Bond Additive Descriptors of Tetrapyrrolic Macrocyclic Nanostructures

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ABSTRACT

Tetrapyrrolic macrocyclic nanoribbons are naturally occurring macrocyclic molecules that are essential to the metabolism of living organisms. These nanostructures are employed in a wide range of industries, including hydrogen storage, cancer therapy, and medicine, due to their unique fundamental characteristics. In this study, the 2D nanostructures of these derivatives are studied with the inclusion of degree-based bond additive descriptors in their molecular structure. Descriptors such as these are vital in the use of QSAR, QSPR, and drug design models. These descriptors are also more suitable to investigate the physiochemical properties of these molecules, and they provide information about the characteristic growth of these nanostructures. We determine the generalized expression of the descriptors for these nanostructures using the edge partition method. We also use Shannon's entropy method to determine the entropy of these nanosheet derivatives to study the complexity of the system. Furthermore, the computed numerical values of these descriptors and their corresponding entropies are applied to demonstrate a predictive model to forecast certain properties of these macrocyclic derivatives. As a result of this study, further structural information regarding tetrapyrrolic macrocycles and their derivatives will be analyzed providing additional insights for future experimental exploration.

Keywords: Degree based descriptors, Edge partition method, Shannon's entropy

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