Topological Characterization and Graph Entropy Measures of Single Layered Cycloarenes and Their Tessellations

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ABSTRACT

The circular arrangement of benzene rings in a D_{6h}-symmetric fashion yields cycloarenes, a subclass of polycyclic aromatic hydrocarbons. Due to the underlying electronic characteristics and quick practical use, these compounds have recently attracted a lot of attention. Topological indices, which are graph-theoretically based metrics that characterize molecular connectivity, offer a powerful tool for building reliable Quantitative Structural Activity Relationship (QSAR) and Quantitative Structural Property Relationship (QSPR) models. The method of graph entropy is used to describe the physical characteristics of chemical compounds and to measure the underlying complexity of graphs. Using an effective edge partition method, this work develops the analytical formulas for different degree-based and neighbourhood degree sum-based topological descriptors for the Cycloarenes and some of its oligomers. By linking the values to various physicochemical features, the predictive power of various indices is examined. Potential topological indices that can yield robust prediction models are selected using regression analysis. Using Shannon's approach, the probabilistic entropies of the structures are thoroughly examined, and conclusions are projected.

Keywords: Topological indices; QSAR; Polycyclic aromatic compounds; Information entropy.

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