

## Abstract

The focus of this research is to investigate algebraic and molecular graphs. We first compute the edge-based partition to calculate the entropy measure of the zero-divisor graph with the help of some examples. Next, we examine the structural characteristics of Fe phthalocyanine (FePc) and explored their various applications across different fields. We compute the topological indices of actinium (III) fluoride. Additionally, a connection has been made between the thermodynamic features of actinium (III) fluoride and Shannon entropy. The numerical and graphical representations of the computed data were combined with curve fitting between the calculated entropies and the heat of formation. We use the Shannon entropy approach to calculate entropies for degree-based topological indices, predict the VCl<sub>3</sub> structure physicochemical correlation capability, and consider its implications for physicochemical and biological aspects. We compute different degree-based indices, and then, using these indices, we compute the entropy measures. Also, we link the indices and entropy (ENT) using the linear regression model. Next, we discuss the concept of subdivision of chemical graphs and their corresponding line chemical graphs. More precisely, we discuss the properties of chemical graph entropies and then construct the chemical structures, namely triangular benzenoid, hexagonal parallelogram, and zigzag edge coronoid fused. Also, we estimate the degree-based entropies with the help of line graphs of the subdivision of the chemical graphs. We examine the structural characteristics of nickel sulfide and explored their various applications across different fields.

This work improves our understanding of star graph structure dynamics and provides a visual framework for interpreting their behaviour.