communications in mathematical
match
and in computer chemistry

no. 38, October 1998

ISSN 0340-6253

MATCDY (38) 33-34 (1998)

ON THE WIENER INDEX OF UNICYCLIC MOLECULAR GRAPHS AND THEIR LINE GRAPHS

A. Gutiérrez

Dpto. de Matemáticas. Universidad Central de Las Villas, Santa Clara 54830, Cuba

Abstract

In a recent paper [I. Gutman and E. Estrada, *J. Chem. Inf. Comput. Sci.* 1996, 36, 541-543] it was shown that in the case of acyclic molecules, the Wiener index of the molecular graph G and the Wiener index of the line graph $\mathcal{L}(G)$ differ by a quantity that depends on the number of vertices only. In this note, a formula for the difference $W(G) - W(\mathcal{L}(G))$ is given for the case of unicyclic molecules.

1 Introduction

Let $G = (V, E)$ be a (molecular) graph, where V is the vertex set and E is the edge set. For any subset A of vertices, E_A denotes the set of edges with both endvertices in A. The distance $d(x, y)$ between two vertices x and y of G is defined as the length of the shortest path between x and y. The Wiener index $W(G)$ [4] of a (molecular) graph G is defined as follows:

$$W(G) = \frac{1}{2} \sum_{x \in V} \sum_{y \in V} d(x, y). \tag{1}$$

Given a nonempty graph G, the line graph $\mathcal{L}(G)$ of G is defined as that graph whose vertices can be put in one-to-one correspondence with the edges of G in such a way that two vertices of $\mathcal{L}(G)$ are adjacent if and only if the corresponding edges of G are adjacent. Thus, the distance $d(e_1, e_2)$ between any two edges e_1 and e_2 in G can be defined as the distance between its corresponding vertices in $\mathcal{L}(G)$.
Set $D(G) = W(G) - W(\mathcal{L}(G))$. In a recent article Gutman and Estrada [1] proved the following result concerning to acyclic (molecular) graphs (i.e trees).

Theorem 1 [1] Let G be a tree of n vertices. Then $D(G) = \binom{n}{2}$.

Here a formula for calculating $D(G)$ for unicyclic (molecular) graphs G is given; as a corollary we obtain the proposition that, for connected unicyclic graphs G on n vertices with cycle length c, $D(G)$ takes any value in an interval whose extrem points depend on n and c (and no value outside this interval).

2 Results

Let G be a graph and set $S(G,\emptyset)=0$. If G is connected, let v be a distinguished vertex of G and define $S(G,v)=\sum_{x\in V(G)} d(v,x)$. If G is a non connected graph and $G_1,\cdots,G_k$ are its connected components,
we define $S(G,\{v_1,\cdots,v_k\})=\sum_{i=1}^{k} S(G_i,v_i)$, where $v_i\in V(G_i)$, $1\le i\le k$. Set $q(n,c)=\binom{c+1}{2}-\binom{c+1}{2}-(n-c)\lceil\frac{c}{2}\rceil$, $l(n,c)=q(n,c)-\binom{n-c+1}{2}$ and $u(n,c)=q(n,c)-(n-c)$.

Theorem 2 Let G be a connected unicyclic graph on n vertices, let C denote its unique cycle, and let c be the length of C. Then

$$l(n,c)\le D(G)=q(n,c)-S(G\setminus E_C,C)\le u(n,c).$$

For each k element of $[l(n,c);u(n,c)]$, there is a connected unicyclic graph G on n vertices with cycle length c such that $D(G)=k$.

The proof (which is omitted) uses induction on the number of vertices of G.

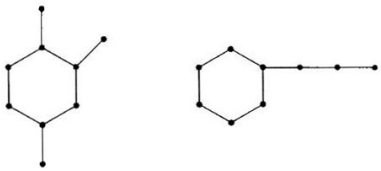

Figure 1: Molecular graphs of 1,2,4-trimethylbenzene (G_1) and propylbenzene (G_2). examples of unicyclic graphs with 9 vertices and cycle length 6.

Example: Let Γ be the class of connected unicyclic graphs with 9 vertices and cycle length 6. From Theorem 2 we have that for any $G\in\Gamma$, $9\le W(G)-W(\mathcal{L}(G))\le 12$. For the (molecular) graphs depicted in Figure 1 it is not difficult to verify that the difference $W(G)-W(\mathcal{L}(G))$ attains its extremal values, that is, $W(G_1)-W(\mathcal{L}(G_1))=12$ and $W(G_2)-W(\mathcal{L}(G_2))=9$.

References

[1] Gutman, I. and Estrada, E. Topological Indices Based on the Line Graph of the Molecular Graph. *J. Chem. Inf. Comput. Sci.* **1996**, 36, 541-543.

[2] Gutman, I.; Yeh, Y. N.; Lee, S. L.; Luo, Y. L. Some Recent Results in the Theory of the Wiener Number. *Indian J. Chem.* **1993**, 32A , 651-661.

[3] Harary, F. *Graph Theory*. Addison-Wesley: Reading, 1969.

[4] Wiener, H. Structural Determination of Paraffin Boiling Points. *J. Am. Chem. Soc.* **1947**, 69, 17-20.