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Some experimental conjectures on energy and Estrada index of $VC_5C_7[4p,8]$ nanotubes

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Let $E(VC_5C_7[4p,8])$ and $EE(VC_5C_7[4p,8])$ denote the energy and Estrada index of $VC_5C_7[4p,8]$ nanotube, where p denotes the period of this C_5C_7 nanotube. In this paper some calculations are given by which it is possible to suggest conjectures about energy and Estrada index of this nanotube. We conjectured $E(VC_5C_7[4p,8]) = 47.4018 + 47.3(p-1)$ and $EE(VC_5C_7[4p,8]) = 99.3238 + 99.2(p-1)$.

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1. Introduction

This paper continues the investigations concerning energy and Estrada index of nanostructures. We begin by some notation which will be kept throughout. Let G be a molecular graph with vertex and edge-sets V(G) and E(G), respectively. A topological index for G is a numeric quantity related to G. The oldest topological index is the Wiener index. Numerous of its chemical applications were reported and its mathematical properties are well understood. For a molecular graph G, the square matrix A_G with $A_G[i, j]$ = the number of edges between vertices v_i and v_j is called adjacency matrix of G. If G is a molecular graph then A_G is a 0-1 matrix. The characteristic polynomial $\chi(G, k)$ is the polynomial of degree n, defined as $\det[\lambda I_n - A(G)]$, where I_n is the unit matrix of order n [1].

Let A be an n × n matrix. 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]

A molecular graph G is called bipartite if there exists a coloring of V(G) by two colors. Here, a coloring of G is a coloring of its vertices such that two adjacent vertices have different colors. 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 its adjacency matrix. This energy is in good linear correlation with the observed heats of formations and it is related to other relevant chemical invariants [2-6].

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 the degree of folding of proteins and other long-chain biomolecules, characterizing the general topological features of complex networks, measuring bipartivity of graphs, modeling of extended atomic branching, and statistical thermodynamics.[7-14] We encourage the reader to consult also papers[15–22] for background material as well as basic computational techniques.

The aim of this paper is to compute the energy and Estrada index of $VC_5C_7[4p,8]$ nanotube, Fig. 1. Our notation is standard and taken mainly from standard books of graph theory and the books of Trinajestic [23].

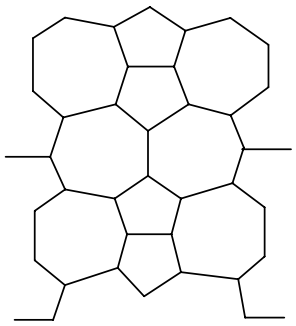

Fig. 1. The $VC_5C_7[4,8]$ Nanotube T.

2. Main results and discussion

In a mechanical system, the stable equilibrium positions minimize the potential energy. The basic geometrical problem of minimizing distance also appears in many contexts. For example, in optics and relativity,

light rays follow the paths of minimal distance the geodesics on the curved space-time. In data analysis, the most fundamental method for fitting a function to a set of sampled data points is to minimize the least squares error, which serves as a measurement of the overall deviation between the sample data and the function.

In this section, the eigenvalues of $VC_5C_7[4p,8]$ nanotube, $1 \le p \le 10$, are computed by the matrix package MATLAB. To do this, we first draw the molecule by HyperChem[24] and then the adjacency matrix of the molecular graph of this nanotube is computed by TopoCluj.[25] In Table I, we give the energy and Estrada index of these nanotubes for $1 \le p \le 10$. Then by curve fitting method, we will find a polynomial of the best degree to approximate the energy and Estrada index of the nanotube.

From now on we shall restrict ourselves to a solution given by the theory of asymptotic series and theory of asymptotic expansions. Here the central theme is the construction and investigation of series which represent given functions asymptotically. The functions are often given by integral representations, or by power series, or else appear as solutions of differential equations; and in the latter case the "variable" of the asymptotic expansions may occur either as the independent variable, or else as a parameter, in the differential equation.

Table 1. The values of E(G) and EE(G) for ten layers of $VC_5C_7[4p,8]$.

No	Energy of $VC_5C_7[4p,8]$	Estrada of $VC_5C_7[4p,8]$
1	47.4017847	99.32283998
2	94.55990061	198.4135016
3	141.9628838	297.6202518
4	189.266535	396.8270025
5	236.587909	496.0337531
6	283.9048423	595.2405037
7	331.2223647	694.4472543
8	378.5399042	793.6540049
9	425.8573567	892.8607555
10	473.1748577	992.0675062

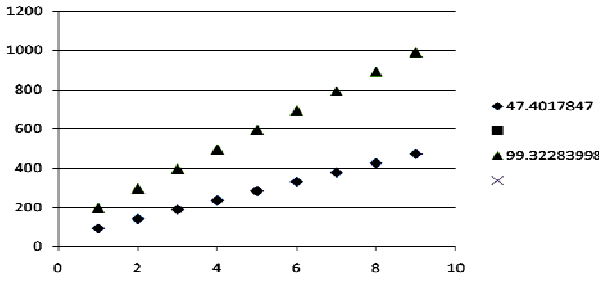

Fig. 2. The diagrams of energy and estrada index.

In Fig. 2, diagrams of our calculations are depicted. From these diagrams we conjecture that the energy is tended to a line, asymptotically. But the Estrada index probably will be curve. Curve fitting is finding a curve which has the best fit to a series of data points and possibly other constraints. We are interested in curve fitting by exponential functions, because polynomials are not good for approximating eigenvalues. Our calculations suggest that the energy and Estrada index of this nanotube can be evaluated by $E(VC_5C_7[4p,8]) = 47.4018 + 47.3(p-1)$ and $EE(VC_5C_7[4p,8]) = 99.3238 + 99.2(p-1)$, respectively.

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