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ESTIMATING THE ENERGY OF NANOHORNS

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ABSTRACT. Let E(NH[n]) denotes the energy of a five pentagons nanohorn, where n is the number of layers of NH[n]. In this paper, some calculations are given in view of estimating the energy of nanohorns.

Keywords: *Energy, nanohorn.*

INTRODUCTION

Fullerenes, carbon nanotubes and carbon nanohorns are three major materials produced by the nanotechnology. Fullerenes are a near spherical cage form of carbon molecule that is neither graphite nor diamond. It was discovered at Rice University in 1985 by R.F. Curl, R.E. Smalley and H.W. Kroto [1]. Carbon Nanotubes (CNTs) were discovered in 1991 by Sumio Iijima [2]. The carbon nanohorns (CNHs) are nanotubes capped by halves of fullerenes. CNHs can serve as vehicles for intracellular delivery and also found interest in photo-voltaic elements because of to their ability to accept electrons and readily diffuse them along the cone. Carbon Nanohorns were first prepared by Harris et al. [3] in 1994. (without this part you loose refs [1] [2] and [3]

Let G be a molecular graph with vertex and edge-sets V(G) and E(G), respectively. The entries in the square matrix A(G) = [a_{ij}] equal 1 if vertices v_i and v_j are neighbors and zero if they are not neighbors or belong to the diagonal. 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 [4].

Let A be an n × n matrix. The scalars λ and vectors x satisfying Ax = λx are called eigenvalues and eigenvectors of A, respectively. 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.

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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. (why do you need bipartite graph IF nanohorn IS NOT bipartite !!!)

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 $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$ of the adjacency matrix A(G). This energy is in good linear correlation with the observed heats of formation of the corresponding conjugated hydrocarbons and it is related to other relevant chemical invariants [5-10].

In a mechanical system, the stable equilibrium positions minimize the potential energy. 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.

The aim of this paper is to investigate the energy of CNH[n] nanohorns, see Figure 1. Notice that the carbon atoms in CNH are entirely sp^+ hybrids, and so our calculations give an approximation of the whole energy of CNH. We encourage the reader to consult papers [11-14] for background material as well as basic computational techniques. Our notation is standard and taken mainly from [4,15].

RESULTS AND DISCUSSION

In this section, the eigenvalues of CNH[n] nanohorn, $1 \leq n \leq 14$, are computed by the matrix package MATLAB. To do this, we first drawn the molecule by HyperChem [16] and then the adjacency matrix of the molecular graphs of nanohorns is computed by TopoCluj software program [17]. In Table 1, we give the energy of these nanohorns for $1 \leq n \leq 14$, according to the Figure 1. Our aim is to apply curve fitting method to find a polynomial of the best degree for approximating the energy of nanohorns.

Suppose F(n) = |V(CNH[n])| and G(n) = |E(CNH[n])|. By solving a simple recursive equation, one can see that $F(n) = n^2 + 20n + 40$ and $G(n) = 3/2\ n^2 + 59/2n + 55$.

Define A[r] = E(CNH[r]), $1 \leq r \leq 14$. We first consider the basic set {A[1], …, A[9]} and apply the least squares method to fit these data by a polynomial F1(x). We have:

$$F(x) = 1.5763\ x^2 + 27.9351\ x + 29.5637. \quad (1)$$

The error of Eq. (1) is E_1 = 3.5219e-004. If we choose the basic set {A[1], …, A[5], A[11], …, A[14]} and apply the least square method then we obtain the following polynomial:

$$G_1(x) = 1.5755\ x^2 + 1.5755\ x + 29.5528. \quad (2)$$

Again the error of Eq. (2) is E_2 = 6.3105e-004. Finally, if we choose the set {A[6],…,A[14]} then we obtain the polynomial $H_1(x) = 1.5746\ x^2 + 27.9574\ x + 29.4968$ with maximum error E_3 = 9.0818e-008.

By using the same data sets for computing polynomials of degree 3, we have:

$$F_2(X) = -0.0004\ x^3 + 1.5829\ x^2 + 27.9073\ x + 29.5927, \quad (3)$$

$$G_2(x) = -0.0001\ x^3 + 1.5783\ x^2 + 27.9256\ x + 29.5751, \quad (4)$$

$$H_2(x) = -0.0000\ x^3 + 1.5748\ x^2 + 27.9553\ x + 29.5031, \quad (5)$$

Then the errors are E_4 = 7.7013e-005, E_5 = 1.9304e-004 and E_6 = 1.7253e-008 for equations (3-5), respectively. Also, it is possible to find four degree polynomials for these data sets, Eqs. (6-8), as follows:

$$F_3(x) = 0.0001\ x^4 - 0.0024\ x^3 + 1.5963\ x^2 + 27.8736\ x + 29.6173, \quad (6)$$

$$G_3(x) = 0.0000\ x^4 - 0.0011\ x^3 + 1.5879\ x^2 + 27.8937 + 29.6031, \quad (7)$$

$$H_3(x) = 0.0000x^4 - 0.0001\ x^3 + 1.5757\ x^2 + 27.9500\ x + 29.5154. \quad (8)$$

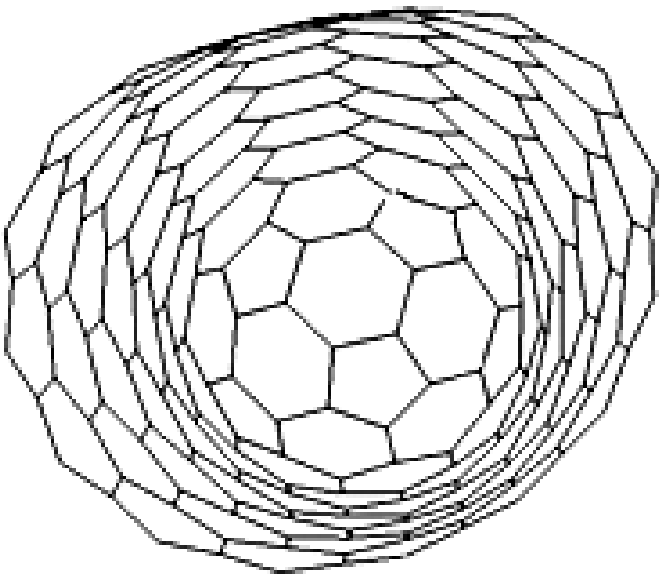

Figure 1. The 3D-Molecular Shape of a Carbon Nanohorn CNH[7].

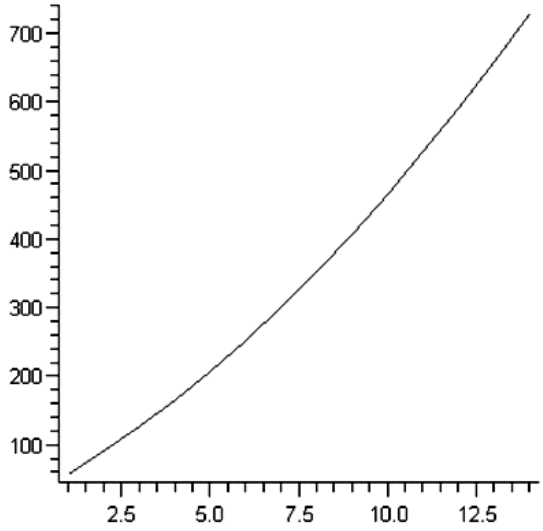

Figure 2. The Diagram of the Energy of Carbon Nanohorn

Table 1. The Energy of CNH[N], $1 \leq N \leq 14$.

n	E(CNH[n])	n	E(CNH[n])
1	59.08575641	**8**	353.9302518
2	91.72904077	**9**	408.6559100
3	127.5493480	**10**	466.5308048
4	166.5226908	**11**	527.5548855
5	208.6496781	**12**	591.7280919
6	253.9269078	**13**	659.0504641
7	302.3537837	**14**	729.5219742

CONCLUSIONS

Suppose A = {A[1], …, A[14]}. If we compute the functions F_1, F_2, F_3, G_1, G_2, G_3, H_1, H_2 and H_3 on the set A and compare them with values of Table 1, then we can see that our functions calculate the energy of nanohorn with almost one digit accuracy. So, it seems that if we want to estimate energy of this nanohorn by polynomials then polynomials of degree 2 is enough exact.

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