

Eccentric Sombor Index of Graphs and Its Role in the Structure-Property Relationship Analysis of Polycyclic Aromatic Compounds

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Abstract

This article focuses on the eccentric Sombor index, a variant of the degree-based Sombor index in which vertex degrees are replaced by their eccentricities. Several bounds for this index are established in terms of other known topological indices. Additionally, the practical utility of the eccentric Sombor index is demonstrated through its application in predicting physicochemical properties of polycyclic aromatic compounds. Our analysis reveals that the index shows a strong linear correlation with a coefficient of determination $R^2 > 0.9$, with key properties such as molecular weight, boiling point, molar refractivity, polarizability, molar volume, and flash point. Furthermore, a comparative study indicates that the eccentric Sombor index offers greater predictive accuracy than the traditional degree-based Sombor index.

Keywords: Eccentricity, Diameter, Radius.
