OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 4, No. 6, June 2010, p. 900 - 901

Automatic generation of adjacency matrix of single-wall carbon nanohorn

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Computing adjacency matrix of the molecular graph of a molecule is the first step to extract math/chemical features of that molecule. Some clusters of molecules grow up in a chain of desired length and so finding adjacency matrix of such long compounds may be so hard. The molecular graphs of carbon nanotubes, nanohorns and nanocones have this property. In this article, the molecular graph of a single-wall carbon nanohorn (SWHN) with different number of carbon atoms is automatically generated and so its adjacency matrix is calculated. Automatic drawing by graphviz, an open source and free software for drawing graph, generate shape of SWHN.

(Received August 13, 2009; accepted June 16, 2010)

Keywords: Automatic graph generation, Nanohorn, SWHN, Wiener index

1. Introduction

In this paper, a new method for semi-automatic generation of some nanohorn graph is presented. Drawing a molecule requires precise molecular specification and calculation of the angles. However, we might not be able to find the precise specification of the molecule under study.

Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. The adjacency matrix of G is an $n \times n$ matrix $A = (a_{ij})$ in which the entry $a_{ij} = 1$ if there is an edge from vertex v_i to vertex v_j and is 0 if there is no edge from vertex v_i to vertex v_j. By the way, a matrix with only zeros and ones as entries is called a (0,1) matrix. It is easy to see that this matrix is uniquely determined by the graph and vice versa. The adjacency matrix of a molecule is defined as the adjacency matrix of its molecular graph. Notice that a given molecule M has too many adjacency matrices that all of them are similar.

To calculate the adjacency matrix of a molecule, we need a labeling of the molecular graph of the molecule involved and we do not need their shapes. In this article, we have proposed a method for creating a graph for a nanohorn. This method is not time consuming, containing development, implementation and execution time. In addition, we have used specific programming language and tools that help us to facilitate the achievement of our goals. This method for creating the graph of nanohorn molecule can be used for other similar molecules. Our programs are accessible from the authors upon request. We encourage the reader to consult papers [1-4] for background materials as well as basic computational techniques.

2. Single walled carbon nanohorn

Nano-structured materials have attracted a great deal of attention in materials science and considerable applications, such as electronic devices and energy-related applications. The Single Walled Carbon Nano Horn (SWNH) is one of the most attractive new forms of nano carbons and has excellent prospects for a wide range of technological applications because of its unique structural properties [5]. SWNHs were found during a chemical research on carbon nanotubes [6].

SWHNs are categorized as nanocones molecules. Cones can be formed by cutting a wedge from planar graphite and connecting the exposed edges in a seamless manner. The opening angle of the wedge, called the disclination angle, is $n(\pi/3)$, with $0 \leq n \leq 6$. This disclination angle is related to the opening angle of the cone by $\square = 2\times\sin^{-1}(1\text{-}n/6)$. Two-dimensional planar structures e. g., a graphene sheet are associated with $n = 0$, and one-dimensional cylindrical structures, such as the nanotubes, are described by $n = 6$. All other possible graphitic cone structures with $0 < n < 6$ have been observed in a sample generated by pyrolysis of hydrocarbons [7]. According to Euler's theorem, the terminating cap of a cone with the disclination angle $n(\pi/3)$ contains n pentagons that substitute for the hexagonal rings of planar graphite [8]. Cone angle of carbon nanohorn is precisely 20^o (corresponding to a $5\pi/3$ disclination) direction of individual cones is radiated out from the center of sphere [9]. It implies that all nanohorns contain exactly five pentagons near the tip [8]. The interlayer spacing between SWNHs approximately is 0.4 nm, about 18% wider than that of graphite [10].

The structure of nanohorns is classified by distinguishing the relative positions of the carbon pentagons at the apex which determine the morphology of the terminating cap [8]. Nano-horns with all five pentagons at the "shoulder" of the cone, yielding a blunt tip, are shown in Figs. 1(a)-(c). Nanohorns with a pentagon at the apex of the tip, surrounded by the other four pentagons at the shoulder, are shown in Figs 1(d)-(f) [8].

3. Molecular graph of nanohorn

Computing adjacency matrix implies having access to the nanohorn graph. Nanohorn graph can be found from precise structure of nanohorn molecule. There is a different method to determine the structural properties of nanohorns such as using the parameterized linear combination of atomic orbitals (LCAO) technique [8] or using hyperboloid geometry within the continuum model [11]. But developing these methods is hard and needs long execution time. Suppose NH[n] denotes the nanohorn with n layers, Figure 1. The proposed method is well described through the following steps:

1. In the first level, there is one pentagon.
2. The second level contains five hexagons, which surrounds the pentagon in the first level.
3. There are four pentagons and six hexagons at the third level.
4. There are 11 hexagons at the fourth level, 12 hexagons at the fifth level, 13 hexagons at the 6th level and so on.
5. From fourth level, eight hexagons are fixed. We call these hexagons type I and the last hexagons are assigned to be type II.
6. *Type I:* Each hexagon is constructed with respect to other hexagons, but they are the same with the corresponding hexagons at the previous level.
7. *Type II:* Each hexagon is constructed similar to other hexagons at this level and similar to hexagons at the previous level. Hence, for the construction of each hexagon of type II the same procedure is used n times, where n is the level number.
8. The graph can be achieved by running instruction on step 6 and 7.

Python programming language and networkx package are used to implement this approach. Graphviz software and pygraphviz package are used for constructing the shape of the graph. The following figures show the resulting graph with a different level. This Fig. 1 is depicted by graphviz.

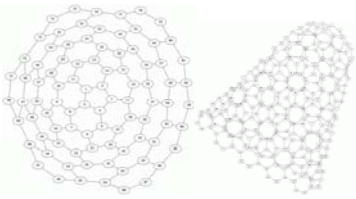

Fig. 1. The molecular graph of nanohorn NH[n], n = 5, 12.

4. Conclusions

In this paper, we have introduced a simple extendable method for calculating the molecular graph of a nanohorn. By this method, we can easily calculate some invariant of a nanohorn graph such as the Wiener index. We are not sure weather or not there exist nanohorn molecule with 19241 carbon atoms, but we can calculate its mathematical properties through the application of the method proposed in this study.

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