MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **62** (2009) 363-370

ISSN 0340 - 6253

PI, Szeged and Edge Szeged Polynomials of a Dendrimer Nanostar

Mahsa Mirzargar

Department of Mathematics, Faculty of Science, University of Kashan, Kashan 87317-51167, I. R. Iran

(Received September 10, 2008)

Abstract

A topological index of a graph G is a numeric quantity related to G which is describe molecular graph G. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper the PI, Szeged and edge Szeged indices of a class of nanostar dendrimers together with their polynomials are computed.

1. Introduction

Let G be a graph with vertex and edge sets V(G) and E(G), respectively. As usual, the distance between the vertices u and v of a connected graph G is denoted by d(u,v) and it is defined as the number of edges in a minimal path connecting the vertices u and v. Throughout the paper, a graph means undirected connected graph without loops and multiple edges.

In chemical graph theory, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory. A chemical graph is a colored graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Its vertices are colored with the kinds of the corresponding atoms and edges are colored with the types of bonds. For particular purposes any of the colorings may be ignored.

A topological index is a numeric quantity from the structure of a graph which is invariant under automorphisms of the graph under consideration. Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffin [1]. Although the topological index, is easily calculable quantity, it does not uniquely correspond to the individual structure of a graph. John Platt was the only person who immediately realized the importance of the Wiener's pioneering work and wrote papers analyzing and interpreting the physical meaning of the Wiener index.

We recall some algebraic definitions that will be used in the paper. The Wiener index of a graph G is defined as the sum of all topological distances between the pair of vertices in which the topological distance between two vertices is the number of edges in a shortest path between them. We encourage the readers to consult two survey articles by Dobrynin and his co-authors [2,3] and references therein for background material and historical aspect of Wiener index.

The PI index is a new topological index defined by Padmakar Khadikar, [4-6]. It is defined as $PI(G) = \sum_{e=uv\in G}[m_u(e)+ m_v(e)]$, where $m_u(e)$ is the number of edges of G lying closer to u than to v and $m_v(e)$ is the number of edges of G lying closer to v than to u. Edges equidistant from both ends of the edge uv are not counted. The Szeged index is another topological index introduced by Ivan Gutman, [7]. To define the Szeged index of a graph G, we assume that e = uv is an edge connecting the vertices u and v. Suppose $n_u(e)$ is the number of vertices of G lying closer to u and $n_v(e)$ is the number of vertices of G lying closer to v. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e=uv\in E(G)}n_u(e)n_v(e)$. Notice that vertices equidistance from u and v are not taken into account. In [8], the authors introduced an edge version of the Szeged index. It is defined as $Sz_e(G) = \sum_{e=uv\in E(G)}m_u(e)m_v(e)$, where $m_u(e)$ is the number of edges of G lying closer to u than to v and $m_v(e)$ is the number of edges of G lying closer to v than to u. Edges equidistant from both ends of an edge are not into account. In the mentioned paper, the main properties of this new index investigated and some open question posed.

Diudea and Nagy in their recent book [9] wrote: “It is well-known that a graph can be described by: a connection table, a sequence of numbers, a matrix, a polynomial or a derived number called a topological index”. In this paper we apply a polynomial approach for studying the molecular graphs. Here, a finite sequence of some graph theoretical properties can be described by so-called counting polynomials $P(G,x) = \sum_k p(G,k)\cdot x^k$, where P(G,k) is the frequency of occurrence of the property partitions of G, of length k, and x is simply a parameter to hold k. The edge Szeged polynomial is a new counting polynomial for graphs defined by $Sz_e(G,x) = \sum_{e=uv} x^{m_u(e)m_v(e)}$, see [10].

The first attempt for studying topological indices of nanostructures was done by Diudea and his co-authors, [11-17]. Recently, Ashrafi and his co-authors, continued the pioneering work of Diudea and his team to compute the PI and Szeged indices of some classes of nanostructures, [18-23]. We also encourage the reader to consult papers [24-27] for more information on this subject.

2. Main Results and Discussion

In recent research in mathematical chemistry, particular attention is paid to distance-based graph invariants. In this section we compute PI and Szeged indices of a nanostar dendrimer NS[n], Figure 1. Using a simple calculation, one can show that $|V(NS[n])| = 75.2^n - 38$ and $|E(NS[n])| = 87.2^n - 45$. We begin with computing $n_u(e)$ for the edges $e = E_1^0 = a_1b_1$, $E_2^0 = a_2b_2$, $E_3^0 = a_3b_3$, $n_{a_r}(E_r^0) = \frac{|V(NS[n])|-1}{3} = 25.2^n - 13$, $1 \le r \le 3$. Now consider the edges $e = uv = E_{jk}^i$, j = 1,2,3, $1 \le i \le n$ and $1 \le k \le 3.2^{i-1}$ Figure 1. For $e = ab = E_{2k}^i$ and $e = cd = E_{3k}^i$, $n_a(e) = n_c(e) = 24(2^{n-i}-1) + (2^{n-i}-1) + 12 = 25.2^{n-i} - 13$ and for $e = gh = E_{1k}^i$, $n_g(e) = 50.2^{n-i} - 25$.

Suppose $e = uv = e_j^i$, $0 \le i \le n$, $1 \le j \le 3.2^i$**.** Then by an inductive argument $n_u(e) = 24(2^{n-i}-1) + (2^{n-i}-1) + 6 = 25.2^{n-i} - 19$. We now consider the edges of hexagons N_{jk}^i, j =1,2; $0 \le i \le n$; $1 \le k \le 3.2^i$, Figure 1. If e = uv is an edge from the hexagon N_{1k}^i, then for six edges of this hexagon $n_u(e) = 24(2^{n-i}-1) + (2^{n-i}-1) + 9 = 25.2^{n-i} - 16$, and for six edges of hexagon N_{2k}^i, $n_u(e) = 24(2^{n-i}-1) + (2^{n-i}-1) + 3 = 25.2^{n-i} - 22$. Using above calculations, we have:

Theorem 1. The Szeged index of the dendrimer NS[n] is computed as follows:

$$Sz(NS[n]) = -18081 + 125712.2^n + 84375.n.4^n - 100125.4^n - 2700.n.2^n.$$

Proof. By our calculations given above, we have:

$$\begin{aligned} Sz(NS[n]) &= \sum\nolimits_{e=uv}[n_u(u)n_v(e)] \\ &= 3(25.2^n - 13)(50.2^n - 25) \\ &\quad + 6\sum\nolimits_{i=1}^{n} 2^{i-1}(25.2^{n-i} - 13)(75.2^n - 25.2^{n-i} - 25) \\ &\quad + 3\sum\nolimits_{i=1}^{n} 2^{i-1}(50.2^{n-i} - 25)(75.2^n - 25.2^{n-i} - 13) \\ &\quad + 3\sum\nolimits_{i=0}^{n} 2^{i}(25.2^{n-i} - 19)(75.2^n - 25.2^{n-i} - 19) \\ &\quad + 18\sum\nolimits_{i=0}^{n} 2^{i}(25.2^{n-i} - 16)(75.2^n - 25.2^{n-i} - 22) \\ &\quad + 18\sum\nolimits_{i=0}^{n} 2^{i}(25.2^{n-i} - 22)(75.2^n - 25.2^{n-i} - 16) \\ &= -18081 + 125712.2^n + 84375.n.4^n - 100125.4^n - 2700.n.2^n. \end{aligned}$$

which proves the theorem. □

Corollary 1. The Szeged polynomial of the dendrimer NS [n] is computed as follows:

$$\begin{aligned} Sz(NS[n],x) = 3\sum_{i=1}^{n} 2^i (&x^{1875.2^{2n-i} - 625.2^{2n-2i} - 1425.2^n + 361} + 6x^{1875.2^{2n-i} - 625.2^{2n-2i} - 150.2^{n-i} - 1200.2^n + 352} \\ &+ 6x^{1875.2^{2n-i} - 625.2^{2n-2i} + 300.2^{n-i} - 975.2^n + 325} + \frac{1}{2}x^{3750.2^{2n-i} - 2500.2^{2n-2i} + 600.2^{n-i} - 1875.2^n + 325} \\ &+ x^{1875.2^{2n-i} - 625.2^{2n-2i} - 300.2^{n-i} - 975.2^n + 325}) + 18x^{1250.4^n - 1350.2^n + 352} + 18x^{1250.4^n - 1500.2^n + 352} \\ &+ 3x^{1250.4^n - 1275.2^n + 325} + 3x^{1250.4^n - 1425.2^n + 361}. \end{aligned}$$

We now compute the PI index of a nanostar dendrimer NS[n]. For the edges $e = E_1^0 = a_1b_1$, $E_2^0 = a_2b_2$, $E_3^0 = a_3b_3$, $m_{a_r}(E_r^0) = \frac{|E(NS[n])|}{3} - 1 = 29.2^{n+1} - 16$, $1 \le r \le 3$. Consider the edges $e = uv = E_{jk}^i$, j=1,2,3; $1 \le i \le n$; $1 \le k \le 3.2^{i-1}$, Figure 1. For edges $e = ab = E_{2k}^i$ and $e = cd = E_{3k}^i$, $m_a(e) = m_c(e) = 26(2^{n-i}-1) + 3(2^{n-i}-1) + 13 = 29.2^{n-i} - 16$ and for $e = gh = E_{1k}^i$, $m_g(e) = 58.2^{n-i} - 30$.

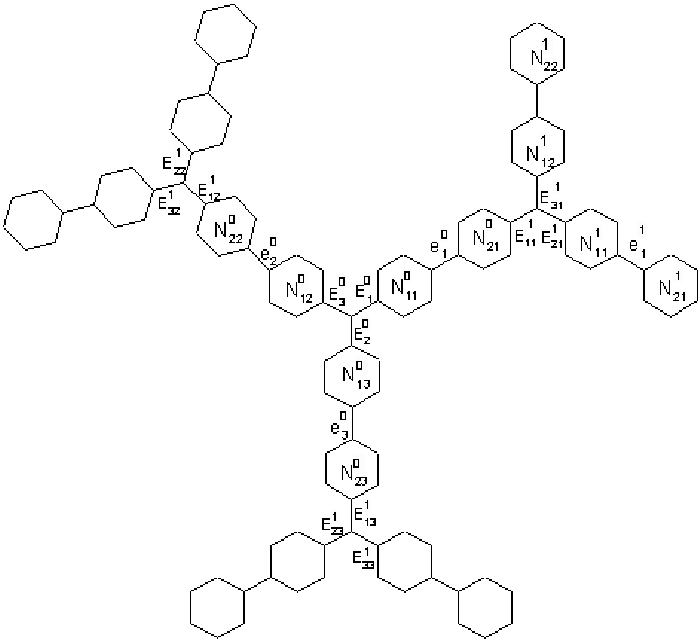

Figure 1. The Nanostar Dendrimer NS[1].

Suppose e = uv = e_j^i, $0 \le i \le n$, $1 \le j \le 3.2^i$, Then by an inductive argument $m_u(e) = 26(2^{n-i}-1) + 3(2^{n-i}-1) + 6 = 29.2^{n-i} - 23$. We now consider the edges of hexagon N_{jk}^i, j = 1, 2; $0 \le i \le n$; $1 \le k \le 3.2^i$, Figure 1. If e = uv is an edge of the hexagon N_{1k}^i, then for six edges of this hexagon $m_u(e) = 26(2^{n-i}-1) + 3(2^{n-i}-1) + 9 = 29.2^{n-i} - 20$, and, for six edgs of hexagon N_{2k}^i, $m_u(e) = 26(2^{n-i}-1) + 3(2^{n-i}-1) + 2 = 29.2^{n-i} - 27$.

Theorem 2. The PI index of the nanostar dendrimer NS[n] is computed as follows:

$$PI(NS[n]) = 7569.4^n - 7989.2^n + 2106.$$

Proof. By our calculations given above, we have:

$$
\begin{aligned}
PI(NS[n]) &= \sum\nolimits_{e=uv} m_u(e) + m_v(e) \\
&= 3.(5.2^n - 3)(87.2^n - 46) \\
&\quad + 36.(2^{n+1} - 1)(87.2^n - 47) \\
&= 7569.4^n - 7989.2^n + 2106.
\end{aligned}
$$

which proves the theorem. □

Corollary 2. The PI polynomial of the nanostar dendrimer NS [n] is computed as follows:

$$PI(NS[n], x) = 3(5.2n - 3)x^{87.2^n - 46} + 36(2^{n+1} - 1)x^{87.2^n - 47}.$$

We now compute the edge Szeged index of the nanostar dendrimer NS[n].

Theorem 3. The Sz_e index of the nanostar dendrimer NS[n] is computed as follows:

$$Sz_e(NS[n]) = -23907 + 177135.2^n - 145116.4^n + 113535.n.4^n.$$

Proof. By our calculations before Theorem 2, one can see that

$$
\begin{aligned}
Sz_e(NS[n]) &= \sum\nolimits_{e=uv} \left[m_u(e) m_v(e)\right] \\
&= 3(29.2^n - 16)(58.2^n - 30) \\
&\quad + 6\sum\nolimits_{i=1}^{n} 2^{i-1}(29.2^{n-i} - 16)(87.2^n - 29.2^{n-i} - 30) \\
&\quad + 3\sum\nolimits_{i=1}^{n} 2^{i-1}(58.2^{n-i} - 30)(87.2^n - 58.2^{n-i} - 16) \\
&\quad + 3\sum\nolimits_{i=0}^{n} 2^{i}(29.2^{n-i} - 23)(87.2^n - 29.2^{n-i} - 23) \\
&\quad + 18\sum\nolimits_{i=0}^{n} 2^{i}(29.2^{n-i} - 20)(87.2^n - 29.2^{n-i} - 27) \\
&\quad + 18\sum\nolimits_{i=0}^{n} 2^{i}(29.2^{n-i} - 27)(87.2^n - 29.2^{n-i} - 20) \\
&= -23907 + 177135.2^n - 145116.4^n + 113535.n.4^n,
\end{aligned}
$$

which proves the theorem. □

Corollary 3. The Sz_e polynomial of the nanostar dendrimer NS [n] is computed as follows:

$$
\begin{aligned}
Sz_e(NS[n], x) = 3\sum_{i=1}^{n} 2^i \Big(& x^{2523.2^{2n-i} - 841.2^{2n-2i} - 2001.2^n + 529} + 6x^{2523.2^{2n-i} - 841.2^{2n-2i} - 203.2^{n-i} - 1740.2^n + 540} \\
& + 6x^{2523.2^{2n-i} - 841.2^{2n-2i} + 203.2^{n-i} - 2349.2^n + 540} + x^{2523.2^{2n-i} - 841.2^{2n-2i} - 406.2^{n-i} - 1329.2^n + 480} \\
& + \frac{1}{2}x^{5046.2^{2n-i} - 3364.2^{2n-2i} + 812.2^{n-i} - 2610.2^n + 480}\Big) + 3x^{1682.4^n - 1798.2^n + 480} + 3x^{1682.4^n - 2001.2^n + 529} \\
& + 18x^{1682.4^n - 1943.2^n + 540} + 18x^{1682.4^n - 2552.2^n + 540}.
\end{aligned}
$$

References

[1] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[2] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta. Appl. Math.* **66** (2001) 211–249.

[3] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta. Appl. Math*. **72** (2002) 247–294.

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

[5] P. V. Khadikar, S. Karmarkar, A novel PI index and its applications to QSPR/QSAR studies, *J. Chem. Inf. Comput. Sci.* **41** (2001) 934–949.

[6] P. V. Khadikar, S. Karmarkar, R. G. Varma, On the estimation of PI index of polyacenes, *Acta. Chim. Slov.* **49** (2002) 755–771.

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

[8] I. Gutman, A. R. Ashrafi, The edge version of the Szeged index, *Croat. Chem. Acta.* **81** (2008) 263–266.

[9] M. V. Diudea, C. L. Nagy, *Periodic Nanostructures*, Springer-Verlag, New York, 2007.

[10] A. R. Ashrafi, M. Mirzargar, The edge Szeged polynomial of graphs, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 897–904.

[11] P. E. John, M. V. Diudea, Wiener index of zig-zag polyhex nanotubes*, Croat. Chem. Acta.* 77 (2004) 127–132.

[12] M. V. Diudea, M. Stefu, B. Pârv, P. E. John, Wiener index of armchair polyhex nanotubes, *Croat. Chem. Acta.* **77** (2004) 111–115.

[13] M. V. Diudea, Toroidal graphenes from 4-valent tori, *Bull. Chem. Soc. Jpn*. **75** (2002) 487–492.

[14] M. V. Diudea, Hosoya polynomial in tori, *MATCH Commun. Math. Comput. Chem.*. **45** (2002) 109–122.

[15] M. V. Diudea, P. E. John, Covering polyhedral tori, *MATCH Commun. Math.Comput. Chem*. **44** (2001) 103–116.

[16] M. V. Diudea, E. C. Kirby, The energetic stability of tori and single-wall tubes, *Fullerene Sci. Technol*. **9** (2001) 445–465.

[17] M. V. Diudea, I. Gutman, Wiener-type topological indices, *Croat. Chem. Acta.* **71** (1998) 21–51.

[18] A. R. Ashrafi, H. Saati, PI and Szeged indices of a one-pentagonal carbon nanocone, *J. Comput. Theor. Nanosci.* **4** (2007) 761–763.

[19] A. R. Ashrafi, A. Loghman, PI index of zig-zag polyhex nanotubes, *MATCH Commun. Math. Comput. Chem*. **55** (2006) 447–452.

[20] A. R. Ashrafi, A. Loghman, Padmakar-Ivan index of $TUC_4C_8(S)$ nanotubes, *J. Comput. Theor. Nanosci.* **3** (2006) 378–381.

[21] A. R. Ashrafi, F. Rezaei, PI index of polyhex nanotori, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 243–250.

[22] A. R. Ashrafi, A. Loghman, PI index of armchair polyhex nanotubes, *Ars Combinatoria* **80** (2006) 193–199.

[23] A. R. Ashrafi, M. Mirzargar, PI, Szeged and edge Szeged indices of an infinite family of nanostar dendrimers, *Indian J. Chem.* **47**A (2008) 538–541.

[24] A. Iranmanesh, B. Soleimani, PI index of $TUC_4C_8(R)$ nanotubes, *MATCH Commun. Math. Comput. Chem*. **57** (2007) 251–262.

[25] A. Iranmanesh, B. Soleimani, A. Ahmadi, Szeged index of TUC4C8(R) nanotube, *J. Comput. Theor. Nanosci.* **4** (2007) 147–151.

[26] A. Iranmanesh, A. R. Ashrafi, Balaban index of an armchair polyhex, $TUC_4C_8(R)$ and $TUC_4C_8(S)$ nanotorus, *J. Comput. Theor. Nanosci*. **4** (2007) 514–517.

[27] A. Heydari, B. Taeri, Szeged index of $TUC_4C_8(R)$ nanotubes, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 463–477.