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On Zagreb indices, Zagreb polynomials of some nanostar dendrimers

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ABSTRACT

Dendrimers are highly branched organic macromolecules with successive layers or generations of branch units surrounding a central core (Ashrafi and Mirzargar, 2008 [3]; Chen et al., 2014 [7]; Klajnert and Bryszewska, 2001 [26]; Yamamoto et al., 2002 [36]). These are key molecules in nanotechnology and can be put to good use. Topological indices are numbers associated with molecular graphs for the purpose of allowing quantitative structure-activity/property/toxicity relationships. These topological indices correlate certain physico-chemical properties like boiling point, stability, strain energy etc of chemical compounds. In this paper, we determine hyper-Zagreb index, first multiple Zagreb index, second multiple Zagreb index and Zagreb polynomials for some nanostar dendrimers.

1. Introduction

In last decade, graph theory has found a considerable use in this area of research of nanobiotechnology. Graph theory has provided chemists with a variety of useful tools, such as topological indices. *Cheminformatics* is a new subject which is a combination of chemistry, mathematics and information science. It studies quantitative structure-activity (QSAR) and structure-property (QSPR) relationships that are used to predict the biological activities and properties of chemical compounds. In the QSAR /QSPR study, physico-chemical properties and topological indices such as hyper-Zagreb index, first multiple Zagreb index, second multiple Zagreb index and Zagreb polynomials are used to predict bioactivity of the chemical compounds.

Molecules and molecular compounds are often modeled by molecular graphs. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. A graph $G(V, E)$ with vertex set V and edge set E is connected, if there exists a connection between any pair of vertices in G. A *network* is simply a connected graph having no multiple edges and no loops. For a graph G, the degree of a vertex v is the number of edges incident with v and denoted by $deg(v)$.

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. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units

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called monomers using a nanoscale fabrication process. Dendrimers are recognized as one of the major commercially available nanoscale building blocks, large and complex molecules with very well defined chemical structure. From a polymer chemistry point of view, dendrimers are nearly perfect monodisperse macromolecules with a regular and highly branched three dimensional architecture. They consist of three major architectural components: core, branches and end groups. New branches emitting from a central core are added in steps until a tree-like structure is created. The nanostar dendrimer is a part of a new group of macroparticles that appear to be photon funnels just like artificial antennas. These macromolecules and more precisely those containing phosphorus are used in the formation of nanotubes, micro and macrocapsules, nanolatex, colored glasses, chemical sensors, modified electrodes and so on [3,8]. A k-polyomino system is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular $4k$-cycle of length one. In other words, it is an edge-connected union of cells [25].

Dendrimer is a synthetic 3-dimensional macromolecule that is prepared in a step-wise fashion from simple branched monomer units see [9]. The nanostar dendrimer is a part of a new group of macromolecules that appear to photon funnels just like artificial antennas.

A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix which represents the whole graph, and these representations are aimed to be uniquely defined for that graph. A topological index is a numeric quantity associated with a graph which characterizes the topology of the graph and is invariant under graph automorphism. There are some major classes of topological indices such as distance based topological indices, degree based topological indices and counting related polynomials and indices of graphs. Among these classes degree based topological indices are of great importance and play a vital role in chemical graph theory and particularly in chemistry. In more precise way, a topological index $Top(G)$ of a graph G, is a number with the property that for every graph H isomorphic to G, $Top(H) = Top(G)$. The concept of topological index came from work done by Wiener [34] while he was working on boiling point of paraffin. He named this index as *path number*. Later on, the path number was renamed as *Wiener index*. The Wiener index is the first and most studied topological index, both from theoretical point of view and applications, and defined as the sum of distances between all pairs of vertices in G, for more details see [10,19,35]. Also in the same paper of Wiener [34], another topological index Wiener polarity index was proposed. Wiener index and Wiener polarity index can characterize the chemical and physical properties of molecules see [11,28,29].

One of the oldest topological index is the first Zagreb index introduced by Gutman and Trinajstic based on degree of vertices of G in 1972 [21]. The first and second Zagreb indices of a graph G are defined as:

$$M_1(G) = \sum_{uv \in E(G)} [deg(u) + deg(v)]$$

$$M_2(G) = \sum_{uv \in E(G)} [deg(u) \times deg(v)]$$

In 2013, Shirdel et al. [33] introduced a new degree based Zagreb index named “hyper-Zagreb index” as

$$HM(G) = \sum_{uv \in E(G)} \left[deg(u) + deg(v)\right]^2 \tag{1}$$

Ghorbani and Azimi defined two new versions of Zagreb indices of a graph G in 2012 [15]. The first multiple Zagreb index $PM_1(G)$, second multiple Zagreb index $PM_2(G)$ and these indices are defined as:

$$PM_1(G) = \prod_{uv \in E(G)} [deg(u) + deg(v)] \tag{2}$$

$$PM_2(G) = \prod_{uv \in E(G)} [deg(u) \times deg(v)] \tag{3}$$

The properties of $PM_1(G)$, $PM_2(G)$ indices for some chemical structures have been studied in [6,12,15,18,27,32].

The first Zagreb polynomial $M_1(G, x)$ and second Zagreb polynomial $M_2(G, x)$ are defined as:

$$M_1(G, x) = \sum_{uv \in E(G)} x^{[deg(u)+deg(v)]} \tag{4}$$

$$M_2(G, x) = \sum_{uv \in E(G)} x^{[deg(u)\times deg(v)]} \tag{5}$$

The properties of $M_1(G, x)$, $M_2(G, x)$ polynomials for some chemical structures have been studied in [17].

Nowadays there is an extensive research activity on $HM(G)$, $PM_1(G)$, $PM_2(G)$ indices, $M_1(G, x)$, $M_1(G, x)$ polynomials and their variants, see also [12,13,15,20–22,33].

For further study of topological indices of various graph families, see [1–5,14,16,22–24,30,31].