 | 0 | 0 |
| [13,3] | 112 | 112 | 0 | 0 |
| [13,5] | 168 | 168 | 0 | 0 |
| [13,7] | 224 | 224 | 0 | 0 |
| [13,9] | 280 | 280 | 0 | 0 |
| [13,11] | 336 | 336 | 0 | 0 |
| [13,13] | 392 | 392 | 0 | 0 |
| [13,15] | 448 | 448 | 0 | 0 |

*Table 10. Inertia, signature and nullity of* $\mathsf{L}$.

| $[m,n]$ | $p(\mathsf{L})$ | $n(\mathsf{L})$ | $s(\mathsf{L})$ | $\eta(\mathsf{L})$ |
|---|---|---|---|---|
| [15,1] | 64 | 64 | 0 | 0 |
| [15,3] | 128 | 128 | 0 | 0 |
| [15,5] | 192 | 192 | 0 | 0 |
| [15,7] | 256 | 256 | 0 | 0 |
| [15,9] | 320 | 320 | 0 | 0 |
| [15,11] | 384 | 384 | 0 | 0 |
| [15,13] | 448 | 448 | 0 | 0 |
| [15,15] | 512 | 512 | 0 | 0 |

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