Computation of Topological Descriptors of Boron Nanosheet

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ABSTRACT

Boron is an element that has many fascinating and complex properties. Boron has only three valence electrons, making it a metal, but enough localized to make it an insulator and lying between metals and insulators. Pure boron is the best option for carbon fullerenes (CFs) and nanotubes (CNTs), which exhibit superior properties, in the form of novel solids and nanostructures, such as quasiplanar clusters, quasi-crystals, nanosheets, nanoribbons, nano chains, and nanotubes. The boron allotropes attract major material researchers since it has properties like thermal conductivity, hardness, and neutron scattering length. In graph theory, topological descriptors analyze network connectivity and chemical structure using structure-based numeric entities. A chemical compound can be modelled as a simple graph, $\boldsymbol{\delta}$ with vertex set $\boldsymbol{V(\delta)}$ and edge set $\boldsymbol{E(\delta)}$. And the valency of vertex $\boldsymbol{k}$ is $\boldsymbol{d_k}$. The neighborhood is defined as $\boldsymbol{N_\delta(i) = \{n \epsilon V(\delta) | ni \epsilon E(\delta)\}}$.A breakthrough was made in degree-based indices by Deutsch and Klavzar introducing the M-polynomial. The concept of graph entropy in molecular structure was introduced by Shannon.

This study investigates the entropies and structural characterization of boron nanosheets using neighborhood degree-based M-polynomial. To compute the indices and entropies, the edge partition and degree counting methods are used. From the derived analytical expression, the numerical representation and graphical comparison are also picturized.

Keywords: Boron nanosheet, Neighbourhood degree-based index, Entropy

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