Digest Journal of Nanomaterials and Biostructures, Vol. 4, No. 1, March 2009, p. 59 - 61

SOME UPPER BOUNDS FOR THE ENERGY OF $TC_4C_8(S)$ NANOTORI

A. R. ASHRAFI• M. FAGHANI[a], S. M. SEYEDALIAKBAR[b]
Institute for Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, Iran
[a]*Department of Mathematics, Paperme Noor University (PNU), Saveh, Iran*
[b]*Department of Industrial Engineering, Islamic Azad University, South Tehran Branch, Tehran, Iran*

Let G be a molecular graph. The energy of G is defined as the sum of absolute vale of the eigen values of G. In this paper, some upper bounds for computing energy of $TC_4C_8(S)$ nanotorus are presented. Using a MATLAB program, the error of $E(TC_4C_8[m,n])$ for nanotori of diameter ≤ 10 are computed.

(Received January 12, 2009; accepted February 12, 2009)

Keywords: Nanotorus, energy, Molecular graph.

1. Introduction

A molecular graph G is a simple graph in which atoms are vertices and bonds are edges of the graph G. In this graph every vertex has a degree ≤ 4.

In linear algebra, every linear transformation can be given by a matrix, which is a rectangular array of numbers arranged in rows and columns. An eigenvector of a linear transformation is a non-zero vector that is either left unaffected or simply multiplied by a scale factor after the transformation. The eigenvalue of a non-zero eigenvector is the scale factor by which it has been multiplied. A real number λ is an eigenvalue of a linear transformation T: V → V if there is a non-zero vector x such that T(x) = λx.

Let G be a molecular graph. The adjacency matrix A(G) of G is a matrix with rows and columns labeled by graph vertices, with a 1 or 0 in position (v_i,v_j) according to whether v_i and v_j are adjacent or not. For a simple graph with no self-loops, the adjacency matrix must have 0s on the diagonal. The eigenvalues of A(G) are called the eigenvalues of G.[1] Following Ivan Gutman[2], the energy, E(G), of a molecular graph G is defined to be the sum of the absolute values of the eigenvalues of G. We encourage the reader to consult papers[2-4] and references therein for background material as well as basic computational techniques.

•Corresponding author: ashrafi@kashanu.ac.ir

Carbon nanotubes are rolled-up sheets of graphite that can act as metals, semiconductors or insulators, depending on their radius and the angle at which the sheets are rolled. If a nanotube is bent so that its ends meet, a nanotorus is produced. The electronic properties of such structures are less well understood and some of its mathematical properties are determined[5-15]. The aim of this paper is to compute some upperbounds for the energy of TC_4C_8 nanotori, Figures 1, 2.

2. Results and discussion

In graph theory, a regular graph is a graph where each vertex has the same number of neighbors, i.e. every vertex has the same degree or valency. A regular graph with vertices of degree k is called a k-regular graph or regular graph of degree k. Suppose G is k-regular graph with exactly n vertices and m edges. Then m = kn/2 and by a well-known theorem in algebraic graph theory for every eigenvalue λ, $|\lambda| \leq k$. Therefore, for such graphs $E(G) \leq nk$.

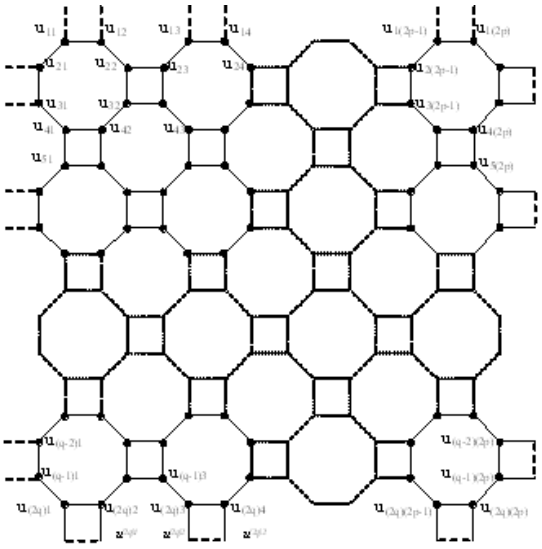
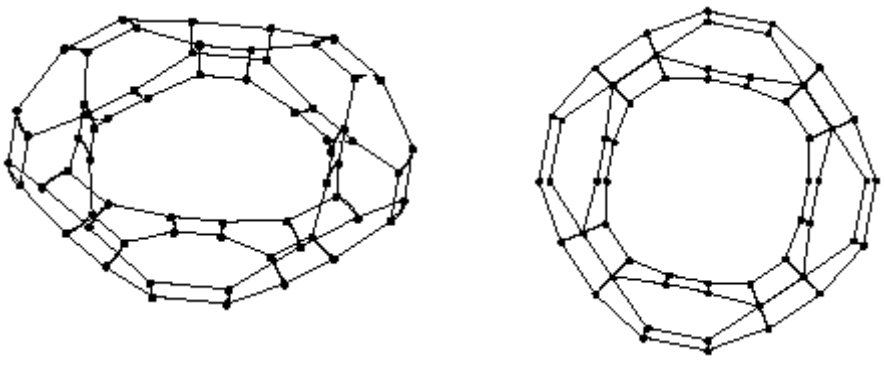


Fig. 1. 2-Dimensional Graph of $C_4C_8(S)$ nanotorus.



(a) (b)

Fig. 2. An $TUC_4C_8(S)$ Nanotorus (a) Side view (b) Top view.

Consider a T(m,n) = $TUC_4C_8(S)$ nanotorus, in which m and n are two times of the number octagons in every row and column, respectively, Figure 2. It is clear that this molecular graph has exactly 2mn vertices and 3mn edges. Since T(m,n) is cubic, E(T(m,n)) ≤ 6mn. On the other hand, by a well-known result on the subject of graph energy, E(G) ≤ k + $\sqrt{k(n-1)(n-k)}$, for n-vertex k-regular graph G. Since T(m,n) is cubic, E(T(m,n)) ≤ 3 + $\sqrt{3(2mn-1)(2mn-3)}$. Our calculations by MATLAB PACKAGE shows that if T(m,n) has diameter ≤ 10 then E(G) ≈ 3 + $\sqrt{3(2mn-1)(2mn-3)}$.

Acknowledgement. This work was partially supported by Institute of NanoSciTech of the University of Kashan.

References

[1] D. M. Cvetkovic, M. Doob, H. Sachs, Spectra of Graph Theory and Applications, VEB Deutscher Berlin; Academic Press, New York, **1979**.
[2] I. Gutman, Ber. Math.-Statist. Sect. Forschungsz. Graz., 103, 1 (**1978**)
[3] R. Balakrishnan, Lin. Algebra Appl. 387, 287 (**2004**).
[4] H. S. Ramane, H. B. Walikar, S. B. Rao, B. D. Acharya, P. R. Hampiholi, S. R. Jog, I. Gutman, Appl. Math. Lett., 18, 679 (**2005**).
[5] M. V. Diudea, B. Parv, E. C. Kirby, MATCH. Commun. Math. Comput. Chem., **47**, 53 (2003).
[6] M. V. Diudea, Bull. Chem. Soc. Japan., **75**, 487 (2002).
[7] M. V. Diudea, MATCH. Commun. Math. Comput. Chem., **45**, 109 (2002).
[8] M. V. Diudea, P. E. John, MATCH. Commun. Math. Comput. Chem., **44**, 103 (2001).
[9] M. V. Diudea, E. C. Kirby, Fullerene. Sci. Technol., **9**, 445 (2001).
[10] A. R. Ashrafi, A. Loghman, J. Comput. Theor. Nanosci. **3**, 378 (2006)
[11] A. R. Ashrafi, F. Rezaei, MATCH Commun. Math. Comput. Chem. **57**, 243 (2007)
[12] S. Yousefi, A. R. Ashrafi, J. Math. Chem. **42**, 1031 (2007).
[13] A. R. Ashrafi, S. Yousefi, Nanoscale Res. Lett. **2**, 202 (2007).
[14] S. Yousefi,A. R. Ashrafi, MATCH Commun. Math. Comput. Chem. **56**, 169 (2006).
[15] A. R. Ashrafi, S. Yousefi, MATCH Commun. Math. Comput. Chem. **57**, 403 (2007).