QSPR Analysis and Complexity Studies of Carbon Allotropes Using Topological Indices and Information Entropies

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ABSTRACT

Molecular descriptors are graph theoretic metrics that are commonly employed to investigate the physicochemical properties of molecular structure. Conjugated carbon nanomaterials have drawn the interest of researchers due to their numerous uses in a variety of industries, including medicine delivery, electronics, composite materials, sensors, field emission devices, energy storage and conversion, etc. In our current research, molecular descriptors are used to conduct a comprehensive analysis of three recently developed carbon allotropes, pentagraphene, phagraphene, and phographene, which are having significant thermal, dynamic, and mechanical stabilities comparable to graphene. Using a graph theory-based technique, the general formulas for the degree and neighbouring degree sum-based indices of these nanosheets are obtained. After a comprehensive QSPR analysis, significant indices are filtered and regression analysis for property prediction models are suggested. Since allotropes with all possible hybridization states and diverse bonding patterns are considered for our analysis, we propose that the derived regression model can be utilized in current and forthcoming allotrope designs. The complexity of various derivatives is contrasted by including topological indices in the definition of Shannon entropy.

Keywords: Molecular descriptors, Edge partition method, Shannon's entropy

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