

On Wiener index of special case of link of fullerenes

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Let Σ be the class of finite graphs. A topological index is a function Top from Σ into real numbers with this property that $Top(G) = Top(H)$, if G and H are isomorphic. is defined as half sum of the distances between all the pairs of vertices in a molecular graph. The goal of this paper is to further the study of Wiener index of special case of a chain of fullerenes.

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1. Introduction

The discovery of C_{60} bucky-ball, which has a nanometer-scale hollow spherical structure in 1985 by Kroto and Smalley revealed a new form of existence of carbon element other than graphite, diamond and amorphous carbon [1, 2]. Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms. Suppose p , h , n and m are the number of pentagons, hexagons, carbon atoms and bonds between them, in a given fullerene F . Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is $n = (5p + 6h)/3$, the number of edges is $m = 3/2n = (5p + 6h)/2$ and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $(5p + 6h)/3 - (5p + 6h)/2 + p + h = 2$, and therefore $p = 12$, $v = 2h + 20$ and $e = 3h + 30$. This implies that such molecules made up entirely of n carbon atoms and having 12 pentagonal and $(n/2 - 10)$ hexagonal faces, where $n \neq 22$ is a natural number equal or greater than 20 [3, 4].

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics [5-7]. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [8]. This theory had an important effect on the development of the chemical sciences. Nowadays hundreds of researchers work in this area producing thousands articles annually.

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. If e is an edge of G , connecting the vertices u and v , then we write $e = uv$ and say " u and v are adjacent". A connected graph is a graph such that there is a path between all pairs of vertices.

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is a function Top from Σ into real numbers with this property that $Top(G) = Top(H)$, if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological index. The Wiener^{9,10} index is the first reported distance based topological index and is defined as half sum of the distances between all the pairs of vertices in a molecular graph. If $x, y \in V(G)$ then the distance $d_G(x, y)$ between x and y is defined as the length of any shortest path in G connecting x and y . Herein, our notation is standard and taken from the standard book of graph theory [8, 11-14].

2. Main results and discussion

As mentioned before, the Wiener index was introduced by H. Wiener in 1947 as follows:

$$W(G) = \sum_{x, y \in V(G)} d(x, y).$$

Let G_1 and G_2 be two simple and connected graphs with disjoint vertex sets. For given vertices $x \in V(G_1)$ and $y \in V(G_2)$, a link of two graphs G_1 and G_2 is defined as the graph $(G_1 \sim G_2)(x, y)$ obtained by joining x and y by an edge (see figure 1). For simply we show the link of G_1 and G_2 by $G_1 \sim G_2$. The link of graphs $G_1, G_2, \dots, G_n$ is $G_1 \sim G_2 \sim \dots \sim G_n$. Furthermore if $G_1 = G_2 = \dots = G_n = G$ we use of the notation $G \overset{n}{\sim} G$. In this section we compute the Wiener index of link graphs. Balakrishnan¹⁵ compute the Wiener index of a graph with exactly n cut-edges. Here we compute the Wiener index of a chain of C_{20} fullerenes by a new method.

Lemma 1. The Wiener index of fullerene C_{20} is $W(C_{20}) = 500$.

Proof. For every vertex u in $V(C_{20})$ it is easy to see that $\sum_{x \in V(C_{20})} d(u, x) = 50$. By definition of Wiener index the proof is completed.

Theorem 2. Consider the chain graph G in figure 1. The Wiener index of G is as follows:

$$W(G \sim G) = 2W(G) + 2|V(G)|D_G(v) + |V(G)|^2,$$

in which, $D_G(u) = \sum_{v \in V(G)} d(u, v)$.

Proof.

$$\begin{aligned} W(G \sim G) &= \sum_{x, y \in V(G \sim G)} d(x, y) = 2 \sum_{x \in V(G_1)} \sum_{y \in V(G_2)} d(x, y) + 2 \sum_{x, y \in V(G_1)} d(x, y) \\ &= 2W(G) + 2 \sum_{x \in V(G_1)} d(x, u) + d(y, v) + 1 \\ &= 2W(G) + |V(G_1)| (D_G(u) + D_G(v)) + |V(G)|^2 \\ &= 2W(G) + 2|V(G)|D_G(v) + |V(G)|^2. \end{aligned}$$

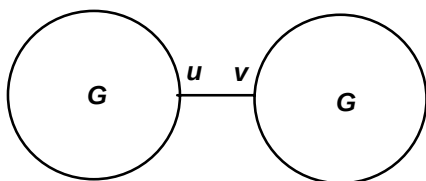


Fig. 1. Link of Graphs $G \sim G$.

Corollary 3. Consider the chain graph G in Fig. 2. The Wiener index of G is as follows:

$$W(G) = 2W(C_{20}) + 450 + 2000 = 3400.$$

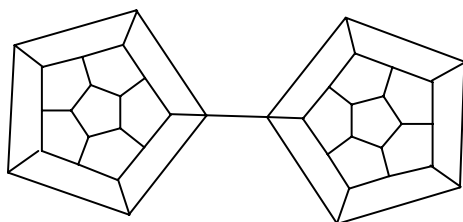


Fig. 2. Link Graph $C_{20} \sim C_{20}$.

Theorem 4. Consider a chain graph of fullerene C_{20} depicted in Fig. 3. Then we have:

$$W(G) = 100n(2n^2 + 6n - 3).$$

Proof. In the following let $G_i = C_{20}$, $(1 \leq i \leq n)$ and

$H = C_{20} \sim C_{20} \sim \dots \sim C_{20}$. One can see that:

$$\begin{aligned} W(H) &= \sum_{x, y \in V(H)} d(x, y) = \sum_{i=1}^n \sum_{x, y \in V(G_i)} d(x, y) \\ &\quad + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{x \in V(G_i)} \sum_{y \in V(G_j)} [d(x, v_{2i-1}) + d(y, v_{2j-2}) + 3(j-i) - 2] \\ &= \sum_{i=1}^n W(G_i) + \sum_{i=1}^{n-1} \sum_{j=i+1}^n [|V(G_j)| D_{G_i}(v_{2i-1}) + |V(G_i)| D_{G_j}(v_{2j-2}) \\ &\quad + |V(G_i)| |V(G_j)| (3(j-i) - 2)]. \end{aligned}$$

On the other hand we know, $|V(G_i)| = 20$, $(1 \leq i \leq n)$ and by lemma 1 for every $v \in V(C_{20})$, we have $D_{G_i}(v) = 50$ and $W(C_{20}) = 500$. This completes the proof.

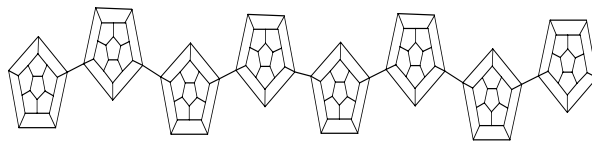


Fig. 3. Link Graph $C_{20} \sim C_{20} \sim \dots \sim C_{20}$.

References

- [1] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R. E. Smalley, *Nature* **318**, 162 (1985).
- [2] H. W. Kroto, J. E. Fichier, D. E. Cox, *The Fullerene*, Pergamon Press, New York, 1993.
- [3] P. W. Fowler, D. E. Manolopoulos, *An Atlas of Fullerenes*, Oxford Univ. Press, Oxford, 1995.
- [4] B. Kostant, *Notices of the AMS* **9**, 959 (1995).
- [5] N. Trinajstić, I. Gutman, *Croat. Chem. Acta* **75**, 329 (2002).
- [6] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, 1986.
- [7] S. J. Cyvin I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons*, Lecture Notes in Chemistry **46**, Springer-Verlag, Berlin, 1988.
- [8] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, FL, 1992.
- [9] H. Wiener, *J. Am. Chem. Soc.* **69**, 17 (1947).
- [10] H. Hosoya, *Disc. Appl. Math.* **19**, 239 (1988).
- [11] M. Ghorbani, A. R. Ashrafi, M. Hemmasi, *Optoelectron. Adv. Mater. – Rapid Comm.* **3**(12), 1306 (2009).
- [12] A. R. Ashrafi, M. Ghorbani, M. Jalali, *Optoelectron. Adv. Mater. – Rapid Comm.* **3**(8), 823 (2009).
- [13] A. R. Ashrafi, M. Ghorbani, *Optoelectron. Adv. Mater. – Rapid Comm.* **3**(6), 596 (2009).
- [14] A. R. Ashrafi, M. Ghorbani, M. Hemmasi, *Digest Journal of Nanomaterials and Biostructures* **4**, 483 (2009).
- [15] R. Balakrishnan, N. Sridharan, K. Wisvanathan Iyer, *Appl. Math. Lett.* **21**, 921 (2008).

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