Computational results on the energy and Estrada index of $TUC_4C_8(R)[m, n]$ nanotubes

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The aim of this paper is to investigate the approximate values of energyand Estrada index of the 2-dimensional lattice of $TUC_4C_8(R)[m, n]$ nanotubes by using computational and statistical tools. Our computations suggest that the energy of this graph can be estimated by the polynomial $1.534\times10^{-6}n^2m^2+3.427\times10^{-4}n^2m+1.713\times10^{-4}m^2+4.565\times10^{-4}n^2+5.875nm+3.725\times10^{-4}nm^2+5.195n-0.6824m-0.6915$ and the Estrada index of this graph can be estimated by $-2.973\times10^{-16}n^2m^2+2.189\times10^{-11}n^2m+2.116\times10^{-11}n^2+1.721\times10^{-4}nm^2+13.53nm+11.51n+1.026\times10^{-5}m^2-2.029m-1.982$.

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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 uncomparable 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 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].

In the H$\ddot{u}$ckel theory of molecular orbitals, the total π-electron energy E_π of a molecular graph G is defined as $E_\pi(G)=\sum_{i=1}^{n}|\lambda_i|$, where $\lambda_1\le\lambda_2\le\cdots\le\lambda_n$ are the eigenvalues of A. The parameter $E_\pi(G)$ is in good correspondence with the molecular orbital energy levels π-electrons in conjugated hydrocarbons [4, 9, 11].

Estrada [6] introduced the notion of Estrada index of a molecular graph G, denoted as $EE(G)$ and defined as $EE(G)=\sum_{i=1}^{n}\exp^{\lambda_i}$. This index has recently found applications in quantifying the degree of folding of proteins and other long-chain biomolecules [5], characterizing the general topological features of complex networks [7] and in measuring bipartivity of graphs [8]. For further information on energy, Estrada index and other notations, the reader is referred to [1, 2, 3, 10, 12, 14].

Let L denote the 2-dimensional lattice of $aTUC_4C_8(R)[m, n]$nanotube. It is composed of n layers ($n\ge1$), where each layer contains $m+2$ cycles of length 4 and each cycle of length 4 is in the form of a rhombus (see Fig. 1). Two consecutive layers are joined by adding edges between the corresponding vertices of the cycles of length 4. Two such layers give us a period of this nanotube, where there are m octagons in each period. We can obtain a next period by adding another layer to the bottom of this nanotube. In this paper, we estimate the energy and Estrada index of the graph L.

2. Computational results

In this section, we explain the computational procedure to calculate the energy and Estrada index of the graph L. The molecules of L are drawn in HyperChem [15] for each value of m and n, $1 \le m,n \le 15$. The adjacency matrices of these molecular graphs are constructed with the help of TopoCluj [13]. Then the energy and Estrada index are calculated using MATLAB. By using "cftoolbox" of MATLAB, a quadratic polynomial is fitted to the exact values of energy and Estrada index of L for $1 \le n \le 15$ and a fixed value of m. The obtained data is arranged in Table 1.

Using the data given in Table 1, a quadratic polynomial is fitted to the coefficients of n^k, where $1 \le m \le 15$ and $k \in \{0,1,2\}$. The results are displayed in Table 2.

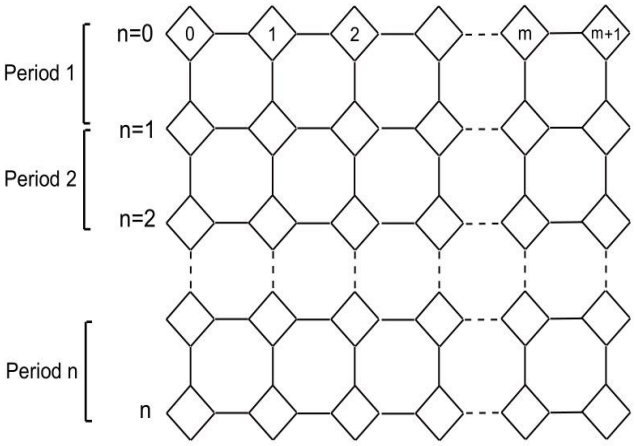

Fig. 1. The graph of a 2-dimensional lattice of $TUC_4C_8(R)[m, n]$ nanotube.

Table 1. The quadratic curves fitted to the Energy and Estrada index of $TUC_4C_8(R)[m, n]$. For each curve, we have a fixed value of m and $1 \le n \le 15$.

$[m,n]$	Energy	Estrada index
$[1,n]$	$0.8665\times10^{-3}n^2+11.1n-1.284$	$4.306\times10^{-11}n^2+25.04n-4.011$
$[2,n]$	$0.9902\times10^{-3}n^2+16.93n-2.226$	$6.495\times10^{-11}n^2+38.57n-6.04$
$[3,n]$	$1.59\times10^{-3}n^2+22.8n-2.617$	$8.684\times10^{-11}n^2+52.1n-8.068$
$[4,n]$	$1.897\times10^{-3}n^2+28.71n-3.55$	$10.87\times10^{-11}n^2+65.64n-10.1$
$[5,n]$	$2.164\times10^{-3}n^2+34.56n-3.958$	$13.06\times10^{-11}n^2+79.17n-12.13$
$[6,n]$	$2.585\times10^{-3}n^2+40.47n-4.886$	$15.25\times10^{-11}n^2+92.7n-14.15$
$[7,n]$	$2.815\times10^{-3}n^2+46.34n-5.372$	$17.44\times10^{-11}n^2+106.2n-16.18$
$[8,n]$	$3.47\times10^{-3}n^2+52.22n-6.185$	$19.63\times10^{-11}n^2+119.8n-18.21$
$[9,n]$	$3.525\times10^{-3}n^2+58.12n-6.791$	$21.82\times10^{-11}n^2+133.3n-20.24$
$[10,n]$	$4.045\times10^{-3}n^2+63.98n-7.525$	$24.01\times10^{-11}n^2+146.8n-22.27$
$[11,n]$	$4.669\times10^{-3}n^2+69.87n-8.136$	$26.19\times10^{-11}n^2+160.4n-24.3$
$[12,n]$	$4.536\times10^{-3}n^2+75.75n-8.891$	$28.38\times10^{-11}n^2+173.9n-26.33$
$[13,n]$	$5.24\times10^{-3}n^2+81.64n-9.512$	$30.57\times10^{-11}n^2+187.4n-28.36$
$[14,n]$	$5.502\times10^{-3}n^2+87.52n-10.25$	$32.76\times10^{-11}n^2+201n-30.38$
$[15,n]$	$5.983\times10^{-3}n^2+93.4n-10.87$	$34.95\times10^{-11}n^2+214.5n-32.41$

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

	Energy	Estrada index
n^2	$1.534\times10^{-6}m^2+3.427\times10^{-4}m+4.565\times10^{-4}$	$-2.973\times10^{-16}m^2+2.189\times10^{-11}m+2.116\times10^{-11}$
n	$3.725\times10^{-4}m^2+5.875m+5.195$	$1.721\times10^{-4}m^2+13.53m+11.51$
1	$-1.713\times10^{-4}m^2+0.6824m+0.6915$	$-1.026\times10^{-5}m^2+2.029m+1.982$

Finally, the general curves in two dimensions, representing the energy and Estrada index of the graph L are given by equation (1) and equation (2), respectively. A comparison between the plots of the two surfaces given by equation (1) and equation (2), has been made in Fig. 2.

$$E(L)=1.534\times10^{-6}n^2m^2+3.427\times10^{-4}n^2m+4.565\times10^{-4}n^2$$

$$+0.0003725nm^2 + 5.875nm + 5.195n + 0.0001713m^2 - 0.6824m - 0.6915 \quad (1)$$

$$EE(L) = -2.973\times10^{-16}n^2m^2 + 2.189\times10^{-11}n^2m + 2.116\times10^{-11}n^2 + 1.721\times10^{-4}nm^2 + 13.53nm + 11.51n + 1.026\times10^{-5}m^2 - 2.029m - 1.982 \quad (2)$$

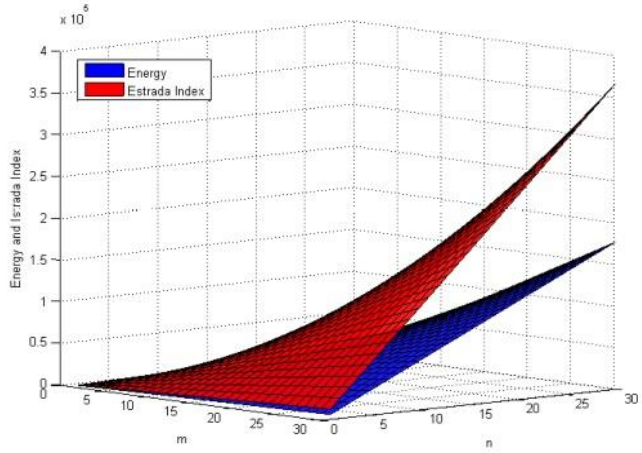

Fig. 2. Energy and Estrada index of $TUC_4C_8(R)[m,n]$ nanotube.

3. Conclusion

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 analyse the general behaviour of data. This makes it possible to estimate the desired values of the data without going through the necessary calculations. The estimated and exact values of energy and Estrada index of the graph L are presented in Table 3 and Table 4, respectively.

It can be seen that the values of desired parameters($E(L)$ and $EE(L)$) can be obtained with small errors. These errors can be reduced by applying a better estimation technique to the data and some other important molecular graphs can also be studied in this perspective, which is open to the readers.

Table 3. Estimated values of Energy and Estrada index of the graph L obtained from (1) and (2).

[m,n]	Energy	Estrada index
[15,1]	175.9424361000000	396.5827535013978
[15,2]	269.3759593500000	611.0814760031450
[15,3]	362.8213669000000	825.5801985055912
[15,4]	456.2786587500000	1040.078921008736
[15,5]	549.7478348999999	1254.577643512580
[15,6]	643.2288953499999	1469.076366017123
[15,7]	736.7218401000000	1683.575088522364
[15,8]	830.2266691499999	1898.073811028305
[15,9]	923.7433824999999	2112.572533534944

Table 4. Exact values of Energy and Estrada index of the graph L.

[m,n]	Energy	Estrada index
[15,1]	176.4719283781837	396.5932571216588
[15,2]	268.9602139104927	611.0965536459598
[15,3]	362.6373316374283	825.5998502177959
[15,4]	456.3125271135441	1040.103146789630
[15,5]	549.4664397693208	1254.606443361467
[15,6]	643.2525811733453	1469.109739933303
[15,7]	736.7771997058154	1683.613036505137
[15,8]	830.2341258472407	1898.116333076973
[15,9]	923.8919048450422	2112.619629648809

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