M-Polynomial Approach to Compute Molecular Descriptors of Conjugated Borane Dendrimer

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ABSTRACT

A recent advancement in mathematical chemistry is the use of topological techniques, notably numerical graph invariants, to describe molecular structure. Recent interest in topological descriptors has increased because of their ease of production and rapid assessment durations, which negate the need for time-consuming laboratory studies. Dendrimers are synthetic macromolecules having tree-like, well-defined branching structure. The three fundamental elements of this structure are the core, inner and outer shells. Each dendrimer's exterior shell has a specified number of functional groups, which may offer a monodispersed platform for creating favourable nanoparticle-drug interactions. Conjugated dendrimers stand out in the category of dendrimers due to their significant molecular architecture. Mathematical chemistry has a lot to offer, including useful tools like polynomials and functions that help predict compound properties. Deutsch and Klavžar proposed the M-polynomial concept in 2015, which resulted in a breakthrough in the mathematical analysis of degree-based topological descriptors. For a finite simply connected graph G having vertex set V(G) and edge E(G), the M-polynomial function of G is defined to be

$$M(G;x,y)=\sum_{i<j} m_{ij}(G)x^i y^j$$

where $m_{ij}(G);\ i,j\geq 1$ be the number of edges $e=uv$ of G such that $\{d_v(G),d_u(G)\}=\{i,j\}$ and $d_v(G),d_u(G)$ denote the degrees of vertices v and u in G. In this study, we have derived the M-polynomial function for the conjugated borane dendrimer BG_nH and subsequently evaluated the topological descriptors. Conjugated borane dendrimers have been intensively explored for applications in a wide range of fields, and they provide viable alternatives to polymers in areas where monodispersity is required. There has been no research done focussing on the relationship between chemical composition and numerical formulations for this dendrimer family. Such conceptual descriptors have also sparked a wide range of applications in QSAR/QSPR studies and are perfect for innovative molecular design, drug development, and risk evaluation of compounds. Furthermore, the M-polynomial function has been analysed graphically and a comparative analysis of various topological descriptors have also been carried out.

Keywords: Borane Dendrimers, M-polynomial, Topological Descriptors

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