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FRUSTRATION INDEX OF HAC_5C_7 NANOTORUS

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Frustration index is the least number of edges whose deletion results in a balanced subgraph. Its complement is the largest size of a balanced subgraph. It has turned out of a molecular graph G and defined the smallest number of edges that have to be deleted from the graph to obtain a bipartite spanning subgraph , which denoted by φ(G). In this paper, this number is computed for HAC_5C_7 nanotorus.

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1. Introduction

In chemical graph theory and in mathematical chemistry, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory.A novel molecular topological index *MTI*(*E*) is proposed, based on edge-distances in molecular graphs. Edge-distances in a graph are equal to distances between vertices of the respective line graph with various physical .A topological index is a numerical value associated with chemical constitution purporting for correlation of chemical structure properties,chemical reactivity or biological activity.

The Hosoya index is the first topological index recognized in chemical graph theory, and it is often referred to as the topological index . Other examples are the Wiener index, Randić's molecular connectivity index, Balaban's J index, and others.

Let G = (V,E) be a simple graph, a molecular 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.

Frustration index is the least number of edges whose deletion results in a balanced subgraph. Its complement is the largest size of a balanced subgraph. It has turned out of a molecular graph G is one of the most important characteristics of molecules and defined the smallest number of edges that have to be deleted from the graph to obtain a bipartite spanning,subgraph which denoted by φ(G).

In [8-11], the frustration as a measure in the context of complex network.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. 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. In this paper, we continue this program to compute the bipartite edge frustration of HAC_5C_7 nanotorus. 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.

2. Results and discussion

Frustration index of a molecular graph is minimum size of a deletion set (least number of edges) that must be removed from graph in order to leave a bipartite graph. In this section the edge frustration number of HAC_5C_7 nanotorus (Figure. 1), is determined.

Theorem. Suppose that G be molecular garph of HAC_5C_7 [r,t] nanotorus. Then

$$\varphi(G)=\begin{cases}8rt-2 & ;\ if\ r\equiv 0\ (\mathrm{mod}\ 2)\ and\ t\equiv 0\ (\mathrm{mod}\ 2)\\ 8rt-r+t; & if\ r\equiv 1\ (\mathrm{mod}\ 2)\ and\ t\equiv 1\ (\mathrm{mod}\ 2)\\ 8rt-t/2+1; & if\ r\equiv 1\ (\mathrm{mod}\ 2)\ and\ t\equiv 0\ (\mathrm{mod}\ 2)\\ 8rt-r/2+1; & if\ r\equiv 0\ (\mathrm{mod}\ 2)\ and\ t\equiv 1\ (\mathrm{mod}\ 2)\end{cases}$$

Proof. We now consider the HC5C7[r,t] nanotorus constructed from t copies of the graph G,depicted in Figure 1. For computing frustration index, we have four cases for r,t.We first consider the case that r is even. In this case,there is two subcases : t is even or odd. we must deleted at least one edge from each pentagon and heptagon. To compute φ(HC5C7[r,t]), we must delete the common edges between all pentagon –pentagon and heptagon – heptagon of the molecular graph of HC5C7[r,t] nanotorus. From Figure 1, the number of these edgesis equal to 8rt-2 and 8rt-r/2+1 . Therefore in this case φ(HC5C7[r,t]), is determined.Another cases is similarly obtained.

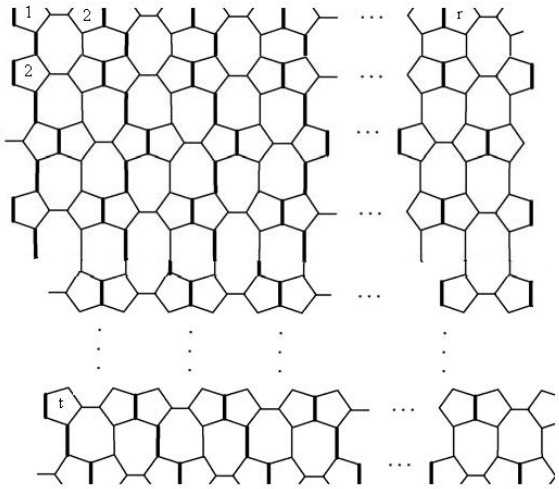

Fig. 1. A molecular Graph of HAC_5C_7 nanotorus.

3. Conclusion

A nanotorus is ideally suited for studying the effects of delocalized deformations and can, in fact, lead to an understanding of the interplay between the mechanical deformation and electronic properties of SWNTs. In this paper, the frustration index of the structural model of carbon nanotorus is determined.

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References

[1] Doslic T, Chem. Phys. Lett.2005, **412,** 336.
[2] Doslic T, Vukicevic D, Discrete Applied Mathematics.2007, **155**, 1294.
[3] Doslic T, J. Math. Chem. 2002, **31,** 187.
[4] Doslic T, Graph Theory Notes NY **XLVI**, 49 (2004).
[5] Fajtlowicz S , Larson C E ,Chem. Phys. Lett.2003, **377,** 485.
[6] Fajtlowicz S, http://www.math.uh.edu/~clarson/#fajt.
[7] Fowler P W , Manolopoulos D E , An Atlas of Fullerenes, Clarendon Press, Oxford, 1995.
[8] Holme P, Liljeros F , Edling G R, Kim B J, Phys. Rev. E.2003, **68**, 056107.
[9] A. Bahrami, J. Yazdani,Digest Journal of Nanomaterials and Biostructures,**4**,141(2009).
[10] H. Yousefi, A. Bahrami, J. Yazdani and A.R. Ashrafi ,J. Comp .Theor .Nanosci ,**4**. (2007).
[11] A. Bahrami, J.Yazdani ,Digest Journal of Nanomaterials and Biostructures**,**3**,265**(2008).
[12] Harary F , Graph Theory, Addison-Wesley, Reading, MA, 1969.