Digest Journal of Nanomaterials and Biostructures Vol. 4, No.2, June 2009, p. 369 – 371

SOME PHYSICO-CHEMICAL CHARACTERISTICS OF Y-JUNCTION CARBON NANOTUBES

Javad Yazdani [a], Amir Bahrami[b]
[a]*Nanoscience and Nanotechnology Research Center, Razi University, Kermanshah , Iran.*
[a]*Young Researchers Club, Islamic Azad University , Garmsar Branch , Garmsar , Iran.*

Y- junction nanotubes can be formed from chemical vapor deposition, welding two crossed nanotubes with an electron beam at high temperature, or using irradiation techniques on an touching tubes to form a Y- tube. In this paper, we propose a method to compute bipartite edge frustration of Y- junction nanotube for first time.

(Received April 29, 2009; accepted May 4, 2009)

Keywords: Molecular graph, Y-tubes, Y- junction nanotubes , Bipartite edge frustration.

1. Introduction

The first structural models for symmetric carbon nanotube Y-junctions based on theoretical calculations [2, 3] were proposed shortly after the discovery of multiwall carbon nanotubes by Iijima [1]. Both models are based on the insertion of non-hexagonal (n-H) rings (at least six heptagons) in the hexagonal network in the region where the three branches of the Y are joined together. All the subsequent structural models [4-9] follow the same construction principle of conserving the sp^2 hybridization of the carbon network, differing only in the kind, number and placement of the n-H rings. These variations make possible the constructions of various symmetric and asymmetric model junctions[8]and various angles from Y to T shapes[4] .A Y-junction is named symmetric if the three carbon nanotubes joining each other in the Y have identical chirality and the distribution of the n-H rings around the Y is symmetric. Such a junction will be constituted from identical branches oriented at 120°, like in Fig.1a. Whenever one of the above conditions is not fulfilled the junction will be asymmetric, a possible example is shown in Fig.1b. For all industrial application of nanotubes, whether single-walled, multiwalled or Y-junctions or other types of nanotubes, efficient and well-controlled synthesis methods are of great importance.

In this paper, the most important Physico-Chemical characteristic called " Bipartite edge frustration "of Structural models of Y-junctions carbon nanotube is computed .Bipartite edge frustration number of a molecular graph *G*, denoted by φ(G), is most important quantity in physicochemistry (particularly in Kekule structures) and defined the minimum number of edges that need to be deleted to obtain a bipartite spanning sub graph. It is a well-known theorem in graph theory that a graph G is bipartite if and only if G does not have odd cycles.

In Refs[10-13] The authors compute φ(G) for some types of fullerenes and nanotubes.In this paper, we continue this program to compute the bipartite edge frustration of Structural models of symmetric Y-junctions carbon nanotube (fig.1(a)) and armchair Y -junction nanotube (fig.1(b)).Throughout this paper ,all graphs considered are finite and simple. Our notation is standard and taken mainly from [14].

* Corresponding author: bahrami@khayam.ut.ac.ir

2. Results and discussion

Edge frustration number 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 Structural models of symmetric Y-junctions carbon nanotube (fig.1(a)) and armchair Y -junction nanotube (fig.1(b))and armchair Y -junction nanotube (fig.1(b)) is determined. For this computation , Suppose that G=YJN[r,r,t] and H=YJAN[r,r,t] be the molecular graph of symmetric and armchair of Y-junctions carbon nanotube (fig.1(a) , 1(b)) respectively.

Theorem. Suppose that G ,H be molecular garph of YJN[r,r,t] and YJAN[r,r,t] ,respectively. Thus

$$\varphi(G)=\varphi(H)=\begin{cases}4rt-r & ;\ if\ r\equiv 0\ (\mathrm{mod}\ 2)\ and\ t\equiv 0\ (\mathrm{mod}\ 2)\\ 4rt-r+2; & if\ r\equiv 1\ (\mathrm{mod}\ 2)\ and\ t\equiv 1\ (\mathrm{mod}\ 2)\\ 2rt; & if\ r\equiv 1\ (\mathrm{mod}\ 2)\ and\ t\equiv 0\ (\mathrm{mod}\ 2)\\ 2rt-r/2+1; & if\ r\equiv 0\ (\mathrm{mod}\ 2)\ and\ t\equiv 1\ (\mathrm{mod}\ 2)\end{cases}$$

Proof . If r and t are even then obviousely the molecular garph G = YJN [r,r,t] , is not bipartite and, We notice that the subgraph H constructed from G by deleting edges e1, ..., e4rt-r is biparetite. This implies that φ(G) ≤ 4rt-r.On the other hand, it is clear that we cannot find less that 4rt-r edges such that the graph constructed from G by deleting them, is bipartite. Thus in this case φ (G) = 4rt-r.In other cases, φ (G) is similarly computed. For molecular graph H, proof is similar.

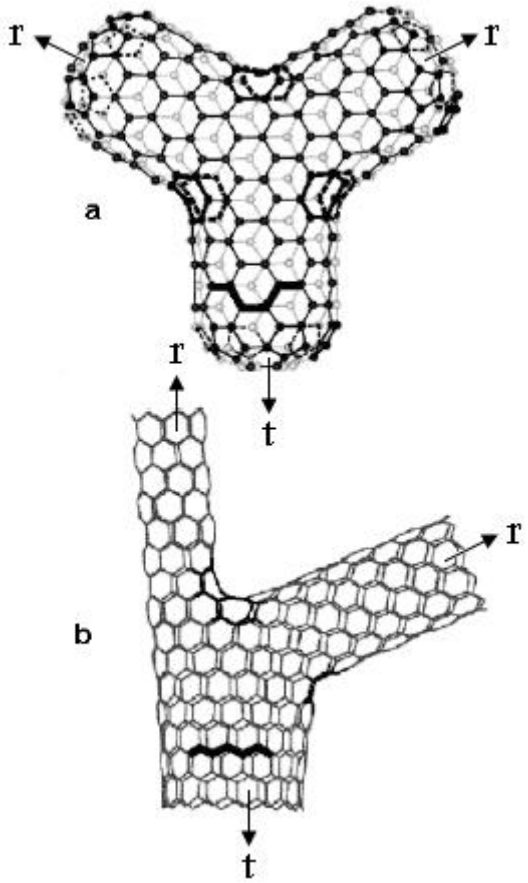

Fig. 1. Structural models of Y-junctions carbon nanotubes. Symetric (a), armchair (b).

3. Conjectures

Conjecture1 . Suppose that n is an arbitrary natural number. There is a Y-junction nanotubes G, such that φ (G) = n.

Conjecture2. Suppose that G and H are two molecular graph of Y-junction nanotubes such that φ(G) = φ(H). Then the molecule of G is isomer by H?

4. Conclusion

Carbon nanotube junctions are of great interest in the fundamental research and nanoelectronic applications. In this paper, the edge frustration number of structural models of carbon nanotube Y-junctions are determined.

Refrences

[1] S. Iijima, Nature, **354**, 56(1991).
[2] G. E. Scuseria., Chem. Phys. Lett,**195**, 534(1992).
[3] L. A. Chernozatonskii. Phys. Lett. A,**172**,173(1992).
[4] M. Menon, D. Srivastava. Phys. Rev. Lett.,**79**,4453(1997).
[5] G. Treboux, P. Lapstun, K. Silverbrook. Chem. Phys. Lett,**306**,402(1999).
[6] A. A. N. Andriotis, M. Menon, D. Srivastava, L. Chernoztatonskii. Appl. Phys. Lett, **79**, 266 (2001).
[7] A. N. Andriotis, M. Menon, D. Srivastava and L. Chernozatonskii. Phys. Rev. Lett,**87**,66802(2001).
[8] V. Meunier, M. Buongiorno Nardelli, J. Bernholc, Th. Zacharia and J.-Ch. Charlier. Appl. Phys. Lett,**81**,5234(2002).
[9] G.E. Scuseria. Chem. Phys. Lett,**195**,534(1992).
[10]T.Doslic, J. Math. Chem, **31,** 187(2002).
[11]S.Fajtlowicz, C.E. Larson ,Chem. Phys. Lett, **377,** 485(2003).
[12]P. Holme, F.Liljeros , G.R.Edling, B.J.Kim, Phys. Rev. E., **68**,56107(2003).
[13] M. Ghojavand, A. R. Ashrafi, Digest Journal of Nanomaterials and Biostructures , **3**, 209 (2008).
[14] F.Harary, Graph Theory, Addison-Wesley, Reading, MA, 1969.