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A Topological Study of Dendrimers by VDB Descriptors

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ABSTRACT

The max-min sdeg index, misbalance indeg index, inverse sum indeg index, and variable sum exdeg index are among the vertex-degree-based (VDB) topological indices which have shown good predictive properties on the testing sets performed by the International Academy of Mathematical Chemistry. This paper is concerned with investigating these topological indices for some infinite families of dendrimers.

KEYWORDS: Dendrimer, Topological index, Vertex degree, Molecular graph.

1 INTRODUCTION

In the fields of 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 labeled graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. A *topological index*, also known as *connectivity index*, is a two-dimensional molecular descriptor that can be calculated from the molecular graphs, and does not depend on the way the graph is depicted or labeled and no need of energy minimization of the chemical structure [1]. Topological indices are used for example in studying correlations between the structure of a molecular compound and its physico-chemical properties or biological activity (QSPR/QSAR) [2]. Some topological indices are *vertex-degree-based* (VDB) which can be defined based on the degrees of vertices of graphs. These indices are useful in analyzing various properties of chemical compounds such as viscosity, entropy, enthalpy of vaporization, gyrational radius, boiling point, etc.

[1]Speaker

In 2010, Vukičević and Gašperov [3] proposed 148 discrete Adriatic indices which showed good predictive properties on the testing sets performed by the International Academy of Mathematical Chemistry. They can be easily encoded in the computer and it may be of interest to incorporate them in the existing software packages for chemical modeling. The *max-min sdeg index* (MMS index), *misbalance indeg index* (MI index) and *inverse sum indeg index* (ISI index) are among this kind of topological indices which are respectively defined for a molecular graph G as

$$MMS(G) = \sum_{uv \in E(G)} \left(\frac{max\{d_u, d_v\}}{min\{d_u, d_v\}}\right)^2,$$

$$MI(G) = \sum_{uv \in E(G)} \left|\frac{1}{d_u} - \frac{1}{d_v}\right| = \sum_{uv \in E(G)} \frac{|d_u - d_v|}{d_u d_v},$$

$$ISI(G) = \sum_{uv \in E(G)} \frac{1}{\frac{1}{d_u} + \frac{1}{d_v}} = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v},$$

where $E(G)$ denotes the edge set of G and d_u stands for the degree of a vertex u of G which is the number of vertices of G adjacent to u. It has been shown in [3] that, the MMS index is a significant predictor of log water activity coefficient for polychlorobiphenyls, MI index is a significant predictor of standard enthalpy of vaporization for octane isomers, and ISI index is a good predictor of total surface area for octane isomers. Furthermore, it was shown that these measures have better quality compared with some previously-stablished measures.

In 2011, Vukičević [4] proposed another VDB topological index namely *variable sum exdeg index* (VSE index). This index is formulated for a molecular graph G as

$$SEI_a(G) = \sum_{uv \in E(G)} \left(a^{d_u} + a^{d_v}\right) = \sum_{u \in V(G)} d_u a^{d_u},$$

in which $V(G)$ denotes the vertex set of G and $a \in (0,1) \cup (1, +\infty)$ is a variable parameter. It was shown in [4] that, for some values of a, SEI_a is a good predictor of the octanol-water partition coefficient for octane isomers.

Dendrimers are hyper-branched macromolecules with a rigorously tailored architecture [5]. They can be synthesized, in a controlled manner, either by a divergent or a convergent procedure. The end groups can be functionalized, thus modifying their physico-chemical or biological properties. Dendrimers have gained a wide range of applications in supra-molecular chemistry, particularly in host-guest reactions and self-assembly processes. Their applications in chemistry, biology, and nano-science are unlimited. Dendrimers have also been studied from the topological point of view, including vertex and fragment enumeration and calculation of some topological descriptors (see, for example, [6-10]). The aim of paper is to study the MMS index, MI index, ISI index, and VSE index for some infinite families of dendrimers.

2 MAIN RESULTS

In this section, we apply the edge partition method to compute the VDB invariants introduced in Section 1 for some infinite families of dendrimers.

Let G_n^1 be the molecular graph of the dendrimer graph depicted in Figure 1, in which n is the growth stages. It is easy to see that, G_n^1 has $136 \times 2^n - 15$ vertices and $152 \times 2^n - 12$ edges.

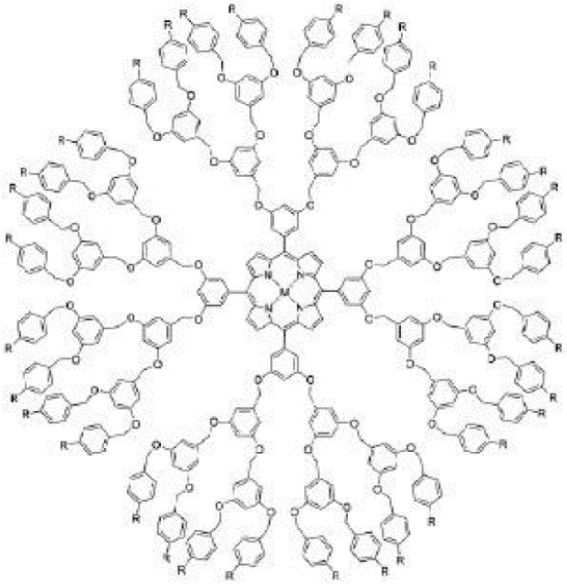

Figure 1: Molecular graph of the dendrimer G_n^1, where $n = 4$.

Theorem 1. The MMS index of G_n^1 is given by

$$MMS(G_n^1) = 85 \times 2^{n+2} - \frac{440}{9}.$$

Theorem 2. The MI index of G_n^1 dendrimer is given by

$$MI(G_n^1) = 3 \times 2^{n+3} - 5.$$

Theorem 3. The ISI index of G_n^1 dendrimer is given by

$$ISI(G_n^1) = \left(\frac{431}{5}\right) 2^{n+1} - \frac{194}{35}.$$

Theorem 4. Let $a \in (0,1) \cup (1, +\infty)$ be a variable parameter. The VSE index of G_n^1 is given by

$$SEI_a(G_n^1) = 2^{n+3}a + (2^{n+6} - 40)a^2 + (2^{n+3} + 12)a^3 + 4a^4.$$

Let G_n^2 be the chemical graph of the dendrimer graph depicted in Figure 2, in which n is the growth stages. It is easy to see that, G_n^2 has $256 \times 2^n - 63$ vertices and $288 \times 2^n - 68$ edges.

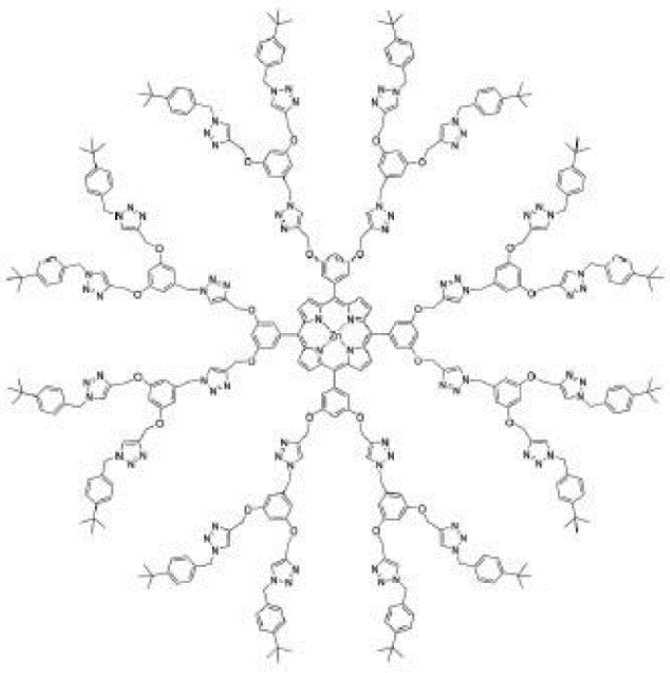

Figure 2: Molecular graph of the dendrimer G_n^2, where $n = 2$.

Theorem 5. The MMS index of G_n^2 is given by

$$MMS(G_n^2) = 185 \times 2^{n+2} - \frac{1484}{9}.$$

Theorem 6. The MI index of G_n^2 is given by

$$MI(G_n^2) = \left(\frac{19}{3}\right) \times 2^{n+3} - 13.$$

Theorem 7. The ISI index of G_n^2 dendrimer is given by

$$ISI(G_n^2) = \left(\frac{819}{5}\right) 2^{n+1} - \frac{498}{7}.$$

Theorem 8. Let $a \in (0,1) \cup (1, +\infty)$ be a variable parameter. The VSE index of G_n^2 is given by

$$SEI_a(G_n^2) = 3 \times 2^{n+3}a + (3 \times 2^{n+5} + 13 \times 2^{n+4} - 104)a^2 + (2^{n+4} + 3 \times 2^{n+3} - 16)a^3 + 4a^4.$$

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