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Computing the Szeged index of 4,4′–bipyridinium dendrimer

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ABSTRACT

Let e be an edge of a G connecting the vertices u and v. Define two sets $N_1(e \mid G)$ and $N_2(e \mid G)$ as $N_1(e \mid G)= \{x \in V(G) \mid d(x,u)< d(x,v)\}$ and $N_2(e \mid G)= \{x \in V(G) \mid d(x,v)< d(x,u)\}$.The number of elements of $N_1(e \mid G)$ and $N_2(e \mid G)$ are denoted by $n_1(e \mid G)$ and $n_2(e \mid G)$, respectively. The Szeged index of the graph G is defined as $Sz(G) = \sum_{e \in E} n_1(e \mid G)\, n_2(e \mid G)$. In this paper we compute the Szeged index of a *4,4′-Bipyridinium* dendrimer.

Keywords: Molecular graph, Dendrimer, Szeged Index**,** *4,4′-Bipyridinium***.**

1 INTRODUCTION

Dendrimers are macromolecular nanoscale objects that are widely recognized as precise, mathematically defined, covalent core-shell assemblies. Since dendrimers are well defined organic molecules in the size range of (1 to 15) nm and are known to act as hosts for guest molecules, they are promising candidates as templates for the formation of inorganic nanoclusters [5–6].

A topological index is a real number related to a molecular graph. It must be a structural invariant, i.e., it does not depend on the labeling or pictorial representation of a graph. There are several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules. Here, we consider only one topological index containing Szeged index of dendrimers. The Wiener index,$W(G)$, of a molecular graph G is defined as the sum of the distances between all pairs of vertices [7]. In other words,

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$$W(G)=\frac{1}{2}\left(\sum_{i=1}^{n}P_i\right),$$

where P_i is the length of the path that contains the least number of edges between vertex i and vertex j in the graph G and n is the maximum possible number of i and j.

Mathematical topological methods occupy an eminent place in the field of prediction of properties and activities of chemical compounds, and even materials. These methods, known under the acronym QSPR/QSAR (quantitative-structure-property or structure-activity relationship) are normally, but not always, based on graph theoretical descriptors, where molecules are seen as chemical graphs, i.e., as a set of vertices attached to each other by a set of non-metrical connections [2]. These descriptors are known also as topological indices. They are the simplest means of describing the structure of a molecule, characterizing it by a simple number [1]. A huge number of topological indices are known [3-4] but in spite of that, interest in topological indices has grown remarkably during recent years.

2 COMPUTATIONS

Let h_i be a hexagon which is in the stage i and $e^{i}_{i-1,j}$ be the edge which is in between h_i and h_{i-1}. Now assume that e is an edge of h_n for all 6 edges: $n_1(e \mid G)$=3, the number of these hexagons is 2^n. If e is an edge of h_{n-1} for 4 of the edges we have $n_1(e|G) = 1\times6+1\times2+3 = 11$ and for the other 2 edges: $n_1(e|G) = 2\times6+2\times2+3 = 19$, the number of these hexagons is 2^{n-1}. We continue until to achieve stage 1. If e is an edge of h_1 for 4 of the edges, we have:

$$\begin{aligned} n_1(e\mid G) &= \left(2^{n-2}+\ldots+2+1\right)\times6+\left(2^{n-2}+\ldots+2+1\right)\times2+3 \\ &= \left(2^{n-1}-1\right)\times6+\left(2^{n-1}-1\right)\times2+3 \end{aligned}$$

and for the other 2 edges, we have:

$$\begin{aligned} n_1(e\mid G) &= \left(2^{n-1}+2^{n-2}+\ldots+2\right)\times6+\left(2^{n-1}+2^{n-2}+\ldots+2\right)\times2+3 \\ &= \left(2^{n}-2\right)\times6+\left(2^{n}-2\right)\times2+3 \end{aligned}$$

andthe number of these hexagons is 2.

Suppose that e is an edge of the hexagonh_0, for all of edges ofh_0, we have:

$$\begin{aligned} n_1(e\mid G) &= \left(2^{n-1}+2^{n-2}+\ldots+2+1\right)\times6+\left(2^{n-1}+2^{n-2}+\ldots+2\right)\times2+4 \\ &= \left(2^{n}-1\right)\times6+\left(2^{n}-2\right)\times2+4 \end{aligned}$$

and the number of these hexagons is 2.

Figure 1, shows a 4,4′-Bipyridinium dendrimer which has grown n stages.

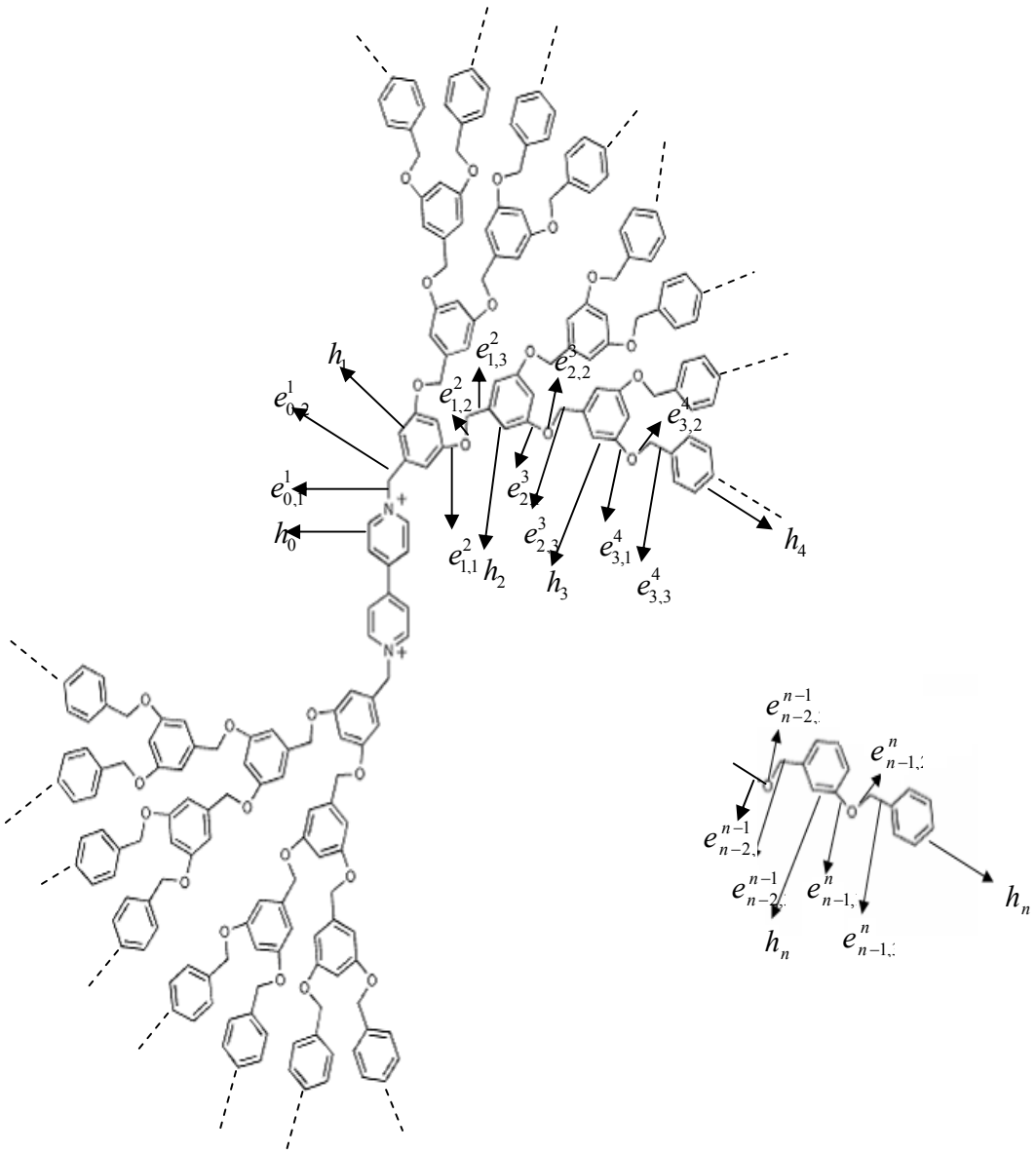

Figure 1. 4,4′-Bipyridinium Dendrimer.

Now we obtain a formula for $\sum_{A}$:

$$\sum_{A} = \sum_{i=1}^{n} 2^i \times \begin{bmatrix} 2\times\left(\left(2^{n+1-i}-2\right)\times 6+\left(2^{n+1-i}-2\right)\times 2+3\right)\times(r-a) \\ +4\times\left(\left(2^{n-i}-1\right)\times 6+\left(2^{n-i}-1\right)\times 2+3\right)\times(r-b) \end{bmatrix}$$
$$+6\times\left[\left(\left(2^n-1\right)\times 6+\left(2^n-2\right)\times 2+4\right)\times(r-a)\right]$$
$$=1024\times \mathrm{n}\times 4^{\mathrm{n}}+768\times 2^n\times \mathrm{n}\text{-}1856\times 4^{\mathrm{n}}+1628\times 2^{\mathrm{n}}+354$$

Now $n_1(e|G)$ is computed for $e^i_{i-1,j}$. Suppose e is the edge of $e^n_{n-1,3}$, we have $n_1\left(e^n_{n-1,3}\,|G\right)=1\times 6=6$, for $e^n_{n-1,2}$: $n_1\left(e^n_{n-1,2}\,|G\right)=7$, for $e^n_{n-1,1}$: $n_1(e^n_{n-1,1}|G)$=8. The number of these edges are 2^n. If e is the edge of $e^{n-1}_{n-2,3}$, we have $n_1\left(e^{n-1}_{n-2,3}\,|G\right)=(2+1)\times 6+2\times 2=22$, for $e^{n-1}_{n-2,2}$: $n_1\left(e^{n-1}_{n-2,2}\,|G\right)=a+1=23$, for $e^{n-1}_{n-2,1}$: $n_1\left(e^{n-1}_{n-2,1}\,|G\right)=a+2=24$. The number of these edges are 2^{n-1}. We continue until to achieve stage 1. If e is the edge of $e^1_{0,2}$, we have:

$$n_1(e^1_{0,2}|G)=(2^{n-1}+2^{n-2}+\ldots+2+1)\times 6+(2^{n-1}+2^{n-2}+\ldots+2)\times 2$$
$$=(2^n-1)\times 6+(2^n-2)\times 2$$

and for $e^1_{0,1}$: $n_1\left(e^1_{0,1}\,|G\right)=a+1$ the number of these edges are 2. Suppose that e is the edge of between two central hexagon, we have:

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

Now we obtain a formula for $\sum_{B}$:

$$\sum_{B} = \sum_{2}^{n} 2^i \times \begin{bmatrix} \left(\left(2^{n+1-i}-1\right)\times 6+\left(2^{n+1-i}-2\right)\times 2\right)\times(r-a) \\ +(a+1)(r-a-1)+(a+2)(r-a-2) \end{bmatrix}$$
$$+2\times\left[\left(\left(2^n-1\right)\times 6+\left(2^n-2\right)\times 2\right)\times(r-b)+(b+1)\times(r-b-1)\right]$$
$$+\left(2^n\times 6+\left(2^n-2\right)\times 2+1\right)\times(r-c)$$
$$=1514\times 2^{\mathrm{n}}+576\times 2^{\mathrm{n}}\times \mathrm{n}+768\times \mathrm{n}\times 4^{\mathrm{n}}\text{-}1696\times 4^{\mathrm{n}}+207$$

Now the Szeged index of the above dendrimer is obtained in the following formula: $Sz\left(G_4\right)=\sum_{A}+\sum_{B}+\sum_{C}$ that A is the set of hexagons edges and B is the hexagons between edges set.

3 CONCLUSION

Let G_n be the graph of a *4,4′-Bipyridinium* dendrimer. The number of vertices of this graph is equal to :r=2×[(2^n-1)×6 +(2^n-2)×2]+14.

In this paper, we can computed the Szeged index of this dendrimer in general case. In fact, the Szeged index of a *4,4′-Bipyridinium* dendrimer when it grows n stages is as follows::

$$Sz\left(G_n\right)=1792\times \mathrm{n}\times 4^{\mathrm{n}}+1344\times 2^{\mathrm{n}}\times \mathrm{n}\text{-}3552\times 4^{\mathrm{n}}+3142\times 2^{\mathrm{n}}+561$$

The Szeged index of 4,4′-Bipyridinium dendrimer which have grown 10 stages is summarized in the following table:

N	$r=2^{n+1}\times 6+\left(2^{n+1}-4\right)\times 2+2$	$Sz\left(G_n\right)$
1	26	437
2	58	15925
3	122	143773
4	250	954381
5	506	5474157
6	1018	2884209
7	2042	143864237
8	4090	691020973
9	8186	3229797037
10	16378	14789547693

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