Experimental results on the energy and Estrada index of HC_5C_7[4p,8] nanotubes

A. R. ASHRAFI
Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I. R. Iran

Let CNC[n] be the molecular graph of a carbon nanocone with n layers. The aim of this paper is to investigate the spectral properties of these nanostructures. Our calculations suggest this conjecture that $E(CNC[n]) = 28.7372(1.2)^{n-1}$ and $E(CNC[n]) = 55.5639(1.2)^{n-1}$, where E(CNC[n]) and EE(CNC[n]) denote the energy and Estrada index of these nanomaterials.

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1. Introduction

Carbon nanotubes are molecular-scale tubes of graphitic carbon with outstanding properties. They are among the stiffest and strongest fibres known, and have remarkable electronic properties and many other unique characteristics. For these reasons they have attracted huge academic and industrial interest, with thousands of papers on nanotubes being published every year. Commercial applications have been rather slow to develop, however, primarily because of the high production costs of the best quality nanotubes.

Let G be an n-vertex molecular graph with V(G) = $\{v_1, v_2, \ldots, v_n\}$. The adjacency matrix A = A(G) is an n × n matrix whose (i, j)-entry is 1 if v_i and v_j are adjacent, and 0 otherwise. The characteristic polynomial of G is the polynomial of degree n, defined as $\chi(\lambda) = \det[\lambda I_n - A(G)]$, where I_n is the unit matrix of order n. The scalars λ and vectors x satisfying Ax = λx are called eigenvalues and eigenvectors of A, respectively. Geometrically, Ax = λx says that under transformation by A, eigenvectors experience only changes in magnitude or sign—the orientation of Ax in $\mathbb{R}^n$ is the same as that of x. The spectrum of A is the multi-set of all eigenvalues of A. The eigenvalues and spectrum of a graph is the eigenvalues and spectrum of its adjacency matrix. All the eigenvalues of a graph are real numbers, and their sum is equal to zero [1].

In the Hückel theory the total π-electron energy of a bipartite molecular graph G is defined as the sum $E_\pi(G) = \sum_{i=1}^{n} |\lambda_i|$ of the absolute values of the eigenvalues $\lambda_1 \le \lambda_2 \le \ldots \le \lambda_n$ of the adjacency matrix A(G) of G. This energy is in good linear correlation with the observed heats of formations of the corresponding conjugated hydrocarbons and it is related with other relevant chemical invariants [2-8].

The Estrada index EE(G) of the molecular graph G is defined as the sum of e^{λ_i}, $1 \le i \le n$. This quantity, introduced by Ernesto Estrada has noteworthy chemical applications [9]. This index recently found applications in seemingly so diverse areas as quantifying of the degree of folding of proteins and other long-chain biomolecules [10, 11], characterizing the general topological features of complex networks [12, 13], measuring bipartivity of graphs [14], modeling of extended atomic branching [15], and statistical thermodynamics [16]. We encourage the reader to consult also papers [17–23] for background material as well as basic computational techniques. The aim of this paper is to compute the energy and Estrada index of one-pentagonal carbon nanocone CNC[n], Fig. 1. Our notation is standard and taken mainly from standard books of graph theory and the books of Trinajestic [24].

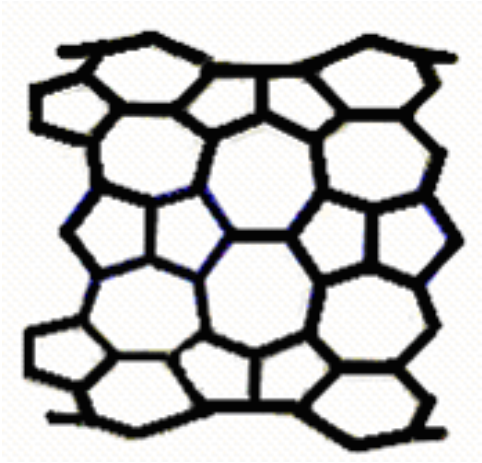

Fig. 1. A HC_5C_7 nanotube.

2. Main results and discussion

In this section, the eigenvalues of the molecular graph of a $HC_5C_7[4p,8]$ nanotube is computed by the matrix package MATLAB. To do this, we first draw the molecule by HyperChem [25]. Then the adjacency matrix of the molecular graph of H[p] = $HC_5C_7[4p,8]$ nanotube is computed by TopoCluj [26].

In Table 1, the energy and Estrada index of some types of this nanotube, $1 \le p \le 10$, are computed. By curve fitting method, two polynomials of the best degree for approximating energy and Estrada index of H[p], respectively, are computed.

Table 1. The Values of E(G) and EE(G) of H[p], $1 \le p \le 10$.

P	E(G)	EE(G)
1	48.09972862	100.5912367
2	95.46260337	202.5909269
3	143.0818336	303.8861851
4	191.023335	405.1815802
5	238.7687923	506.4769752
6	286.3886887	607.7723702
7	334.2478136	709.0677653
8	381.9931283	810.3631603
9	429.6566714	911.6585554
10	477.4797063	1012.95395

Data Mining is a part of computer science investigates method for finding a good curve which has the best fit to a series of data points. DataFit is a software for simplifies the tasks of data plotting, regression analysis (curve fitting) and statistical analysis. This package is applied for solving our problem. In most of problems related to eigenvalues the curve fitting by exponential functions is more important, because polynomials are not good for approximating eigenvalues. It seems that the data of Table 1 can be fitted by polynomials of degree one. Hence we conjecture that the curve of data given in Table 1 has an asymptotic line. Our calculations suggest that the energy and Estrada index of this nanotube can be evaluated by $E(HC_5C_7[4p,8]) = 48.1 + 47.7(n-1)$ and $EE(HC_5C_7[4p,8]) = 100.6 + 101.3(n-1)$. In Fig. 1, a diagram is depicted to show difference between energy and Estrada index of the nanotube.

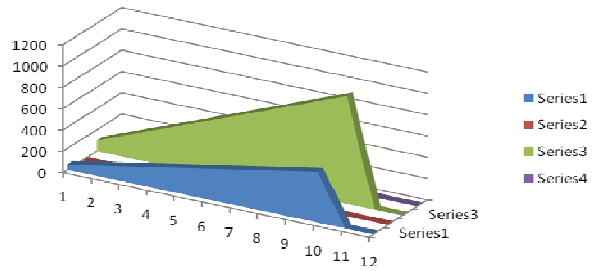

Fig. 2. The diagram of energy and Estrada index of $HC_5C_7[4p,8]$.

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*Corresponding author: alir.ashrafi@gmail.com