OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 4, No. 12, December 2010, p. 2190 - 2193

Szeged and PI indices of Naphthalene dendrimer

ALI IRANMANESH *, N. GHOLAMI, ALI AHMADI[a]
Department of Mathematics, Tarbiat Modares University P.O. Box: 14115-137, Tehran, Iran
[a]Mathematics and Informatics Research Group, ACECR, Tarbiat Modares University P.O. Box: 14115-343, Tehran, Iran

In this paper, we compute the Szeged and Padmakar-Ivan indices of Naphthalene dendrimer.

(Received October 31, 2010; accepted November 29, 2010)

Keywords. Dendrimer, Szeged index, PI index, Naphthalene

1. Introduction

Dendrimers constitute a fascinating class of monodisperse, highly branched

Macromolecules which are the object of continuously increasing interest. The possibility of introducing selected chemical units in predetermined sites of the dendritic structure gives rise to the possibility of performing specific functions at the molecular level. The interest on dendrimer chemistry has evolved from the simple construction of these intriguing molecules to their characterization, and finally toward their functionalization, in view of potential applications in many different fields, such as chemistry, physics, engineering, biology and medicine.

Let *G* be a simple molecular graph without loops, directed and multiple edges.

The vertex and edge sets of G are represented by V(*G*) and E(*G*), respectively. A topological index is a numeric quantity derived from the structural graph of a molecule. Usage of topological indices in chemistry began in 1947, when Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of the type of alkanes known as paraffins [1]. Let *G* be a connected molecular graph and *e*=*uv* an edge of *G*, $n_{eu}(\mathrm{e}\mid \mathrm{G})$ denotes the number of edges lying closer to the vertex *u* than the vertex *v*, and $n_{ev}(\mathrm{e}\mid \mathrm{G})$ is the number of edges lying closer to the vertex *v* than the vertex *u*. The Padmakar-Ivan (PI) index of a graph G is defined as follows [2]: $\mathrm{PI}(\mathrm{G}) = \sum_{\mathrm{e}\in \mathrm{E}(\mathrm{G})}\left[n_{eu}(e\mid G)+n_{ev}(e\mid G)\right]$,.

2. Results

In Fig. 1, we show a Naphthalene dendrimer. The number of edge for this graph is $\left|E(G)\right| = 18\times 2^{n}+15$.

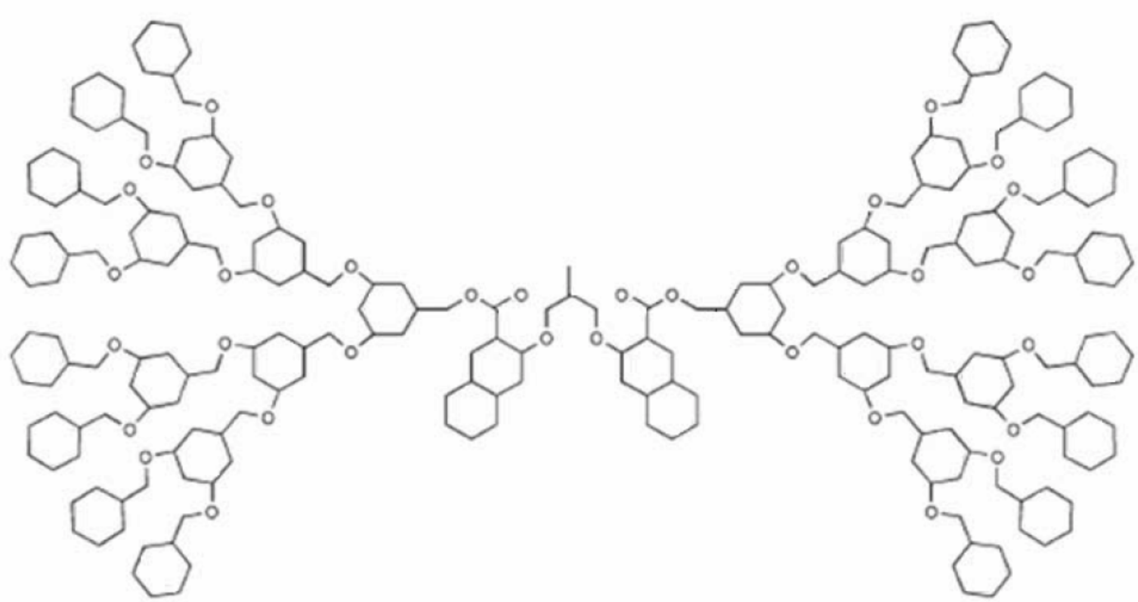

Fig. 1. Naphthalene dendrimer

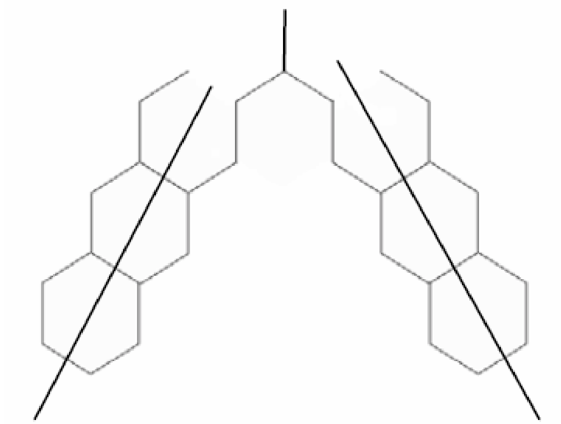

Fig. 2. Core.

In this core, for 11 edges $n(e)=1$ and for 6 edges $n(e)=3$ and for 19 edges $n(e)=2$. So the PI index is computed as follows:

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

$$= (18\times 2^n + 15)^2 - \left(\begin{array}{l} (2\times 2^{n+1}-2) \\ \times 6\times 2 + 6\times 2^n - 6 + 11 + 6\times 3 + 19\times 2 \end{array} \right)$$

$$= 324\times 4^n + 486\times 2^n + 188$$

3. Discussion and conclusion

Let e be an edge of a G connecting the vertices u and v. Define two sets $N_1(e|G)$ and $N_2(e|G)$ as

$$N_1(e|G) = \{x \in V(G) | d(x,u) < d(x,v)\}$$

and

$$N_2(e|G) = \{x \in V(G) | d(x,v) < d(x,u)\}.$$

The number of elements of $N_1(e|G)$ and $N_2(e|G)$ are denoted by $n_1(e|G)$ and $n_2(e|G)$ respectively. The Szeged index of the graph G [3] is defined as : $Sz(G) = \sum_{e\in E} n_1(e|G) n_2(e|G)$.

Up to now, topological indices of many nanbotubes and dendrimers computed. For example see [4-18].

In this section, we compute the Szeged index of Naphthalene Dendrimer.

Fig. 3, shows a Naphthalene Dendrimer which has grown 4 stages.

Let this dendrimer has grown n stage. At first, we compute $n_1(e|G)$. Let e be an edge of h_n. For all six edges, we have $n_1(e|G)$=3. The number of these hexagons in the n-th stage are equal to 2^n.

Let e be an edge of h_{n-1}. For two edges, we have $n_1(e|G) = 2\times 6 + 2\times 2 + 3$ and for another of four edges, we have $n_1(e|G) = 1\times 6 + 1\times 2 + 3$. The number of these hexagons in the n-1-th stage is equal to 2^{n-1}. If we continue this procedure for all stages n-1, n-2, …, 1, then in the first stage for two edges we have:

$$n_1(e|G) = (2^{n-1} + 2^{n-2} + \dots + 2)\times 6 + (2^{n-1} + 2^{n-2} + \dots + 2)\times 2 + 3$$

$$= (2^n - 2)\times 6 + (2^n - 2)\times 2 + 3$$

and for another four edges we have :

$$n_1(e|G) = (2^{n-2} + 2^{n-3} + \dots + 1)\times 6 + (2^{n-2} + 2^{n-3} + \dots + 1)\times 2 + 3$$

$$= (2^{n-1} - 1)\times 6 + (2^{n-1} - 1)\times 2 + 3$$

The number of these hexagons in the first stage is equal to 2.

Now, we obtaine $n_1(e|G)$ for all of edges between the hexagons.

If e is the edge $e^n_{n-1,3}$, then $n_1(e|G) = 6$. If e is the edge $e^n_{n-1,1}$, then $n_1(e|G) = 6+2$. We continue this procedure till received the first stage. If e is the edge $e^n_{n-1,3}$, then

$$n_1(e|G) = \left(2^{n-1}+2^{n-2}+\ldots+2+1\right)\times 6+\left(2^{n-1}+2^{n-2}+\ldots+2\right)\times 2$$
$$=\left(2^n-1\right)\times 6+\left(2^n-2\right)\times 2$$

If e is the edge $e^1_{0,2}$, then $n_1(e|G)=a+1$. If e is the edge $e^1_{0,1}$, then $n_1(e|G)=a+2$. Therefore, we can obtain the Szged index of this dendrimer as follows: $Sz(G_3)=\sum_A+\sum_B+\sum_C$ where A is the set of all edges of hexagon, B is the set of all edges between hexagon and C is the set of all edges in central core.
Therefore, we have:

$$\sum_A = \sum_{i=1}^{n} 2^i \times \left[\begin{array}{l} 2\times\left(\begin{array}{l}\left(2^{n+1-i}-2\right)\times 6+\\ \left(2^{n+1-i}-2\right)\times 2+3\end{array}\right) \\ \left(r-\left(\begin{array}{l}\left(2^{n+1-i}-2\right)\\ \times 6+\left(2^{n+1-i}-2\right)\times 2+3\end{array}\right)\right) \\ +4\times\left(\begin{array}{l}\left(2^{n-i}-1\right)\times 6+\\ \left(2^{n-i}-1\right)\times 2+3\end{array}\right) \\ \left(r-\left(\begin{array}{l}\left(2^{n-i}-1\right)\times 6+\\ \left(2^{n-i}-1\right)\times 2+3\end{array}\right)\right)\end{array}\right]$$

$$= -2240\times 4^{\mathrm{n}}+76\times 2^{\mathrm{n}}+1024\times \mathrm{n}\times 4^{\mathrm{n}}+2048\times \mathrm{n}\times 2^{\mathrm{n}}+2164$$

$$\sum_B = \sum_{i=1}^{n} 2^i \times \left[\begin{array}{l} \left(\begin{array}{l}\left(2^{n+1-i}-1\right)\times 6+\\ \left(2^{n+1-i}-2\right)\times 2\end{array}\right) \\ \left(r-\left(\begin{array}{l}\left(2^{n+1-i}-1\right)\times 6\\ +\left(2^{n+1-i}-2\right)\times 2\end{array}\right)\right) \\ +\left(\begin{array}{l}\left(2^{n+1-i}-1\right)\times 6+\\ \left(2^{n+1-i}-2\right)\times 2+1\end{array}\right) \\ \left(r-\left(\begin{array}{l}\left(2^{n+1-i}-1\right)\times 6+\\ \left(2^{n+1-i}-2\right)\times 2+1\end{array}\right)\right) \\ +\left(\begin{array}{l}\left(2^{n+1-i}-1\right)\times 6+\\ \left(2^{n+1-i}-2\right)\times 2+2\end{array}\right) \\ \left(r-\left(\begin{array}{l}\left(2^{n+1-i}-1\right)\times 6+\\ \left(2^{n+1-i}-2\right)\times 2+2\end{array}\right)\right)\end{array}\right]$$

$$=386\times 2^{\mathrm{n}}-1632\times 4^{\mathrm{n}}+768\times \mathrm{n}\times 4^{\mathrm{n}}+1536\times \mathrm{n}\times 2^{\mathrm{n}}+1246$$

$$\sum_C = 5\times 3\times(r-3)+4\times 7\times(r-7)+2\times(a+9)(r-a-9)+(a+14)(r-a-14)+(a+15)(r-a-15)+(a+16)(r-a-16)+2(r-1)+(a+4)(r-a-4)$$

$$=1392\times 2^{\mathrm{n}}+486+384\times 4^{\mathrm{n}}$$

Thus the Szeged index of Naphthalene dendrimer is:

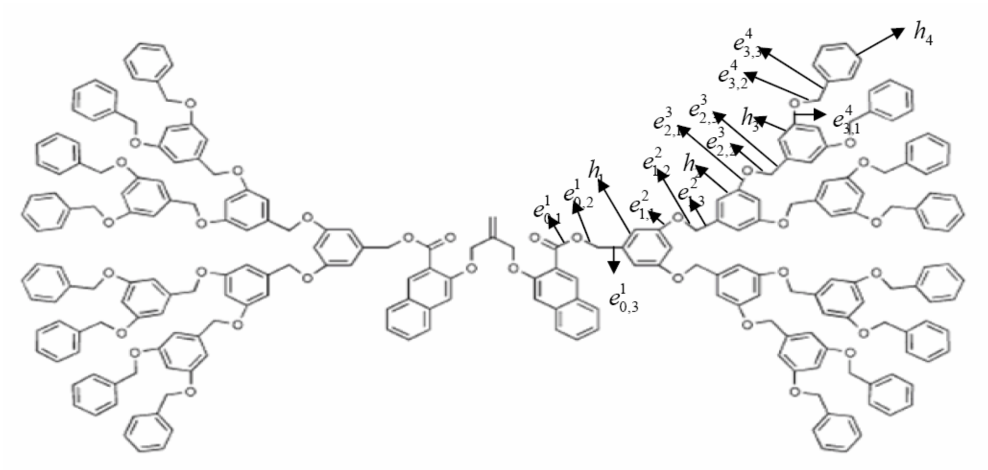

Fig. 3. Naphthalene Dendrimer which has grown 4 stages.

References

[1] H. Wiener, J. Am.Soc. **69**, 17 (1947).
[2] P. V. Khadikar, S. Karmakar, Acta Chim. Slov. **49**, 755 (2002).
[3] A. A. Dobrynin, I. Gutman, S. Klavzar, P. Z.igert, Acta Appl. Math. **72**, 247 (2002).
[4] A. Iranmanesh, N. Gholami, Micro & Nano Letters, **2**(4), 107 (2007).
[5] Ali Iranmanesh, Ivan Gutman, Omid Khormali and Anehgaldi Mahmiani, The edge versions of the wiener index, Math Commun. Math. Comput. Chem. 61 663(2009).
[6] A. Iranmanesh, B. Soliemani, MATCH Communications in Mathematical and in Computer Chemistry **57,** 251 (2007).
[7] A. Iranmanesh, B. Soliemani, A. Ahmadi, Journal of Computational and Theoretical Nanoscience**,** **4,** 147 (2007).
[8] A. Iranmanesh, A. R. Ashrafi, Journal of Computational and Theoretical Nanoscience, **4,** 514 (2007).
[9] A. Iranmanesh, Y. Pakravesh, Ars Combinatorics, **84,** 247 (2007).
[10] A. Iranmanesh, Y. Pakravesh, Utilitas Mathematica, **75**, 89 (2008).
[11] Anehgaldi Mahmiani, Omid Khormali, A. Iranmanesh, Optoelectron. Adv. Mater. Rapid Commun. **2**, 252 (2010).
[12] Anehgaldi Mahmiani, Omid Khormali, A. Iranmanesh, Ali Ahmadi, Optoelectron. Adv. Mater. Rapid Commun. **2**, 256 (2010).
[13] A. Iranmanesh, Y. Pakravesh, Optoelectron. Adv. Mater. Rapid Commun. **2**, 264 (2010).
[14] A. Iranmanesh and O. Khormali, J. Comput. Theor. Nanosci., **5**(1), 131(2008).
[15] A. Tehranian, A. Iranmanesh and Y.Alizadeh, Optoelectron. Adv. Mater. Rapid Commun. **7**, 1043 (2010).
[16] A. R. Ashrafi, M. Jalali, M. Ghorbani, Optoelectron. Adv. Mater-Rapid Commun. **3**(8), 823 (2009).
[17] A. R. Ashrafi, M. Ghorbani**,** Optoelectron. Adv. Mater-Rapid Commun. **3**(6), 596 (2009).
[18] A. Iranmanesh, A. Soltani, O. Khormali, Optoelectron. Adv. Mater.-Rapid Commun. **4**(2), 242 (2010).

*Corresponding author: iranmanesh@modares.ac.ir