Calculation of the Wiener, Szeged, and PI indices of a certain nanostar dendrimer

M. R. Darafsheh, M. H. Khalifeh
School of Mathematics, College of Science,
University of Tehran, Tehran, Iran
E-mail: darafsheh@ut.ac.ir

Abstract

Let $G = (V, E)$ be a simple connected graph with vertex set V and edge set E. The Wiener index of G is defined by $W(G) = \sum_{\{x,y\}\subseteq V} d(x,y)$, where $d(x,y)$ is the length of the shortest path from x to y. The Szeged index of G is defined by $Sz(G) = \sum_{e=uv\in E} n_u(e|G)n_v(e|G)$, where $n_u(e|G)$ (resp.$n_v(e|G)$) is the number of vertices of G closer to u(resp. v) than v(resp. u). The Padmakar-Ivan index of G is defined by $PI(G) = \sum_{e=uv\in E}[n_{eu}(e|G) + n_{ev}(e|G)]$, where $n_{eu}(e|G)$(resp.$n_{ev}(e|G)$) is the number of edges of G closer to u (resp. v) than v (resp. u). In this paper we will consider the graph of a certain nanostar dendrimer consisting of a chain of hexagons and find its topological indices such as the Wiener, Szeged, and PI index.

1 Introduction

The graphs considered in this paper are simple and connected. Let $G = (V, E)$ be a graph with vertex set V and edge set E. We will assume that G

Mathematics subject classification: Primary 05C12, 05CO5, Secondary 05C90.
Key words: Nanostar; Topological index, Wiener index; Szeged index; PI-index.

is a finite graph, i.e. both V and E are finite sets. For $u,v \in V$, the length of the shortest path from u to v is denoted by $d(u,v)$ and is called the topological distance between u and v. The Wiener index of G is denoted by $W(G)$ and is defined by: $W(G) = \sum_{\{u,v\} \subseteq V} d(u,v)$.

If for a vertex $v \in V$ the sum of distances between v and all other vertices of G is denoted by $d(v)$, i.e. $d(v) = \sum_{x \in V} d(v,x)$, then $W(G) = \frac{1}{2} \sum_{v \in V} d(v)$.

H. Wiener was the first one who considered the above index in connection with chemical graphs [18]. The Wiener index is one of the oldest descriptors concerned with the molecular graph and is concerned with the determination of the boiling points of paraffins. We remark that Wiener defined this index only for arcylic molecules in a different way, but the definition of $W(G)$ in terms of distances between vertices of a graph G was first defined by Hosoya in [11].

In mathematical research, the Wiener index has been first studied in [6], and for a long time mathematicians were not aware of the importance of the Wiener index in mathematical chemistry. However, because of the chemical facts about the Wiener index and also because it is an invariant of the graph, that is: it is invariant under the automorphism of the graph, hence various researchers found methods to calculate this index. Among the important works on finding the Wiener index of a general graph the reader is referred to the papers by Gutman et al. [5], [3], [9], and [10].

In theoretical chemistry molecular structure descriptor, also called topological indices, are used to understand properties of chemical compounds. By now there exist many different types of such indices for a general graph $G = (V, E)$. Here, apart from the Wiener index, we are interested in indices such as the Szeged and the Padmakar-Ivan index, the so called PI-index of a graph.

The Szeged index [7], [8], and [13] is a topological index closely related to the Wiener index of a graph $G = (V, E)$. Let $e = uv$ be an edge of G. By $n_u(e|G)$ we mean the number of vertices lying closer to u than v and similarly we define $n_v(e|G)$. Therefore if we define the following sets: $N_u(e|G) = \{w \in V \mid d(w,u) < d(w,v)\}$ and $N_v(e|G) = \{w \in V \mid d(w,v) < d(w,u)\}$.

Then $n_u(e|G) = |N_u(e|G)|$ and $n_v(e|G) = |N_v(e|G)|$. The Szeged index of G is defined by the following formula: $Sz(G) = \sum_{e=uv\in E} n_u(e|G)n_v(e|G)$.

In [15] basic properties of Szeged index and its analogy to the Wiener index is discussed. It is proved that for a tree T the Wiener index of T is equal to its Szeged index.

Since the Szeged index takes into account how the vertices of the graph G are distributed, it is natural to define an index that takes into account the distribution of the edges of G. The padmakar-Ivan (PI) index, [12] and [14], is another important index which is assigned to a graph G and takes into account the distribution of edges of the graph and therefore complements the Szeged index in a certain sense. Let the number of edges in the graphs induced by $N_u(e|G)$ and $N_v(e|G)$ be denoted by $n_{eu}(e|G)$ and $n_{ev}(e|G)$, respectively. The PI index of G is defined by: $PI(G) = \sum_{e\in E} (n_{eu}(e|G) + n_{ev}(e|G))$.

We remark that the edges equidistant from both ends of the edge uv are not counted in the above expression for $PI(G)$. It is easy to see that if $N(e)$ denotes the number of all the edges equidistance from e, then $N(e) + n_{eu}(e|G) + n_{ev}(e|G) = |E|$, hence we have: $PI(G) = \sum_{e\in E}(E - N(e)) = |E|^2 - \sum_{e\in E} N(e)$. Therefore to compute $PI(G)$ it is enough to know the number of edges of G and the numbers $N(e)$ for each edge e of G.

All the indices mentioned above, when applied to chemical graphs have many chemical applications and it was shown that the PI index is related to the Szeged and the Wiener index of a graph, and all of them have connections with the physicochemical properties of many complex compounds.

For the topological indices associated to a graph two groups of problems can be distinguished in the theory of topological indices. One is to ask the dependence of the index to the graph and the other is the calculation of these indices efficiently. The greatest progress in solving the above problems was made for trees and hexagonal systems by Gutman et al. in [3] and [5]. Because of the importance of the above indices important methods have been developed to compute them. For example one can refer to [1], [2], [4], [16], and [17].

In this paper we will consider the graph of a certain nanostar dendrimer consisting of a chain of hexagons and find its topological indices such as the Wiener, Szeged, and PI indices. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. The nanostar dendrimer is part of a new group of molecules that appears to be photon funnels just like artificial antennas.

2 Preliminaries

Let $G = (V, E)$ be a simple connected graph with vertex set V and edge set E. We recall that the distance between two vertices u and v is denoted by $d(u, v)$ and it is the length of the shortest path from u to v. If we want to specify the graph in question then the distance between u and v is denoted by $d_G(u, v)$. If H is a subgraph of G, then this fact is denoted by the symbol $H \leq G$ and H is called an isometric subgraph if $d_H(u, v) = d_G(u, v)$ for all vertices u and v of H, and if this is the case then we write $H << G$.

Let V_1 and V_2 be non-empty subsets of the vertex set V of G. The distance between V_1 and V_2 is denoted by $d_G(V_1, V_2)$ and is defined as follows $d_G(V_1, V_2) = \sum_{u \in V_1} \sum_{v \in V_2} d_G(u, v)$. If $V_2 = V$ then we write $d_G(V_1, V) = d(V_1, G)$. With this notation the Wiener index of the graph G can be written as $W(G) = \frac{1}{2} d_G(V, G)$.

If $\{F_i\}_{i=1}^{r}$ is a partition of the vertex set V, then it is easy to see that: $W(G) = \frac{1}{2} \sum_{i=1}^{r} \sum_{j=1}^{r} d_G(F_i, F_j)$. Also if $H << G$, then: $W(H) = \frac{1}{2} d_H(V(H), V(H))$ and $W(G) = \frac{1}{2} d(V(G), G)$, where $V(H)$ and $V(G)$ denote the vertex sets of H and G, respectively.

The graph we will consider in this paper is denoted by $G(n)$, $n \geq 0$, which is a kind of nanostar dendrimer. In the following we draw the picture for $G(2)$. O_1 and O_2 are the initial vertices which are joined by an edge. Then two isomorphic graphs $L_1(n)$ and $L_2(n)$ consisting of hexagons are built as above. The following facts can be proved by induction.

$|V(G(n))| = 12(2^{n+1} - 1)$, $|V(L_1(n))| = |V(L_2(n))| = 6(2^{n+1} - 1)$, $|E(G(n))| = 7.2^{n+2} - 15$. The number of edges of $G(n)$ not contained in a hexagon is $2^{n+2} - 3$.

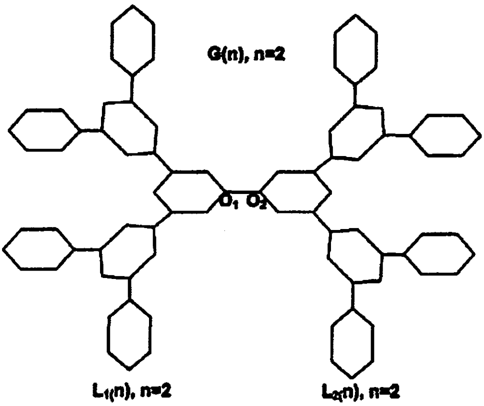

Figure 1

3 Main results

Let us fix the notations used so far. In this section first of all we will compute the Wiener index of the graph $G(n)$ in terms of a function of n. To start we will prove some auxiliary lemmas.

Lemma 1 $W(G(n)) = 2W(L_1(n)) + 2\,|V(L_1(n))|\,d(O_1, L_1(n)) + |V(L_1(n))|^2$.

Proof. Referring to the graph $G(n)$ at stage n it is clear that $L_1(n) << G(n)$ and $L_2(n) << G(n)$. Since $V(L_1(n))$ and $V(L_2(n))$ are partitions of $V(G(n))$ and the graphs $L_1(n)$ and $L_2(n)$ are isomorphic we can write:

$W(G(n)) = d_G(V(L_1(n)), V(L_2(n))) + d_G(V(L_1(n)), V(L_1(n))) +$
$d_G(V(L_2(n)), V(L_2(n))) = d_G(V(L_1(n)), V(L_2(n))) + 2W(L_1(n))$. (1)

If $u \in V(L_1(n))$ and $v \in V(L_2(n))$, then $d_G(u,v) = d_{L_1(n)}(u, O_1) + d_G(O_1, O_2) + d_{L_2(n)}(O_2, v) = d_{L_1(n)}(u, O_1) + d_{L_2(n)}(O_2, v) + 1$.

Therefore $d_G(V(L_1(n)), V(L_2(n))) = \sum_{u \in V(L_1(n))} \sum_{v \in V(L_2(n))} d_G(u,v)$
$= \sum_{u \in V(L_1(n))} \sum_{v \in V(L_2(n))} (d_{L_1(n)}(u, O_1) + d_{L_2(n)}(O_2, v) + 1) =$
$\sum_{u \in V(L_1(n))} (|V(L_2(n))|\, d_{L_1(n)}(u, O_1) + d(O_2, L_2(n)) + |V(L_2(n))|) =$
$|V(L_2(n))|\, d_{L_1(n)}(O_1, L_1(n)) + |V(L_1(n))|\, d(O_2, L_2(n)) +$
$|V(L_1(n))|\, |V(L_2(n))| = 2\,|V(L_1(n))|\, d(O_1, L_1(n)) + |V(L_1(n))|^2$. (2)

Now if we substitute the equality (2) in (1) we will obtain the formula stated in the lemma. ■

Lemma 2 $W(L_1(n)) = 432n.4^n + 216n.2^n - 792.4^n + 810.2^n + 9$, $n \geq 0$.

Proof. We consider the binary tree T_n, $n \geq 0$, whose shape is drawn as follows at the stage $n = 2$:

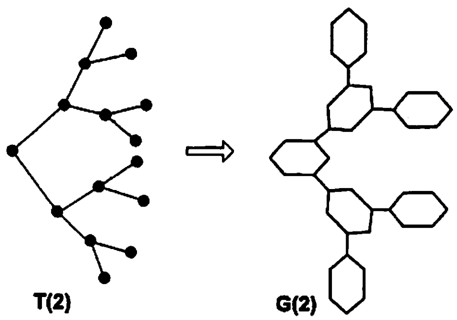

Figure 2

Now we may replace each vertex of T_n by a hexagon C_6 so that to obtain $L_1(n)$ or $L_2(n)$. In this case the C_6 corresponding to a vertex v of T_n is denoted by C_v. It is easy to prove the following equality for all distinct $u, v \in V(T_n)$:

$d_{L_1(n)}(C_u, C_v) = 36(d_{T_n}(u,v) + 2(d_{T_n}(u,v) - 1)) + 108 = 108d_{T_n}(u,v) + 36$, and also $d_{L_1(n)}(C_v, C_v) = 27$.

Since $\{V(C_v)\}_{v \in V(T_n)}$ is a partition of the set of vertices of $L_1(n)$, we have:

$W(L_1(n)) = \sum_{\{u,v\} \in V(T_n)} d_{L_1(n)}(V(C_u), V(C_v)) + \sum_{u \in V(T_n)} 27 =$
$\sum_{\{u,v\} \in V(T_n)} (108d_{T_n}(u,v) + 36) + 27\,|V(T_n)| =$
$108W(T_n) + 36\binom{|V(T_n)|}{2} + 27\,|V(T_n)|$ (3)

But we have $|V(T_n)| = \sum_{i=0}^{n} 2^i = 2^{n+1} - 1$.

Since the Wiener index of a tree is equal to its Szeged index we can compute $W(T_n)$ as follows:

$W(T_n) = Sz(T_n) = \sum_{e=uv \in E(T_n)} n_u(e|T_n) n_v(e|T_n) =$
$\sum_{i=0}^{n} 2^i\,|V(T_{n-i})|\,(|V(T_n)| - |V(T_{n-i})|) =$

$\sum_{i=0}^{n} 2^i(2^{n+1-i}-1)(2^{n+1}-2^{n+1-i}) = 4n.4^n + 2n.2^n - 8.4^n + 8.2^n$.

Now substituting the value of $W(T_n)$ in (3) we obtain: $W(L_1(n)) = 432n.4^n + 216n.2^n - 792.4^n + 810.2^n + 9$, for all $n \geq 0$, and the lemma is proved. ■

Lemma 3 $d(O_1, L_1(n)) = 36n.2^n - 18.2^n + 27$.

Proof. With regard to the construction of $G(n)$ from T_n mentioned in Lemma 2 we can write: $d_{L_1(n)}(O_1, C_u) = 6(2d_{T_n}(O_1, u) + d_{T_n}(O_1, u)) + 9 = 18d_{T_n}(O_1, u) + 9$. But it easy to calculate that:

$d(O_1, L_1(n)) = \sum_{u \in V(T_n)} d_{L_1(n)}(O_1, C_u)$

$= \sum_{u \in V(T_n)} (18d_{T_n}(O_1, u) + 9)$

$= 18d(O_1, T_n) + 9\,|V(T_n)|$ (4)

But is can be shown that: $d(O_1, T_n) = \sum_{i=0}^{n} i2^i = 2n.2^n - 2.2^n + 2$, and substituting the value in (4) we will obtain:

$d(O_1, L_1(n)) = 18(2n.2^n - 2.2^n + 2) + 9(2^{n+1} - 1) = 36n.2^n - 18.2^n + 27$

■

Theorem 1 $W(G(n)) = (1728n - 1872)4^n + 2340.2^n - 270$, $n \geq 0$.

Proof. By Lemma 1 we have:

$W(G(n)) = 2W(L_1(n)) + 2\,|V(L_1(n))|\,d(O_1, L_1(n)) + |V(L_1(n))|^2$.

Now by Lemmas 2 and 3 the values of $W(L_1(n))$ and $d(O_1, L_1(n))$ are known, and since $|V(L_1(n))| = 6(2^{n+1} - 1)$, we will obtain the value of $W(G(n))$ as written in the theorem. ■

Next we calculate the PI-index of $G(n)$.

Theorem 2 $PI(G(n)) = 784.4^n - 852.2^n + 232$, $n \geq 0$.

Proof. By definition of the PI-index, as indicated in the introduction, we can write: $PI(G) = |E(G(n))|^2 - \sum_{e \in E} N(e)$, where $N(e)$ is the number of edges of $G(n)$ equidistance from e. Now it is easy to see that if e is an edge of a hexagon, then $N(e) = 2$, and if e is an edge joining any two hexagons, then $N(e) = 1$. But the number of hexagons in $G(n)$ is equal to $2(2^{n+1} - 1)$ and the number of edges of $G(n)$ not contained in a hexagon is $2^{n+2} - 3$. Therefore:

$PI(G) = (7.2^{n+2} - 15)^2 - 2.2(2^{n+1} - 1) - (2^{n+2} - 3) = 784.4^n - 852.2^n + 232$ as required. ■

Finally we will compute the Szeged index of $G(n)$.

Theorem 3 $Sz(G(n)) = (2880n - 3024)4^n + 3816.2^n - 432$, $n \geq 0$.

Proof. As we mentioned in the introduction the Szeged index of a graph, say $G(n)$, is defined by: $Sz(G) = \sum_{e=uv\in E} n_u(e|G(n))n_v(e|G(n))$, where $n_u(e|G(n))$ is the number of vertices of $G(n)$ lying closer to u than v. The number $n_v(e|G(n))$ is defined similarly.

Since no two vertices of each two hexagons C_6 are involved in a circuit, the graph $G(n)$ should be bipartite. Now for every bipartite graph G for an edge $e = uv$ we have:

$n_u(e|G) + n_v(e|G) = |V(G)| \qquad (5)$

Now for each edge $e = uv$ of $G(n)$ which is not involved in a circuit, using (5), we obtain:

$n_u(e|G(n))n_v(e|G(n)) = |V(L_1(n-1))|.(|V(G(n))| - |V(L_1(n-1))|)$.

But the number of such edges is 2.2^i for $1 \leq i \leq n$, and is 1 for $i = 0$. If we consider an arbitrary C_6 as in Fig. 3.

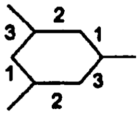

Figure 3

Then for each parallel arbitrary edges $e = uv$ and $f = ab$, because of their symmetry we can write: $n_a(f|G(n))n_b(f|G(n)) = n_u(e|G(n))n_v(e|G(n))$. On the other hand we can see easily that for edges numbered 2 in Fig. 3, using (5) we obtain: $n_u(e|G(n))n_v(e|G(n)) = (|V(L_1(n-i))| - 3)(|V(G(n))| - |V(L_1(n-i))| + 3)$. And for edges numbered 1 and 3, using (5) we obtain $n_u(e|G(n))n_v(e|G(n)) = (|V(L_1(n-i-1))| + 3)(|V(G(n))| - |V(L_1(n-i))| - 3)$ where the number of such edges in $G(n)$ is 2.2^i for $0 \leq i \leq n$. Therefore:

$Sz(G(n)) = |V(L_1(n))|^2 + \sum_{i=1}^{n} |V(L_1(n-i))|.(|V(L_1(n))| - |V(L_1(n-i))|)2.2^i + \sum_{i=1}^{n} 2.2^i\{(|V(L_1(n-i))| - 3)(|V(G(n))| - |V(L_1(n-i))| + 3) + 2(|V(L_1(n-i-1))| + 3)(|V(G(n))| - |V(L_1(n-i-1))| - 3)\}$.

Taking into account the fact that $V(L_1(n)) = 6(2^{n+1}-1)$, and summing up the expressions in (2) we obtain the formula stated in the theorem for $Sz(G(n))$. ∎

Acknowledgement. The first author was supported by the reaserch council of the college of science of the University of Tehran through grant #610-3014-1-05.

References

[1] M. R. Darafsheh, Computation of topological indices of some graphs, Acta Appl. Math. 110 (2010), no. 3, 1225-1235.

[2] H. Deng and S. Chen, PI indices of pericondensed benzenoid graphs, J. Math. Chem. 43 (2008), no. 1, 19-25.

[3] A. A. Dobrynin, R. Entringer and I. Gutman, Wiener index of trees: Theory and applications, Acta Appl. Math. 66 (2001), 211-249.

[4] A. A. Dobrynin and I. Gutman, Congruence relations for the Szeged index of hexagonal chains, Univ. Beograd. Publ. Elektrotehn. Fak. Ser. Mat. 8 (1997), 106-113.

[5] A. A. Dobrynin, I. Gutman, S. Klavzar and P. Zigert, Wiener index of hexagonal systems, Acta Appl. Math. 72 (2002), 247-294.

[6] R. C. Entringer, D. E. Jackson, and D. A. Snyder, Distance in graphs, Czechoslovak Math. J. 26 (1976), 283-296.

[7] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, Graph Theory Notes, New York 27 (1994), 9-15.

[8] I. Gutman and A. A. Dobrynin, The Szeged index - a success story, Graph Theory Notes, N. Y. 34 (1998), 37-44.

[9] I. Gutman, S. Klavzar and B. Mohr (Eds.), Fifty years of the Wiener index, MATCH Commun. Math. Comput. Chem. 35 (1997), 1-259.

[10] I. Gutman, Y. N. Yeh, S. L. Lee, and J. C. Chen, Wiener numbers of dendrimers, MATCH Commun. Math. Comput. Chem. 30 (1994), 103-115.

[11] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, Bull. Chem. Soc. Jpn. 4 (1971) 2332-2339.

[12] P. V. Khadikar, On a novel structural descriptor PI, Nat. Acad. Sci. Lett. 23 (2000) 113-118.

[13] P. V. Khadikar, N. V. Deshpande, P. P. Kale, A. A. Dobrynin, and I. Gutman, The Szeged index and an analogy with the Wiener index, J. Chem. Inf. Comput. Sci. 35 (1995), 547-550.

[14] P. V. Khadikar, S. Karmarkar and V. K. Agrawal, Relationship and relative correction potential of the Wiener, Szeged and PI indexes, Nat. Acad. Sci. Lett. 23 (2000)165-170.

[15] S. Klavzar, A. Rajapakse, and I. Gutman, On the Szeged and Wiener index of graphs, Appl. Math. Lett. 9 (1996), 45-49.

[16] N. Prabhakara Rao and A. Laxmi Prasanna, On the Wiener index of pentachains, Appl. Math. Sci. 2 (2008), no. 49, 2443-2457.

[17] Z. Tang and H. Deng, The (n, n)-graphs with the first three extremal Wiener indices, J. Math. Chem. 43 (2008), no. 1, 60-74.

[18] H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc. 69 (1947), 17-20.