Calculation of Wiener index for some single-wall carbon nanohorn

A. Yoosofan , A. Ashrafi

Department of computer engineering, Faculty of engineering, University of Kashan, Kashan 87317-51167, I. R. Iran
Department of Mathematics, Faculty of Science, University of Kashan, Kashan 87317-51167, I. R. Iran

Abstract

Let G be a simple graph and V(G) and E(G) be vertices and edges of G, respectively. The distance between each of the two vertecies (u,v) is defined as the minimum number of vertices which should be traversed so that they can reach each other. The Wiener index of this graph, denoted by W(G), is defined as the sum of all distances between unordered pairs of vertices[1] . A conjunction of nanocone and cylindrical carbon cluster is recognized as the single-wall carbon nanohorn (SWHN) [2]. In this article, the Wiener index of some nanohorn is calculated.

1 Introduction

In this paper, a new method is used for semi_automatic generation of some nanohorn graph. Drawing one nano 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.
To Calculate Wiener index of such new melocules, we need the graph of the molecules involved and and we do not need their shapes. In this article, we have proposed a method for creating a graph for one nanohorn. This method is not time consuming(development, implementation and execution time). It is interesting that the graphs which are shown with some tools look like the real molecule in case they are expanded.
Also, we have used specific programming language and tools which help us facilitate the achivement of goals. This method for creating the graph of nanohorn molecule can be used for other similar molecules.

2 Single wall 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 Wall Carbon Nano Horn (SWNH) is one of the most attractive new forms of nanocarbons and has excellent prospects for a wide range of technological applications because of its unique structural properties[3]. SWNHs were found during a chemical research on carbon nanotube[4].

SWHNs are categorized as nanocones melecules. 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 $0<=n<=6$. This disclination angle is related to the opening angle of the cone by $\Theta=2\sin^{-1}(1-n/6)$. 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

[5]. According to Euler's rule, 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

[6] 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[7] . It implies that all nanohorns contain exactly five pentagons near the tip[6]. The interlayer spcaing between SWNHs approximatiely is 0.4 nm, about 18% wider than that of graphite [8] .

Structure of nanohorns is calssified by distinguishing the relative positions of the carbon pentagons at the apex which determine the morphology of the terminating cap[6]. 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). [6]

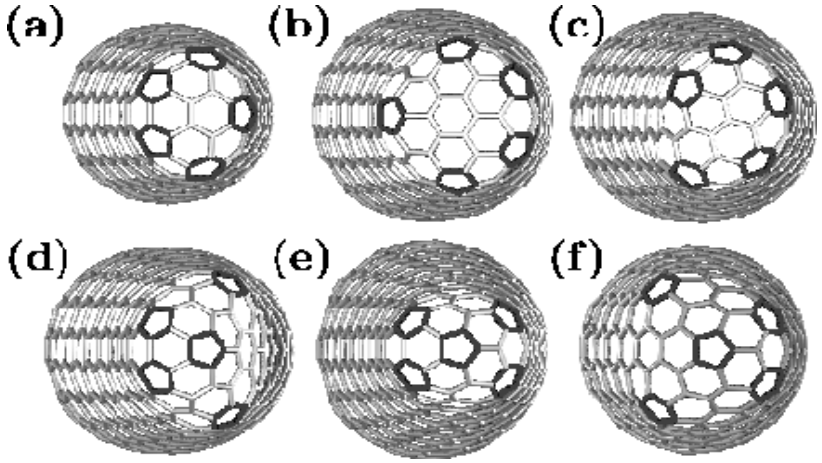

FIG1.

Structure of six carbon nanohorn [6]

In this paper we work on nanohorn whose structure is shown in fig1(e).

3 Graph of nanohorn

Adjacent matrix of nanohorn graph is needed to find Wiener index. Finding the adjacent matrix implies having access to the nanohorn graph. Nanohorn graph can be found from precise structure of nanohorn moloecule. There is a different method to determine the structural properties of nanohorns such as using the parameterized linear combination of atomic orbitals (LCAO) technique [6] or using hyperboloid geometry within the

continuum model [9] . But developing these methods is hard and needs long execution time.

The proposed method is well described through the following steps:

1. At the first level there is one pentagon.
2. The second level contains five pentagons which surround the pentagon of first level.
3. There are four pentagons and six hexagons at the third level.
4. There are eleven hexagons at the fourth level, twelve 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 eight hexagons Section I and the last hexagones are assigned to Section II.
6. In section I, construction of each hexagon is different with respect to other hexagons in this section but are the same with the coresponding hexagons at the previous level.
7. In section II. construction of each hexagon is similar to other hexagons at this level and similar to hexagons at the previous level. Hence, for the construction of each hexagon in section II the same procedure is used n times, where n is level number.
8. The graph can be achived by runnig 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 showing the shape of the graph. The following figures show the resulting graph with a different level.

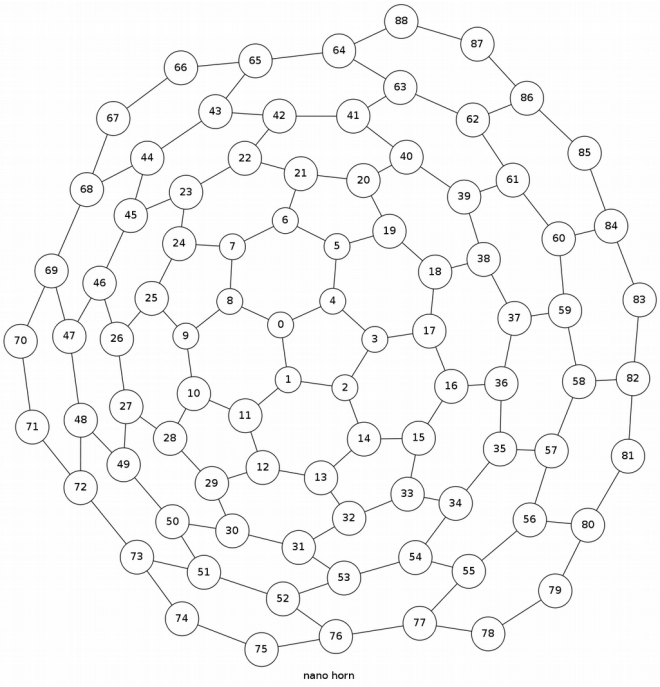

Fig 2graph of nanohorn with 6 level

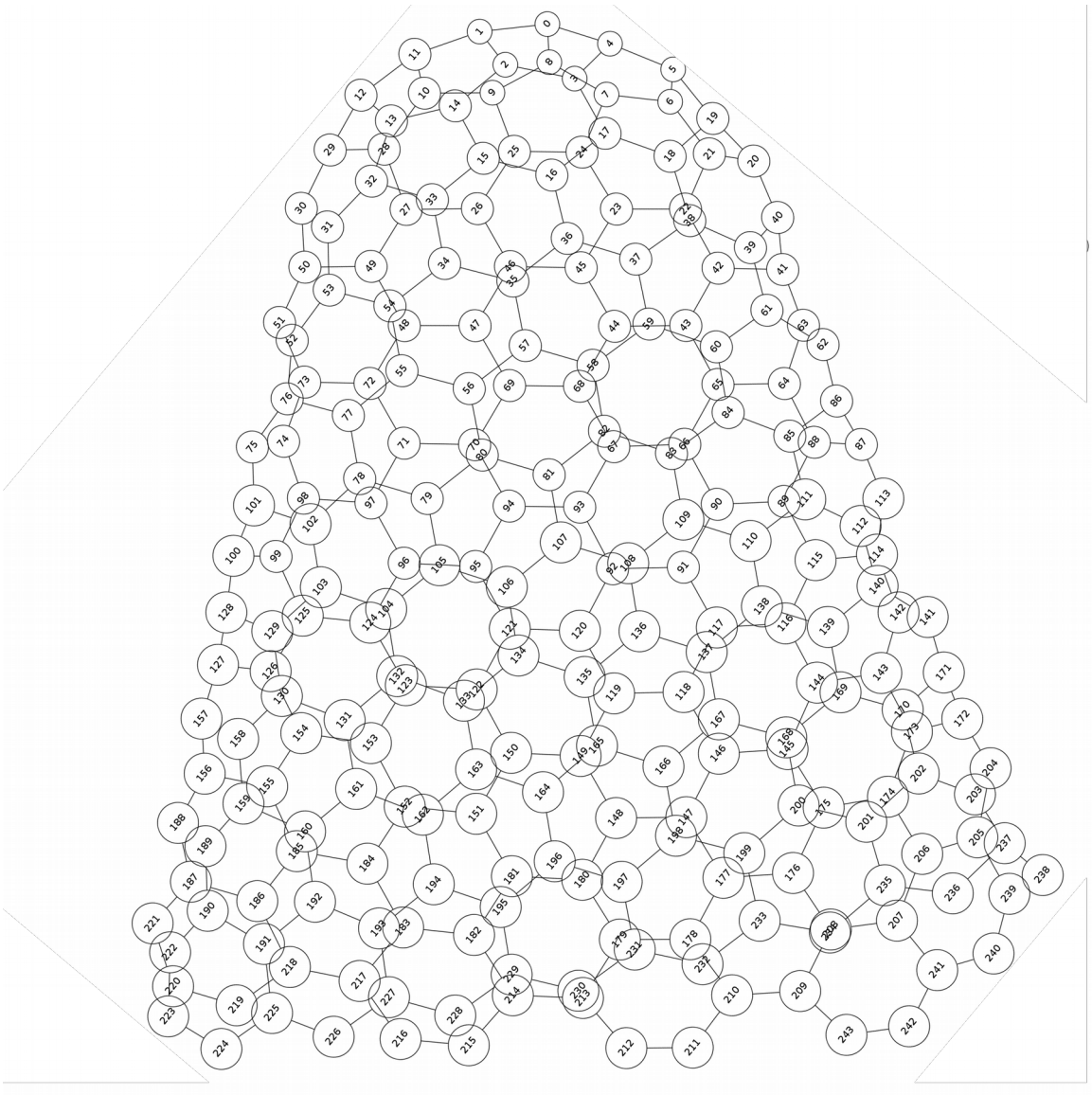

Fig 3 graph of nanohorn with 9 leve 1

Fig 3 Shows that automatic shape is generated with our method which looks like the real nanohorn molecule.

4 Calculation of Winer index

Let G be a connected graph with vertex and edge sets V(G) and E(G), respectively. As usual, the distance between the vertices u and v of G is denoted by d(u,v) and it is defined as the number of edges in a minimal path connecting the vertices u and v.

A topological index is a real number related to a graph. It must be a structural invariant, i.e., it does not depend on the labeling or the pictorial representation of a graph. There are several topological indices have been defined and many of them have found applications as means for modeling chemical, pharmaceutical and other properties of molecules[10].

The Wiener index W was the first topological index to be used in chemistry. It was introduced in 1947 by Harold Wiener, as the path number for characterization of alkanes [11]. In chemical language, the Wiener index is equal to the sum of all shortest carbon–carbon bond paths in a molecule. In graph theoretical language, the Wiener index is equal to the count of all shortest distances in a graph. For more information on the Wiener index and its applications we encourage the reader to consult papers by Dobrynin and co-authors [12] and [13] and references therein.

The following table shows the Wiener index of nanohorn graph with different level.

Table 1: Wiener index of nanohorn with different level

Level	n vertex	Wiener	Level	N vertex	Wiener	Level	N vertex	Wiener
1	5	15	20	704	4367111	100	11584	5024205143
2	20	615	21	761	5317447	101	11801	52663443519
3	41	3683	50	3284	212468623	120	16304	11826616651
4	64	11014	51	3401	232017099	130	18964	17266373455
5	89	24658	70	6004	967070631	131	19241	17904729571

5 Conclusion

In this paper, we have introduced a simple but precise and generalizable method for delivering a nanohorn graph. Therefore we can easily calculate the mathematical aspects of a nanohorn graph such as Wiener index. Probably there is no real nanohorn molecule with 19241 carbon on its structure, but we can calculate its mathematical properties through the application of the method proposed in this study.

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