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Reduced Forgotten Topological Indices of some Dendrimers Structures

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Abstract : In computational chemistry, the molecular structures are modeled as graphs which are called the molecular graphs.A massive of early drug tests implies that there exist strong inner relationships between the bio-medical and pharmacology characteristics of drugs and their molecular structures. Dendrimers are highly branched nanostructures and are considered a building block in nanotechnology with a variety of suitable applications. Chemical graph theory is a branch of mathematical chemistry in which different tools from graph theory are used to model chemical phenomena mathematically. Dendrimers have a very well-defined chemical structure with three major architectural components. Dendrimers are considered one of the most important, commercially available building blocks in nanotechnology. A topological index can be considered as the transformation of chemical structure into a real number. Dendrimers are highly-branched star-shaped macromolecules with nanometer-scale dimensions. Dendrimers are defined by three components: a central core, an interior dendritic structure (the branches), and an exterior surface with functional surface groups. In this paper, we determine Reduced Forgotten Topological indices of poly(propyl) ether imine, porphyrin, and zinc-porphyrin dendrimers.

Keywords and phrases : Topological index, Molecular graph, Degree Dendrimers.

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Introduction : 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. In the chemical literature, several dozens of vertex-degree-based topological indices have been and are currently considered and applied in QSPR/QSAR studies. Graph theory is used to model molecules mathematically in order to gain insight into the physical properties of these