Digest Journal of Nanomaterials and Biostructures Vol. 3, No.4, December 2008, p. 209 - 214

COMPUTING BIPARTITE EDGE FRUSTRATION OF SOME NANOTUBES

Masoumeh Ghojavand, Ali Reza Ashrafi*
Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I. R. Iran

The smallest number of edges that have to be deleted from a molecular graph G to obtain a bipartite spanning subgraph is called the bipartite edge frustration of G, denoted by φ(G). In this paper this number is computed for some important classes of nanotubes.

(Received September 12, 2008; accepted September 22, 2008)

Keywords: Bipartite edge frustration, polyhex nanotube, C_4C_8 nanotube, C_5C_7 nanotube.

1. Introduction

Let G = (V,E) be a simple graph, a graph without multiple edges and loops. A subgraph S of G is a graph whose set of vertices and set of edges are all subsets of G. A spanning subgraph is a subgraph that contains all the vertices of the original graph. The graph G is called bipartite if the vertex set V can be partitioned into two disjoint subsets V_1 and V_2 such that all edges of G have one endpoint in V_1 and the other in V_2. Bipartite edge frustration of a graph *G*, denoted by φ(G), is the minimum number of edges that need to be deleted to obtain a bipartite spanning subgraph.

It is easy to see that φ(G) is a topological index and G is bipartite if and only if φ(G) = 0. Thus φ(G) is a measure of bipartivity. It is a well-known fact that a graph G is bipartite if and only if G does not have odd cycles. Holme, Liljeros and Edling introduced the edge frustration as a measure in the context of complex network, [8].

In [5,6] Fajtlowicz claimed that the chemical stability of fullerenes is related to the minimum number of vertices/edges that need to be deleted to make a fullerene graph bipartite. We mention here that before publishing the mentioned papers of Fajtlowicz, Schmalz et al. [10] observed that the isolated pentagon fullerenes (IPR fullerenes) have the best stability. Doslic [1], presented some computational results to confirm this relationship. So it is natural to ask about relationship between the degree of non-bipartivity of nanotubes and their stability.

Throughout this paper all graphs considered are finite and simple. Our notation is standard and taken mainly from [7,9]. We encourage the reader to consult papers by Doslic [1-4] for background material and more information on the problem. Our main results are the following two theorems:

Theorem 1. Suppose E = $TUC_4C_8(R)[p,q]$, Figure 1, and F = $TUC_4C_8(S)[p,q]$, Figure 2, are C_4C_8 nanotubes in which p and q are the number of rhombs and squares in each row and column, respectively. Then φ(F) =0 and

$$\varphi(E) = \begin{cases} 0 & 2 \mid p \\ q & 2 \nmid p \end{cases}.$$

Theorem 2. Suppose A = $HC_5C_7[r,t]$, B = $VC_5C_7[r,t]$, C = $SC_5C_7[r,t]$ and D = $HAC_5C_7[r,t]$ are C_5C_7 nanotubes, where 2r is the number of pentagons in each period and t is the number of periods, Figures 3-7. Then φ(B) = φ(C) = φ(D) = 2rt and we have:

* Corresponding author: alir.ashrafi@gmail.com

$$\varphi(A)=\begin{cases}2rt-\frac{r}{2} & 2\mid\frac{r}{2}\\ 2rt-\frac{r}{2}+1 & 2\nmid\frac{r}{2}\end{cases}.$$

We encourage the reader to consult papers by Diudea and his co-author for some background material as well as basic computational methods on mathematical properties of nanomaterials, [11-13].

2. Results and discussion

In this section the edge frustration number of five infinite class of nanotubes containing $TUC_4C_8(R)[p,q]$, $TUC_4C_8(S)[p,q]$, $HC_5C_7[r,t]$, $VC_5C_7[r,t]$, $SC_5C_7[r,t]$ and $HAC_5C_7[r,t]$ are computed. At first, we compute $\varphi(TUC_4C_8(R))$, Figure 1. If p is even then obviousely the molecular garph of $TUC_4C_8(R)[p,q]$ is bipartite and so $\varphi(TUC_4C_8(R)) = 0$. Suppose p is odd. Then E has a cycle of length 3p and so it is not bipartite. We notice that the subgraph H constructed from G by deleting edges $e_1, ..., e_q$, Figure 1, is biparetite. This implies that $\varphi(TUC_4C_8(R)) \leq q$. On the other hand, it is clear that we cannot find less that q edges such that the graph constructed from G by deleting them, is bipartite. Thus $\varphi(TUC_4C_8(R)) = q$.

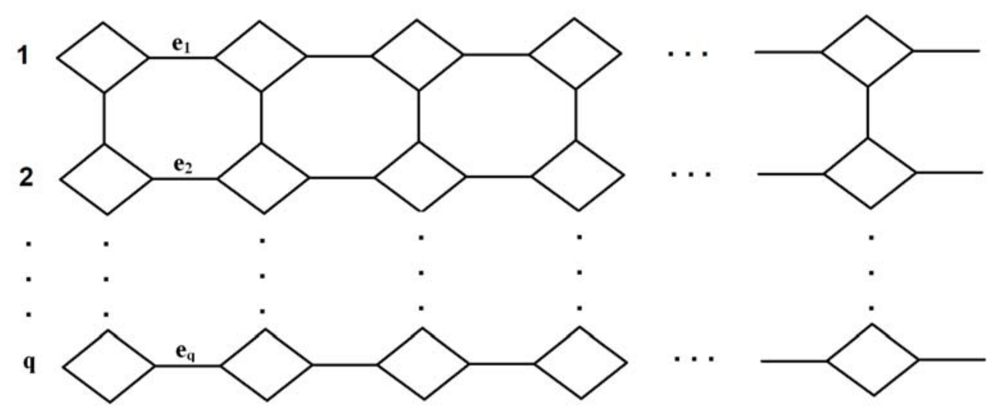

Fig. 1. The 2-dimensional Lattice of $TUC_4C_8(R)[p,q]$.

In Figure 2, a 2-colouring of the graph $TUC_4C_8(S)[p,q]$ is presented and so $\varphi(TUC_4C_8(S)) = 0$.

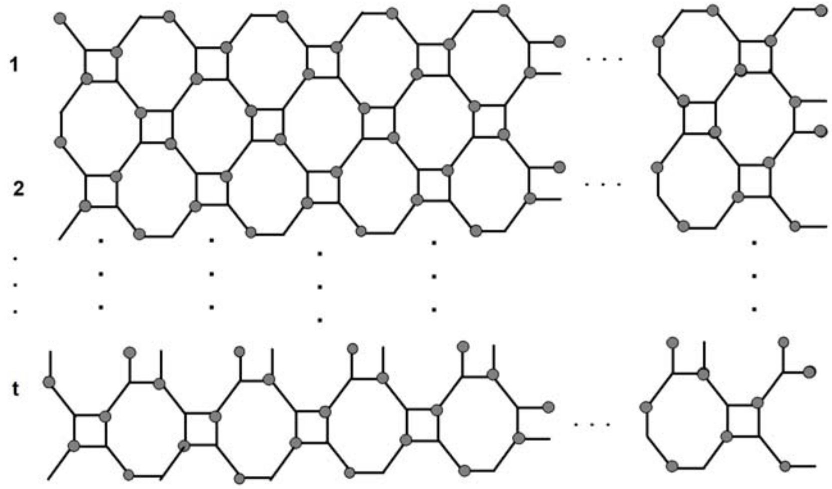

Fig. 2. The 2-dimensional Lattice of $TUC_4C_8(S)[p,q]$.

We now consider the $HC_5C_7[r,t]$ nanotube constructed from t copies of the graph L depicted in Figure 3. Obviously r is even. We first consider the case that r/2 is even. In Figure 3, a 2-dimensional representation of this graph is depicted. In this case, the odd length cycles have exactly 5 and 7 edges. Therefore, we must deleted at least one edge from each pentagon and heptagon. To compute $\varphi(HC_5C_7[r,t])$, we must delete the common edges between all pentagon – pentagon and heptagon – heptagon of the molecular graph of $HC_5C_7[r,t]$ nanotube. From Figure 4, one can see that there are rt edges between pentagon-pentagon and tr/2 + (t-1)r/2 edges between heptagon – heptagon of the graph. Therefore, $\varphi(HC_5C_7[r,t]) = 2rt - r/2$.

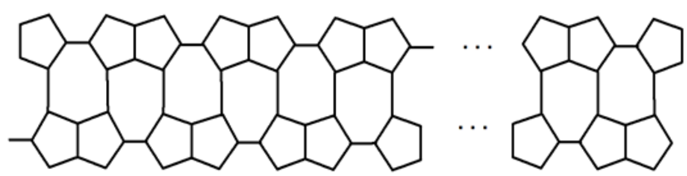

Fig. 3. The Graph L.

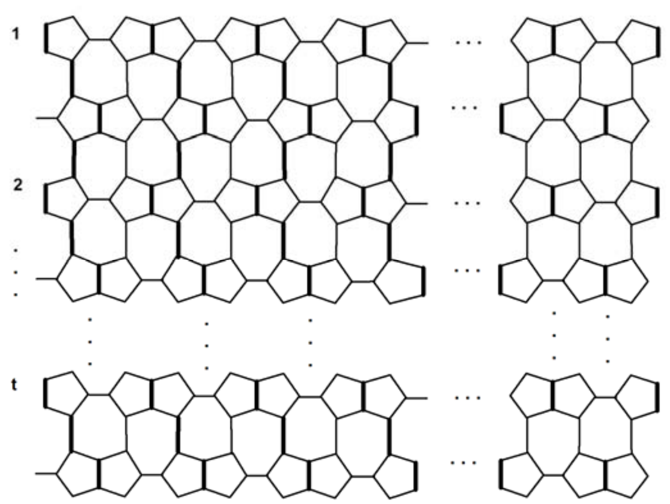

Fig. 4. The 2-Dimensional Lattice of $HC_5C_7[r,t]$ when r/2 is even.

We now assume that r/2 is odd. In this case there are other odd cycles of length 5r/2. To delete these cycles, we must change our algorithm. In Figure 5, our deletion algorithm is depicted. By this figure, one can prove $\varphi(HC_5C_7[r,t]) = 2rt - r/2 + 1$.

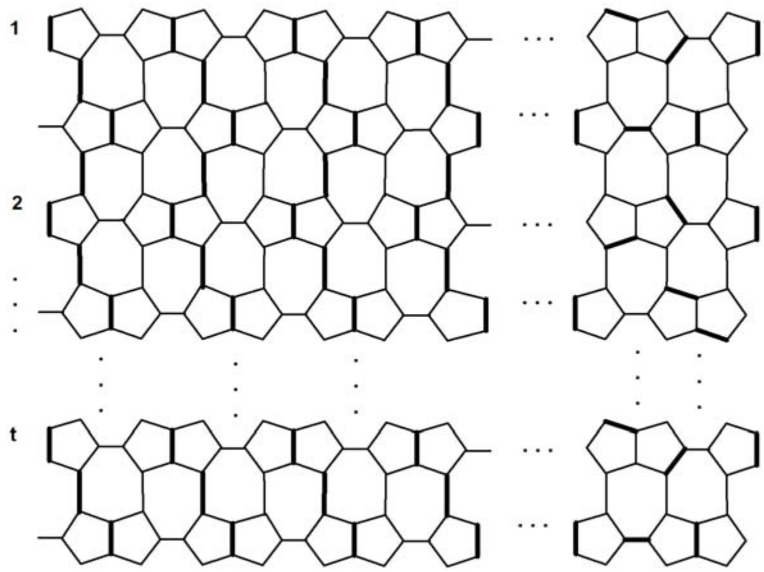

Fig. 5. The 2-Dimensional Lattice of $HC_5C_7[r,t]$ when r/2 is Odd .

Considet the molecular graph of $VC_5C_7[r,t]$ nanotube. The only odd cycles of this graph are pentagons and heptagons. Using a similar method as in $HC_5C_7[r,t]$, we delete edges between adjacent pentagons and adjacent heptagons to construct a bipartite graph. From Figure 6, one can see that $\varphi(VC_5C_7[r,t]) = rt + rt = 2rt$.

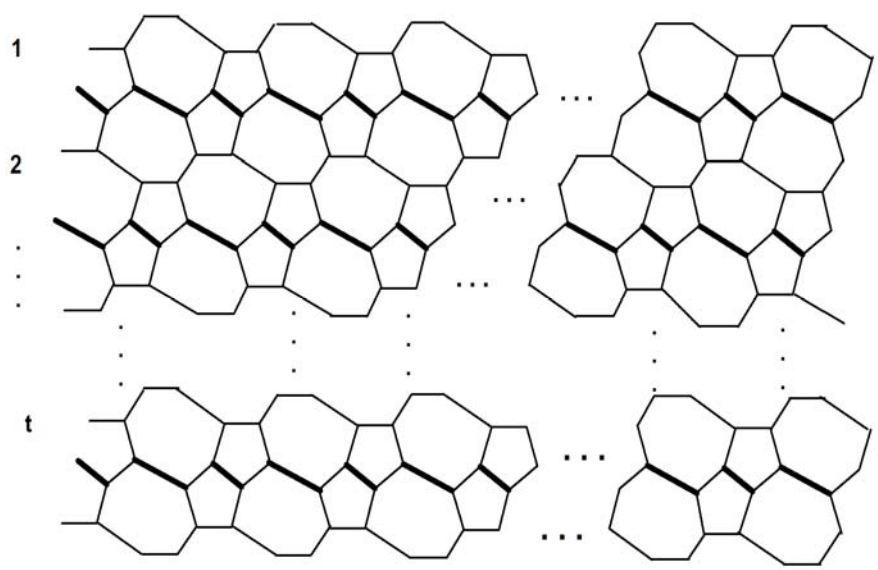

Fig. 6. The 2-dimensional Lattice of $VC_5C_7[r,t]$.

Finally, we consider the molecular graph of $SC_5C_7[r,t]$ and $HAC_5C_7[r,t]$. These molecular graphs have exactly three types of odd cycles containing pentagons, heptagons and cycles of a lengths j. It is possible to choose edges e_i's for deletion such that e_i's are edges of pentagons and heptagons, see Figures 7,8. Therefore, φ(SC_5C_7[r,t]) = φ(HAC_5C_7[r,t]) = 2rt.

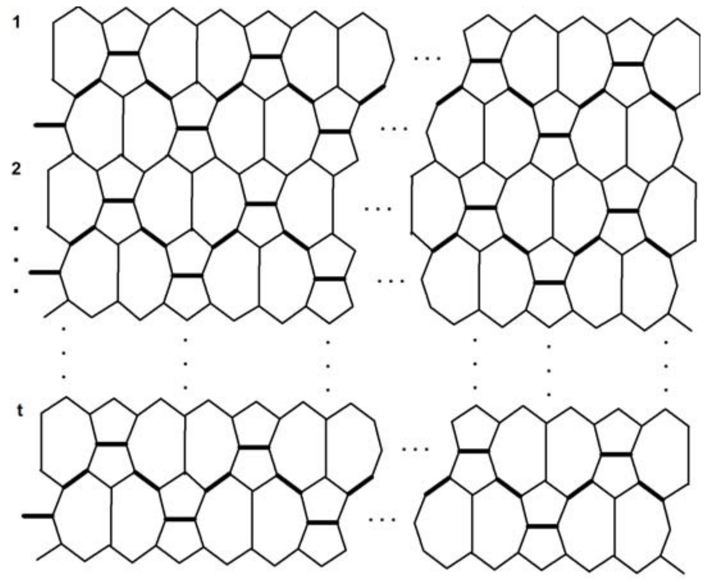

Fig. 7. The 2-dimensional Lattice of $SC_5C_7[r,t]$.

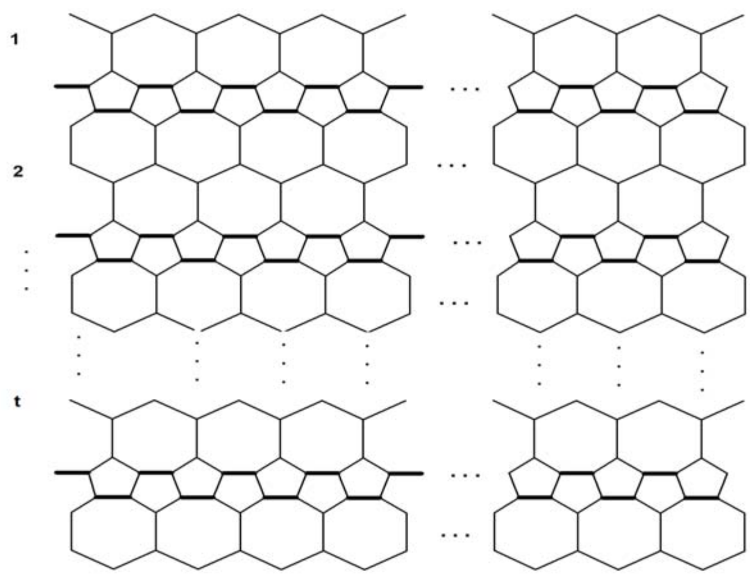

Fig. 8.The 2-dimensional Lattice of $HAC_5C_7[r,t]$.

Acknowledgement

This research was in part supported by a grant from the Center of Excellence of Algebraic Methods and Applications of Isfahan University of Technology.

References

[1] T. Doslic, Chem. Phys. Lett. **412,** 336 (2005).
[2] T. Doslic, D Vukicevic, Discrete Applied Mathematics **155**, 1294 (2007).
[3] T. Doslic, J. Math. Chem. **31,** 187 (2002).
[4] T. Doslic, Graph Theory Notes NY **XLVI**, 49 (2004).
[5] S. Fajtlowicz, C. E. Larson, Graph-theoretic independence as a predictor of fullerene stability, Chem. Phys. Lett., **377** (2003) 485–490.
[6] S. Fajtlowicz, http://www.math.uh.edu/~clarson/#fajt.
[7] P. W. Fowler, D. E. Manolopoulos, An Atlas of Fullerenes, Clarendon Press, Oxford, 1995.
[8] P. Holme, F. Liljeros, G.R. Edling, B.J. Kim, Phys. Rev. E **68**, 056107 (2003).
[9] F. Harary, Graph Theory, Addison-Wesley, Reading, MA, 1969.
[10] T. G. Schmalz, W. A. Seitz, D. J. Klein, G. E. Hite, Chem. Phys. Lett. **130,** 203 (1986).
[11] M. V. Diudea, MATCH Commun. Math. Comput. Chem. **45,** 109 (2002).
[12] M. V. Diudea, P. E. John, MATCH Commun. Math. Comput. Chem. **44,** 103 (2001).
[13] M. V. Diudea, M. Stefu, B. Pârv, P. E. John, Croat Chem Acta **77,** 111 (2004).