THE WIENER, SZEGED AND PI-INDICES OF A PHENYLAZOMETHINE DENDRIMER

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A new type of phenylazomethine with a tetraphenylmethane core which was first investigated by Osamu Enoki et. al. is considered and its topological indices such as Wiener, Szeged and PI-index are found using a new method.

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1. Preliminaries

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The function $d: V(G) \times V(G) \to \mathbb{N} \cup \{0\}$ which assigns to each pair of vertices x, y in $V(G)$, the length of minimal path from x to y, is called the distance function between two vertices. The distance function between and edge and a vertex is $d': E(G) \times V(G) \to \mathbb{N} \cup \{0\}$ where for $e = uv \in E(G)$ and.$w \in V(G)$, $d'(e, w) = \min\{d(u, w), d(v, w)\}$.

The Wiener index of a graph G is denoted by $W(G)$ and is defined by $W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v)$.In general this kind of index is called a topological index, which is a distance based quantity assigned to a graph. This is an invariant of the graph G in the sense that if a graph H is isomorphic to G then $W(H) = W(G)$. The Wiener index for the first time was introduced by H. Wiener in [11] and is related to chemical substances. The definition of the Wiener index in terms of distance between vertices of a graph for the first time was given by Hosoya in [6]. This index is extensively studied by various authors, and we may refer the reader to [5] and [1] in which a new method is found to calculate the Wiener index of a graph.

Another index that will be investigated in this paper is the Szeged index, which is defined as follows:

$$Sz(G) = \sum_{e=uv \in E(G)}' n_u(v) n_v(u)$$

where for the two vertices u and v we define

$$N_u(v) = \{w \in V(G) | d(v, w) < d(u, w)\}$$

and $n_u(v) = |N_u(v)|$. The set $N_v(u)$ and the quantity $n_v(u)$ is defined similarly. We refer the reader to [4] to see more properties of the Szeged index of a graph.
Similar to the definition of the Szeged index we define the vertex PI-index as follows

$$PI_v(G) = \sum_{e=uv \in E(G)} [n_u(v) + n_v(u)].$$

For more information we refer the reader to [8].

Since a bipartite graph G has no cycle of odd length, for each edge $e = ur$ we have

$$N_u(v) \cup N_v(u) = V(G),$$

and if G is not bipartite, then there is an edge $e = ab$ such that $N_a(b) \cup N_b(a) \subset V(G)$. Hence

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$$PI_v(G) \leq |E(G)||V(G)|,$$

and it is proved in [8] that the equality $PI_v(G) = |E(G)||V(G)|$ holds if and only if G is bipartite. If G has n vertices, then

$$Sz(G) \leq Sz(K_{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil})$$

where $K_{r,s}$ denotes the complete bipartite graph. For more details see [2] and [10].

Another index that we will define here is the edge PI-index which was defined in[9]. In a graph G two edges $e = uv$ and f are called parallel, and is written by symbol $e \parallel f$, if

$$d'(f,u) = d'(f,v).$$

In general the relation $\parallel$ is not reflexive, but in a bipartite graph it is reflexive. We set

$$M_u(v) = \{e \in E(G) | d'(e,u) d'(e,v)\},$$

and $m_u(v) = |M_u(v)|$, and define $M_u(v)$ and $m_u(v)$ similarly. Furthermore, for and edge $e = uv$ we define

$$n(e) = |\{f \in E(G) | e \parallel f\}|$$

$$m_u(v) + m_v(u) = |E(G)| - n(e).$$

Next we define the edge PI-index as follows:

$$PI_e(G) = \sum_{e=uv \in E(G)} [m_u(v) + m_v(u)]$$

$$= |E(G)|^2 - \sum_{e \in E(G)} n(e)$$

2. Main results

In this section our aim is to compute the above indices for a new type of phenylazomethine dendrimer with a tetraphenylmethane core which is investigated in [3] whose graph is given below and is denoted by G_n, where $n = 0,1,2,\cdots$. In figure 1 below the graph $G_0 - G_4$ are drawn in such a way that $G_0 \subset G_1 \subset G_2 \subset G_3 \subset G_4$.

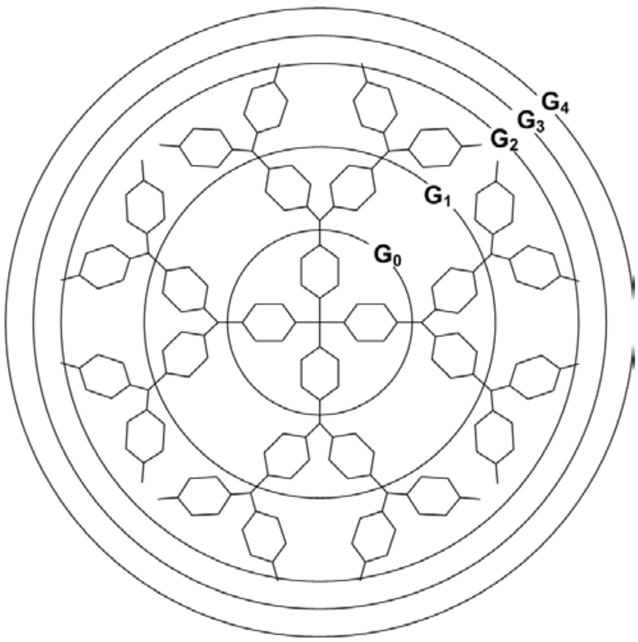

Fig. 1. structure of the TPM dendrimer.

The graph G_n has 4 arms, and we choose one of the arms and call it H_n. Clearly H_n is a subgraph of G_n and in figure 2 the graphs $H_0 - H_4$ are drawn.

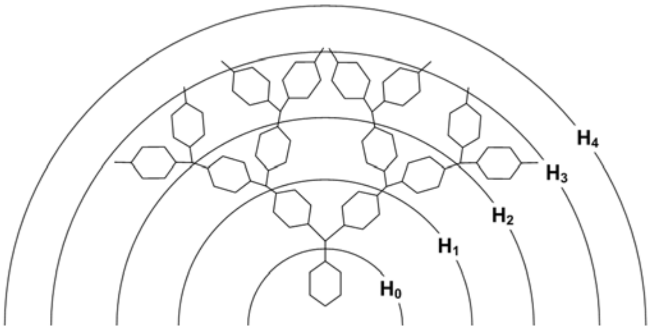

Fig. 2. H_n *a subgraph of* G_n

With this setting the graph G_n is obtained by joining four copies of H_n together. Both graphs G_n and H_n are bipartite because they don't include an odd cycle.

If g_n and h_n denote the number of vertices in G_n and H_n respectively then it is easy to find that

$$h_n = 7\sum_{i=0}^{n} 2^i - 2^n = 13 \times 2^n - 7, n \geq 0,$$

$$g_n = 4h_n + 1 = 26 \times 2^{n+1} - 27, n \geq 0.$$

We want to compute the mentioned indices of the graph G_n using a new method. To do this we will introduce the following concept.

Definition 1. Let G be a simple graph. A subgraph K of G is called convex if for every two vertices u and v in K, then K contains all the edges and vertices of all the minimal paths from u to v in G.

Theorem 1. Let G be a simple graph. If there exists a partition of the edge set of G like $\{F_i\}_{i=1}^{k}$ such that $G - F_i$ is a graph with two connected components G_i^1 and G_i^2, $1 \leq i \leq k$, and each of G_i^1 and G_i^2 is a convex graph then

$$(a) \quad W(G) = \sum_{i=1}^{k} |V(G_i^1)||V(G_i^2)|$$

$$(b) \quad Sz(G) = \sum_{i=1}^{k} |V(G_i^1)||V(G_i^2)||F_i|$$

$$(c) \quad PI_e(G) = |E(G)|^2 - \sum_{i=1}^{k} |F_i|^2$$

Proof. For the proof we refer the reader to [7] and [12].

Theorem 2. $PI_v(G_n) = 3120 \times 4^n - 3284 \times 2^n + 864$.

Proof. It is proved in [8] that if G is bipartite graph, then $PI_v(G) = |E(G)||V(G)|$. Therefore to calculate $PI_v(G_n)$ it is enough to compute the number of edges of G_n. But the number of edges of G_n is easily computed as

$|E(G_n)| = 4(|E(H_n)| + 1) = 15 \times 2^{n+2} - 32.$

Hence using. $PI_v(G_n) = |E(G_n)||V(G_n)|$.the result follows. ■

Theorem 3. $PI_e(G_n) = 3600 \times 4^n - 3948 \times 2^n + 1080.$

Proof. In the graph G_n if we delete an edge which is not contained in a cycle, we will obtain a graph with two components. Since each edge acts as a bridge, the two components are convex. From the other hand in each cycle C_6 contained in G_n, for each edge there is a different edge of C_6 which is parallel to it. If we delete and edge of C_6 and the edge parallel to it, then we again will obtain a graph with two components such that each component is a convex subgraph of G_n.

Hence, in this way we will obtain a partition $\{F_i\}$ of the edge set of G_n which satisfies the conditions of Theorem 1. Furthermore we have

$$|F_i| = \begin{cases} 1, & \text{if } F_i \text{ is not contained in a cycle,} \\ 2, & \text{if } F_i \text{ is a subset of a } C_6. \end{cases}$$

It can be calculated that the number of edges in C_6 cycles contained in G_n is equal to $C = 24\sum_{i=0}^{n} 2^i = 24(2^{n+1} - 1)$, the rest of edges of G_n, $|E(G_n)| - C = 6 \times 2^{n+1} - 8$, are not contained in any cycle. Therefore using Theorem 1 (c) we can write

$$PI_e(G_n) = |E(G_n)|^2 - \sum_{i=1}^{|E(G_n)|-C} 1 - \sum_{i=1}^{\frac{\sigma}{2}} 4$$

$= |E(G_n)|^2 - \ |E(G_n)| - C = 3600 \times 4^n - 3948 \times 2^n + 1080.$ ■

Theorem 4. $W(G_n) = 13520n \times 4^n - 1820n \times 2^n - 14040 \times 4^n + 181616 \times 2^n - 3328.$

Proof. Let us fix the notation used in the proof of Theorem 3. If $F_i \subseteq E(H_n)$ and $|F_i| = 1$, then one of the components of $G - F_i$ has either $h_\alpha - 6$ or $h_{\alpha-1}$ vertices, and the other component has either $g_n - (h_\alpha - 6)$ or $g_n - (h_{\alpha-1})$ vertices respectively.

The number of such edges F_i is $4 \times 2^{n-\alpha}$ or $8 \times 2^{n-\alpha}$ respectively, where $0 \leq \alpha \leq n$.

For these edges we can write

$$S_n = \sum_{\substack{|F_i|=1 \\ F_i \subseteq E(H_n)}} |V(G_i^1)||V(G_i^2)|$$

$$= 4\sum_{i=0}^{n-1} [2^i(h_{n-i} - 6)(g_n - (h_{n-i} - 6)) + h_{n-i-1}(g_n - h_{n-i-1})]$$

$= 9422 \times 2^n - 7644 \times 4^n - 728 \times n \times 2^n + 5408 \times n \times 4^n - 1848.$

Now if $|F_i| = 2$, one of the components of $G - F_i$ has $h_\alpha - 3$ vertices and the other component has $g_n - (h_\alpha - 3)$ vertices and the number of such edges is equal to $12 \times 2^{\alpha-1}$ where $0 \leq \alpha \leq n$.

Therefore

$$T_n = \sum_{|F_i|=2} |V(G_i^1)||V(G_i^2)| = 4\sum_{i=0}^{n} 3 \times 2^i \times (h_{n-i} - 3)(g_n - (h_{n-i} - 3))$$

$$= 11256 \times 2^n - 8424 \times 4^n - 1092n \times 2^n + 8112 \times n \times 4^n - 2040$$

Now we have 4 more edges that are not contained in $E(H_n)$, $(g_n - h_n)g_n = |V(G_i^1)||V(G_i^2)|$.

By Theorem 1 (a) we can write:

$W(G_n) = S_n + T_n + 4h_n(g_n - h_n)$,

and by substituting the values of S_n, T_n, g_n, and h_n the result will be proved. ■

Theorem 5. $Sz(G_n) = 15548n \times 4^n - 2093n \times 2^n - 16146 \times 4^n + 2143 \times 2^n - 3838.$

Proof. By Theorem 1 (b) we can write $Sz(G_n) = W(G_n) + T_n = S_n + 2T_n + 4h_n(g_n - h_n)$, and again by substituting the result follows. ■

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