Wiener index of organosilicon dendrimer

H. YOUSEFI-AZARI[a] A. R. ASHRAFI[b,*], M. H. KHALIFEH[a]
[a]*School of Mathematics, Statistics and Computer Science, University of Tehran, Tehran, I. R. Iran*
[b]*Department of Nanocomputing, Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I. R. Iran*

The Wiener index of a molecular graph *G* is defined as the sum of all distances between the atoms of G. Here, distance between two atoms is defined as the length of a minimum path connecting them. Nakayama and Lin in [*Tetrahedron Letters*, **38** (34) (1997), 6043-6046] prepared the organosilicon dendrimer composed of 16 thiophene rings, $C_{64}H_{44}S_{16}Si_5$. In this paper the Wiener index of the general form of this dendrimer is computed for the first time.

(Received August 12, 2013; accepted September 11, 2014))

Keywords: Organosilicon dendrimer, Wiener index

1. Introduction

A *graph G* is defined as a pair $G = (V,E)$, where V is defined to be a finite non-empty set of vertices and E is the set of edges. A *molecular graph* is a graphical model for a molecule in which atoms are the set of vertices and edges are bonds between them. The distance between the vertices x and y, $d(x,y)$, is defined as the length of a shortest path connecting them. The Wiener index is defined as the half-sum of all distances in the hydrogen-depleted graph representing the skeleton of the molecule [1]. We encourage the reader to consult papers [2,3] for more information on chemical meaning and mathematical properties of the Wiener index.

Dendrimers are highly branched macromolecules. These molecules constructed from a core and some similar branches connected to the core in a mathematical progression [4]. Diudea and his co-workers [5-10] considered the topological properties of some infinite classes of dendrimers. In some recent papers [11-16] the authors spent their times for computing exact formulas for the Wiener type indices of dendrimers. In the present article, a new efficient method is presented by which it is possible to compute the Wiener index of graphs constructed from independent cycles. Here two cycles are said to be independent if they don't have common edge. We apply our method for the general form of an organosilicon dendrimer G[n], Fig. 1 [17].

Throughout this paper, our notation is standard and taken mainly from the standard books of graph theory.

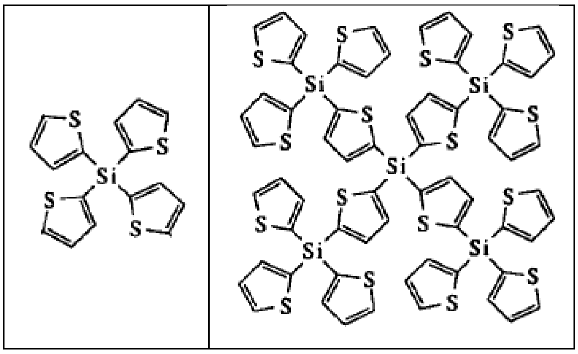

Fig. 1. The Molecular Graph of G[1] (left) and G[2] (right).

2. Results and discussion

The aim of this section is to compute the organosilicon dendrimer $G[n]$, $n \geq 1$. This dendrimer is first synthesized in 1997 [17]. The molecular graph of $G[n]$ is containing $4\sum_{i=0}^{n-1} 3^i = 2(3^n - 1)$ pentagons and so $G[n]$ is not bipartite. It also has $4\sum_{i=0}^{n-2} 3^i + 1 = 2 \times 3^{n-1} - 1$ vertices outside pentagons. If g_n denotes the number of vertices of organosilicon dendrimer $G[n]$ then

$$g_n = 4\left(\sum_{i=0}^{n-1} 6 \times 3^i - 3^{n-1}\right) + 1 = 32 \times 3^{n-1} - 11.$$

From the molecular graph of organosilicon dendrimer, one can see that $G[n]$ is constructed from four isomorphic branches having a common vertex. So, each branch has exactly $8(3^{n-1} - 3)$ vertices. We now describe our method. Let G be a connected graph and $\mathcal{R}$ be a set of shortest paths in G such that for each vertex $x, y \in V(G)$, there is a unique shortest path in $\mathcal{R}$ connecting x and y. Suppose e is an edge of G and $n_R(e)$ is the number of paths in $\mathcal{R}$ passing e. Then

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v) = \sum_{e\in E(G)} n_R(e) \qquad (1)$$

In the following results we fix a set $\mathcal{R}$ of shortest paths in *G* and assume that for a natural number *d*, $d^c = g_n - d$. Moreover, a pentagon P in G[n] is called terminal, if it has exactly four vertices of degree 2. Otherwise, we call P to be internal.

Lemma 1. Suppose $A[n]$ denotes the set of edges of $G[n]$ outside pentagons. Then

$$\sum_{e\in A[n]} n_R(e) = 2048 \times n \times 3^{2n-2} - 320 \times 9^n + 416 \times 3^n - 96.$$

Proof. From the Fig. 1, it is easy to see that for each non-boundary internal pentagon P of G[n] there are two cut edges of G[n] connecting to P. By deleting these cut edges of G[n], we obtain two components where one of them has exactly S_r or $S_r - 5$ vertices, $1 \le r \le n - 1$. Here, r denotes distance from core. We denote by $(S_r)^c$ or $(S_r - 5)^c$ the number of vertices of other component. Suppose e is such a cut edge. Then each shortest path connecting vertices from two components mentioned above traverse e. So, $n_R(e) = S_r \times (S_r)^c$ or $(S_r-5) \times (S_r-5)^c$ and the number of such edges is $4\times 3^{n-r}$. Therefore,

$$\sum_{e\in A[n]} n_R(e) = 4 \times 5 \times 5^c \times 3^{n-1} + 4 \times \Big[\sum_{i=0}^{n-2} 3^i \,(S_{n-i} \times (S_{n-i})^c + (S_{n-i} - 5) \times (S_{n-i} - 5)^c)\Big] = 2048 \times n \times 3^{2n-2} - 320 \times 9^n + 416 \times 3^n - 96.$$

A pentagon P of G[n] is called terminal, if it has exactly four vertices of degree 2. Otherwise, we call P, internal.

Lemma 2. Suppose U[n] is the set of all edges of G[n] on cycles of length five. Then

$$\sum_{e\epsilon U[n]} n_R(e) = 2^{11} \times n \times 9^{n-1} - \frac{896}{3} 9^n + 1178 \times 3^{n-1} - 94.$$

Proof. Consider an internal pentagon P of G[n] depicted in Fig. 2. Using a similar method as those are given in the proof of Lemma 1, there exists a positive integer r such that:

$n_R(e_1) = (S_r - 3)((S_r - 3)^c - 2) + 1$ and $n_R(e_2) = (S_r - 4)((S_r - 4)^c - 2) + 1$.

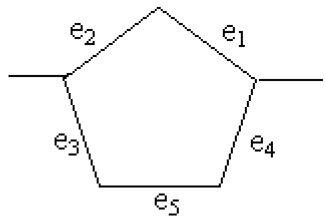

Fig. 2. An Internal Pentagon in G[n].

Since the elements of $\mathcal{R}$ are shortest paths of G[n], we have:

$n_R(e_3) = 2(S_r - 4) + 1$, $n_R(e_4) = 2(S_r - 1)^c + 1$, $n_R(e_5) = (S_r - 4) + (S_r - 1)^c + 1$.

By the Fig. 1, the numbers of internal pentagons are $4 \times 3^{n-r}$, $2 \le r \le n$. We now consider a terminal pentagon Q as depicted in Fig. 2.

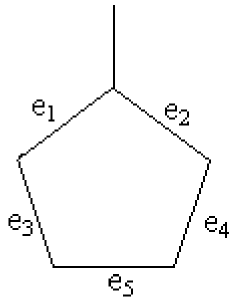

Fig. 2. A Terminal Pentagon in G[n].

One can easily seen that $n_R(e_5) = 3$, $n_R(e_3) = n_R(e_4) = g_n - 2$, $n_R(e_1) + n_R(e_2) = 4(g_n - 4) + 2$. On the other hand the numbers of terminal pentagons are $4 \times 3^{n-1}$. Since $W(G[n]) = \sum_{e\epsilon U[n]} n_R(e)$, we have:

$$W(G[n]) = 4 \times \Big[\sum_{i=0}^{n-2} 3^i\big((S_{n-i} - 3)\times((S_{n-i} - 3)^c - 2) + (S_{n-i} - 4)\times((S_{n-i} - 4)^c - 2) + 2(S_{n-i} - 4) + 2(S_{n-i} - 1)^c + (S_{n-i} - 4) + (S_{n-i} - 1)^c + 5\big) + 3^{n-1}(4(g_n - 4) + 2(g_n - 2) + 5)\Big].$$

To prove the lemma, it is enough to substitute g_n and S_{n-i}, in above equation.

We are now ready to prove the main result of this paper.

Theorem. The Wiener index of G[n] is computed as follows:

$$W(G[n]) = 2^{12} \times n \times 9^{n-1} - \frac{1856}{3} 9^n + 2426 \times 3^{n-1} - 190.$$

Proof. By choosing a set $\mathcal{R}$ of shortest paths for G[n] and Eq. 1, we have:

$$W(G[n]) = \sum_{e\epsilon E(G[n])} n_R(e) = \sum_{e\epsilon U[n]} n_R(e) +$$

$\sum_{e \in A[n]} n_R(e)$.

To prove theorem, it is enough to apply Lemmas 1 and 2.

Acknowledgment

We are indebted to the referee for reading carefully our paper and his/her suggestions and helpful remarks. This research is partially supported by Iran National Science Foundation (INSF) (Grant No. 86043/17).

References

[1] H. Wiener, J. Am. Chem. Soc. **69**, 17 (1947).
[2] A. A. Dobrynin, R. Entringer, I. Gutman, Acta Appl. Math., **66**, 211 (2001).
[3] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Acta Appl. Math.**, 72**, 247 (2002).
[4] G. R. Newkome, C. N. Moorefield, F.Vögtle, Dendrimers and Dendrons, Eds. Wiley-VCH Publishers, New York, 2001.
[5] M. V. Diudea, B. Parv, J. Chem. Inf. Comput. Sci., **35**, 1015 (1995).
[6] M. V. Diudea, A. E. Vizitiu, M. Mirzargar, A. R. Ashrafi, Carpath. J. Math., **26**, 59 (2010).
[7] A. Karbasioun, A. R. Ashrafi, M. V. Diudea, MATCH Commun. Math. Comput. Chem., **63**, 239 (2010).
[8] A. R. Ashrafi, A. Karbasioun, M. V. Diudea, MATCH Commun. Math. Comput. Chem., **65**, 193 (2011).
[9] K. Nagy, C. L. Nagy, M. V. Diudea, MATCH Commun. Math. Comput. Chem., **65**, 163 (2011).
[10] N. Dorosti, A. Iranmanesh, M. V. Diudea, MATCH Commun. Math. Comput. Chem., **62**, 389 (2009).
[11] A. Iranmanesh, N. Dorosti, MATCH Commun. Math. Comput. Chem., **65**, 209 (2011).
[12] Z. Yarahmadi, G. H. Fath-Tabar, MATCH Commun. Math. Comput. Chem., **65**, 201 **(**2011).
[13] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, Indian J. Chem., **47A**, 1503 (2008).
[14] M. H. Khalifeh, H Yousefi-Azari, A. R. Ashrafi, Dig. J. Nanomat. Biostruct., **4**, 63 (2009).
[15] A. Karbasioun, A. R. Ashrafi, Macedonian J. Chem. Chem. Eng., **28**, 49 **(**2009).
[16] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, Comput. Math. Appl., **60**, 2460 (2010).
[17] J. Nakayama, J.-S. Lin, Tetrahedron Lett., **38**, 6043 (1997).

*Corresponding author: ashrafi@kashanu.ac.ir