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Further Results on Wiener Polarity Index of Graphs

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ABSTRACT

The Wiener polarity index $W_p(G)$ of a molecular graph G of order n is the number of unordered pairs of vertices u, v of G such that the distance d(u,v) between u and v is 3. In an earlier paper, some extremal properties of this graph invariant in the class of catacondensed hexagonal systems and fullerene graphs were investigated. In this paper, some new bounds for this graph invariant are presented. A relationship between Wiener and Wiener polarity index of some classes of graphs are also presented.

Keywords: Fullerene graph, Wiener index, Wiener polarity index.

1 INTRODUCTION

Let G be a connected simple graph with vertex and edge sets $V = V(G)$ and $E = E(G)$, respectively. The distance between vertices u and v of G, $d(u,v)$, is defined as the length of a shortest path connecting u and v. The quantity $d(G,k)$ is defined as the number of unordered pairs of vertices u and v of G such that $d_G(u,v) = k$. A topological index is a graph invariant applicable in chemistry. The first studied distance-based topological index is the famous Wiener index which is defined as the summation of distances between all pairs of vertices of the respective graph [1].

The Wiener polarity index of a molecule whose molecular graph G is defined as $W_p(G) = d(G,3)$. With the best of our knowledge, the Wiener had some information about applicability of this topological index. Using the Wiener polarity index, Lukovits and Linert [2] demonstrated quantitative structure property relationships in hydrocarbons. Hosoya [3] found a physico-chemical interpretation of $W_p(G)$. The first Zagreb index,

$M_1(G)$, is defined as the summation of squares of the degrees of the vertices, and the second Zagreb index, $M_2(G)$, is the sum of the products of the degrees of pairs of adjacent vertices of the molecular graph G. These topological indices were introduced by Gutman and Trinajstić [4]. For mathematical properties of these topological indices we refer to [5–7].

Throughout this paper our notations is standard and taken mainly from [8–10]. The diameter of a graph G, $d(G)$, is the maximum distance between vertices of G.

2 MAIN RESULTS

In this section we prove a relationship between the Wiener polarity index and the first and second Zagreb indices of connected graphs. We begin by mathematical formulation of these topological indices. To do this, we assume that G is a connected graph and the vertex set $V(G)$ is equal to $\{1, 2, \ldots, n\}$. Then one can see that,

$$W_p(G) = |\{\{u,v\} \subseteq V(G) \mid d(u,v) = 3\}|,$$
$$M_1(G) = \Sigma_{1 \le i \le n} deg(i)^2,$$
$$M_2(G) = \Sigma_{ij \in E(G)} deg(i)deg(j).$$

Lemma 1. If G is a connected graph then $W_p(G) \le n(n-1)/2 - ½\, M_1(G)$ with equality if and only if $d(G) = 3$.

Proof. Since G is connected, $d(G,1) + d(G,2) + d(G,3) \le n(n-1)/2$. So,

$$W_p(G) \le n(n-1)/2 - ½\, M_1(G).$$

The equality holds if and only if $d(G,4) = 0$, proving the lemma. ∎

Corollary 2. If $d(G) \le 3$ then $W(G) = 3/2n(n-1) - ½\, M_1(G) - m$.

Lemma 3. $W(G) \le 2n(n-1) - W_p(G) - M_1(G) - m$ with equality if and only if $d(G) \le 4$.

Proof. Since $d(G,1) + d(G,2) + d(G,3) + d(G,4) \le n(n-1)/2$, $M_1(G) + 2W_p(G) + 2d(G,4) \le n(n-1)$. Therefore, $2d(G,4) \le n(n-1) - 2W_p(G) - M_1(G)$ and so $W(G) \le 2n(n-1) - W_p(G) - M_1(G) - m$. ∎

Lemma 4. If T is a tree then

1) $W_p(L(T)) = d(T,4)$,
2) $W_p(T) + W_p(L(T)) \le n(n-1)/2$ with equality if and only if $d(T) \le 4$,
3) $W(T) \le 4W_p(L(T)) + 3W_p(T) + M_1(G) - m$ with equality if and only if $d(T) \le 4$.

Proof. Suppose u and v are vertices such that $d(u,v) = 4$ and $u = u_1, e_1, u_2, e_2, u_3, e_3, u_4 = v$ is a shortest path connecting u and v. Then $d_{L(T)}(e_1,e_2) = 3$. Conversely, if $e = xy$ and $f = rs$ are two edges such that $d_{L(T)}(e,f) = 3$ then one of the quantities d(a,r), d(x,s), d(y,r) or d(y,s) is equal to 3. This completes (1). To prove (2), we notice that $d(T,1) + d(T,2) + d(T,3) + d(T,4) \leq n(n-1)/2$ and so $2m + M_1(T) - 2m + 2W_p(T) + 2W_p(L(T)) \leq n(n-1)$. Thus $W_p(T) + W_p(L(T)) \leq n(n-1)/2$. Clearly, the equality holds if and only if $d(T) \leq 4$. Finally, (4) is a direct consequence of $d(T,3) = W_p(T)$ and $d(T,4) = W_p(L(T))$. ■

Lemma 5. If T is a tree then $W(T) \leq 1/2(5n-2)(n-1) - 2W_p(T) - 3W_p(L(T)) - 3/2M_1(T)$ with equality if and only if $d(T) \leq 5$.

Proof. It is clear that $d(T,1) + d(T,2) + d(T,3) + d(T,4) + d(T,5) \leq n(n-1)/2$. Since $d(T,1) = m$, $d(T,2) = 1/2M_1(T) - m$, $d(T,3) = W_p(T)$ and $d(T,4) = W_p(L(T))$,

$$d(T,5) \leq m + (1/2M_1(T) - m) + W_p(T) + W_p(L(T)) \tag{1}$$

By Eq. (1) and this fact that $W(T) \leq d(T,1) + d(T,2) + d(T,3) + d(T,4) + d(T,5)$, the lemma is proved. ■

A unicyclic graph is a connected graph such that $|V(G)| = |E(G)|$. The girth of G, g(G), is defined to be the number of edges in the unique cycle of G. In the following lemma the Wiener polarity index of a unicylic graph is computed.

Lemma 6. Suppose G is a unicyclic graph. Then we have,

1. If $g(G) \geq 7$ then $W_p(G) = M_2(G) - M_1(G) + n$,
2. If $g(G) = 6$ then $W_p(G) = M_2(G) - M_1(G) + n - 3$,
3. If $g(G) = 5$ then $W_p(G) = M_2(G) - M_1(G) + n - 5$,
4. If $g(G) = 4$ and $\{v_1, v_2, v_3, v_4\}$ are vertices of the cycle of G then
   $W_p(G) = M_2(G) - M_1(G) + n + 4 - (\deg(v_1) + \deg(v_2) + \deg(v_3) + \deg(v_4))$,
5. If $g(G) = 3$ and $\{v_1, v_2, v_3\}$ are vertices of the cycle of G then
   $W_p(G) = M_2(G) - M_1(G) + n + 9 - 2(\deg(v_1) + \deg(v_2) + \deg(v_3))$.

Proof. The proof is similar to the main result of [9] and so it is omitted. ■

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