OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 3, No. 8, August 2009, p. 821 - 822

A numerical method for computing energy and estrada index of one-pentagonal carbon nanocones

A. R. ASHRAFI*, M. SADATI
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 $E(CNC_5[n]) = 28.7372(1.2)^{n-1}$ and $EE(CNC_5[n]) = 55.5639(1.2)^{n-1}$, where $E(CNC_5[n])$ and $EE(CNC_5[n])$ denote the energy and Estrada index of these nanomaterials.

(Received May 05, 2009; accepted July 20, 2009)

Keywords: Carbone nanocone, Energy, Estrada index

1. Introduction

Let G be a molecular graph without loops and multiple edges and n and m be, respectively, the number of vertices and edges of G. The adjacency matrix A(G) of the graph G is the square matrix of order n whose (i, j)-entry is 1 if the i-th and j-th vertices of G are adjacent, and 0 otherwise. 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. The spectrum of G is formed by the n solutions of the equation $\chi(G, k) = 0$. Each solution of this equation is called an eigenvalues of G. All the eigenvalues of a graph are real-valued numbers, and their sum is equal to zero [1]. The eigenvalues of G are usually denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$ and are assumed to be labeled in a non-increasing sequence $\lambda_1 \le \lambda_2 \le \ldots \le \lambda_n$.

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 biparticity of graphs [14], modeling of extended atomic branching [15], and statistical thermodynamics [16]. We encourage the reader to consult also papers [17-21] 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 [22].

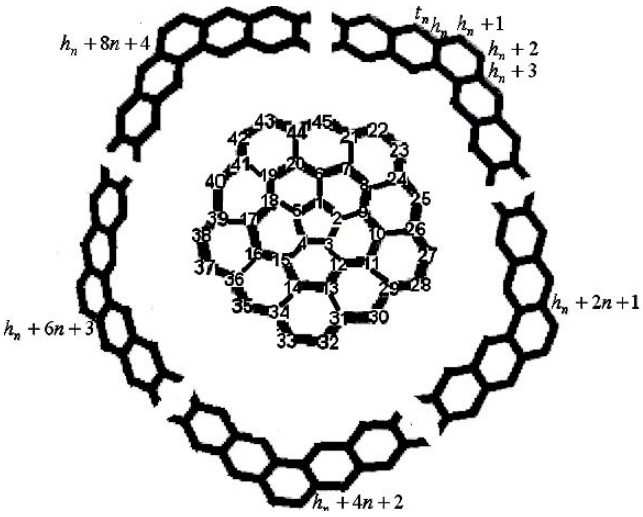

Fig. 1. The one-pentagonal carbon nanocone $CNC_5[4]$.

2. Main results and discussion

In this section, the eigenvalues of the molecular graph of a nanohorn is computed by the matrix package MATLAB. To do this, we first draw the molecule by HyperChem.[23] Then the adjacency matrix of the molecular graph of nanocone $CNC_5[n]$ is computed by TopoCluj. In Table I, we calculate the energy and Estrada index of these nanomaterials for $1 \le n \le 11$. Then by curve fitting method, we find a polynomial of the best degree to approximate the energy and Estrada index of $CNC_5[n]$.

Table 1. The values of E(G) and EE(G) for eleven layers of $CNC_5[n]$.

n	E(G)	EE(G)
1	28.7372	55.5639
2	66.4306	132.3316
3	119.8436	241.8130
4	177.1510	344.3944
5	273.6709	558.9171
6	374.1501	766.5397
7	490.3667	1006.8760
8	622.311	9261.1279
9	769.996	1585.69
10	933.4196	1924.1675
11	1112.5855	2295.3588

Curve fitting is finding a curve which has the best fit to a series of data points and possibly other constraints. DataFit is a science and engineering tool that simplifies the tasks of data plotting, regression analysis (curve fitting) and statistical analysis. This package is applied for solving our problem. The interested readers can check "http://www.oakdaleengr.com/datafit.htm" for further information on this tool. We are interested in curve fitting by exponential functions, because polynomials are not good for approximating eigenvalues. We search for the best exponential function to fit data of Table I. Our calculations suggest that the energy and Estrada index of this nanocone are computed as $E(CNC[n]) = 28.7372(1.2)^{n-1}$ and $E(CNC[n]) = 55.5639(1.2)^{n-1}$. Our method is general and can be applied to compute the energy and Estrada index of nanostructures.

References

[1] D. Cvetkovic, M. Doob, H. Sachs, Spectra of Graphs-Theory and Application, third ed., Johann Ambrosius Barth Verlag, Heidelberg, Leipzig, 1995.

[2] R. Balakrishnan, Linear Algebra Appl., **387**, 287 (2004).

[3] I. Gutman, Ber Math. Statist, Sek. Forsch-ungszentram Graz., **103**, 1 (1978).

[4] I. Gutman, N. Trinajstic, Chem. Phys. Lett. **17**, 535 (1972).

[5] I. Gutman, Topics Curr. Chem. **162**, 29 (1992).

[6] I. Gutman, In: A. Betten, A. Kohnert, R. Loue, A. Wassermann (Eds.), Algebraic Combinatorics and Applications, Springer-Verlag, Berlin, 196 (2001).

[7] A. R. Ashrafi, P. Nikzad, Digest Journal of Nanomaterials and Biostructures **4**, 383 (2009).

[8] A. R. Ashrafi, M. Faghani, S. M. Seyedaliakbar, Digest J. of Nanomaterials and Biostructures **4**, 59 (2009).

[9] E. Estrada, Chem. Phys. Lett. **319**, 713 (2000).

[10] E. Estrada, Bioinformatics **18**, 697 (2002).

[11] E. Estrada, Proteins **54**, 727 (2004).

[12] E. Estrada, J. A. Rodrıguez-Velazquez, Phys. Rev. E **71**, 056103 (2005).

[13] E. Estrada, Phys. Rev. E **75**, 016103 (2007).

[14] E. Estrada, J. A. Rodrıguez-Velazquez, Phys. Rev. E **72**, 046105 (2005).

[15] E. Estrada, J. A. Rodrıguez-Velazquez, M. Randic, Int. J. Quant. Chem. **106**, 823 (2006).

[16] E. Estrada, N. Hatano, Chem. Phys. Lett. **439**, 247 (2007).

[17] I. Gutman, E. Estrada, J. A. Rodrıguez-Velazquez, Croat. Chem. Acta **80**, 151 (2007).

[18] Y. Yiang, H. Zhu, H. Zhang, I. Gutman. Chem. Phys. Lett. **159**, 159 (1989).

[19] I. Gutman, A. Graovac, Chem. Phys. Letters **436**, 294 (2007).

[20] I. Gutman, S. Radenkovic, A. Graovac and D. Plavsic, Chem. Phys. Letters **446**, 233 (2007).

[21] G. H. Fath-Tabar, A. R. Ashrafi, I. Gutman, Bulletin de l'Academie Serbe des Sciences et des Arts **33**, 1 (2008).

[22] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, FL, 1992.

[23] Hyper Chem. package Release 7.5 for Windows, Hypercube Inc., 1115 NW 4th Street, Gainesville, Florida 32601, USA 2002.

[24] M. V. Diudea, O. Ursu, Cs. L. Nagy, TOPOCLUJ, Babes-Bolyai University, Cluj, 2002.

*Corresponding author: alir.ashrafi@gmail.com