Computing PI index of micelle-like chiral dendrimers

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A map taking graphs as arguments is called a graph invariant or topological index if it assigns equal values to isomorphic graphs. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper, the PI index of the micelle-like chiral dendrimers is computed.

Keywords: Micelle-like chiral dendrimer, molecular graph, PI index.

1 INTRODUCTION

The basic assumption for all molecule based hypotheses is that similar molecules have similar activities. This principle is also called structure-activity relationship (SAR). Quantitative structure-activity relationship, QSAR, is the process by which chemical structure is quantitatively correlated with a well defined process, such as biological activity or chemical reactivity.

A molecular graph is a simple graph in which vertices are the atoms and edge are bonds between them. A topological index for a molecular graph G is a numerical value for correlation of chemical structure with various physical properties, chemical reactivity or biological activity [1]. The Wiener index [2] is the first topological index introduced by chemist Harold Wiener. This index is defined as the sum of all topological distances between the pair of vertices. Khadikar *et al.* [3] defined a new topological index, named PI index. 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.

It is worthy to mention here that Khadikar and his co-workers [4-11] examined variety of cases in that the PI index was found more useful than many of the other distance-based topological indices in QSAR/QSTR analysis. They established the success of PI index with rigorous examples. Khadikar and his team observed that in many cases the biological activity is well correlated with PI index.

The PI index has more and more applications in nanoscience. Khadikar [12] established the

(a)

(b)

(c)

(d)
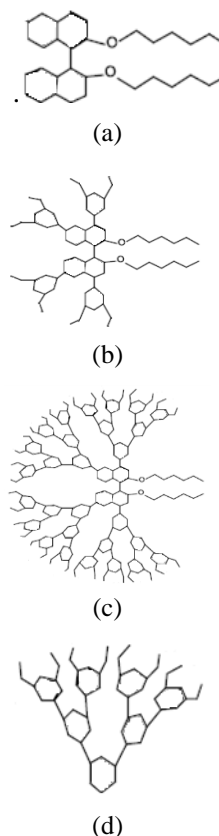
Fig. 1. a) The Core of Micelle-Like Chiral Dendrimer G[n];
b) The Molecular Graph of G[0];
c) The Molecular Graph of G[2];
d) A Branch of G[2].

importance of PI index in nanotechnology. The present article is an extension of our earlier work in demonstrating the applicability of PI index to model dendrimers and to investigate relative

potential of PI index in such studies. We encourage the readers to consult paper [13-18] for background material as well as basic computational techniques. Our calculations are done with the help of GAP System.

2 PI Index of Micelle-Like Chiral Dendrimers

Nanobiotechnology is a rapidly advancing area of scientific and technological opportunity that applies the tools and processes of nanofabrication to build devices for studying biosystems. Dendrimers are one of the main objects of this new area of science. Here a dendrimer is a synthetic 3-dimensional macromolecule that is prepared in a step-wise fashion from simple branched monomer units, the nature and functionality of which can be easily controlled and varied. The aim of this article is mathematical study of this class of nano-materials.

Consider the molecular graph of micelle-like chiral dendrimer G[3] depicted in Figure 1. We extend this molecular graph to the case that there exists a maximal chain of length n from the core to the end hexagon and denote its molecular graph by G[n].

Suppose e is an edge of G[n] and N(e) denotes the number of parallel edges to e. Then $N(e) = M - (m_u(e) + m_v(e))$, where M is the number of edges in G[n]. We first notice that $PI(G) = M^2 - \sum_{e \in E(G)} N(e)$. From the molecular graph of this dendrimer, Figure 1, we can see that the core of G[n] has exactly 37 edges and by considering its branches we have:

$$M = 4 \times [1 + 10 + 2 \times (5 + 4) + 2^2 \times (5 + 4) + \ldots + 2^{n-1}(5 + 4)] + 37 = 9 \times 2^{n+2} + 9.$$

From Figure 1, one can see that there are three types of edges as follows: the edges with N(e) = 1, the edges satisfy N(e) = 2 and the edges with N(e) = 3. To compute the PI index of this dendrimer, it is enough to compute the number of edges in each case. Suppose m_i, denote the number of edge e such that N(e) = i, $1 \le i \le 3$. Then we have $m_1 = 3 \times 2^{n+2} + 7$, $m_2 = 3 \times 2^{n+3} - 8$ and $m_3 = 6$. By these calculations, $PI(G[n]) = 81 \times 2^{2n+4} + 72 \times 2^{n+3} - 1$.

3 CONCLUSIONS

In this paper a method for computing PI index of a dendrimer is presented by which it is possible to calculate this topological index for dendrimer molecules, in general. Our method is efficient for dendrimers and we apply on micelle-like chiral dendrimer.

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ИЗЧИСЛЯВАНЕ НА PI ИНДЕКС НА МИЦЕЛОПОДОБНИ ХИРАЛНИ ДЕНДРИМЕРИ

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(Резюме)

Матрица с графи за параметри се нарича графова инварианта или топологичен индекс ако присвоява равни стойности на изоморфен граф. Дендримерът е изкуствено получена или синтезирана молекула, изградена от разклоняващи се структури, наречени мономери. В настоящата статия се изчислява PI индексът на мицелоподобни хирални дендримери.