On Topological Entropies of Zeolite Frameworks and its QSPR Modelling with Molecular Interactions

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ABSTRACT

Chemical graph theory is a significant area of applied chemistry that investigates the underlying connection between atoms and bonds using graph theoretical approaches such as vertex and edge partitioning. Topological indices are scalar numerical values related to molecular constitutions involved in the process of correlating chemical structure with physical properties, chemical reactivity, or biological activity. Bond additive or degree-based topological indices are useful in predicting the physico-chemical properties of chemical compounds. In QSAPR studies, topological indices can be used in determining quantum chemically derived metrics like molecular hardness, polarizability, atomic charges, and so on. Some of the well-known degree-based indices with high correlation factors are Zagreb, Randić, Atom Bond Connectivity, Harmonic, and Geometric–Arithmetic index. Shannon introduced the concept of entropy in order to obtain the measure of uncertainty of the system. Later the concept of entropy was introduced in graph theory by Rashevsky. A graph's entropy is a function that depends on the graph's vertex set and its probability distribution. These measures are used in developing advanced QSAPR models which have potential applications in determining the bond energies and stability of the compounds. Microporous aluminosilicate crystals consisting of silicon cations (Si^{4+}) and aluminum cations (Al^{3+}) arranged in tetrahedral shapes surrounded by four oxygen anions (O^{2-}) are known to be zeolites. Currently, there exist more than 240 variants of zeolites which are characterized by their Silicon-Aluminium composition which gives its 3D complex structure consisting of tunnels and cages. Zeolites have served as multifunctional microporous materials and have been utilized as ion exchangers, catalysts, and adsorbents. In this study, we derive the generalized expressions to compute bond additive indices of selected 3D zeolite framework and its entropy measures using Shannon's entropy model. Further, we use statistical tools to investigate the relationship between the entropy values and potential energies of zeolites.

Keywords: Zeolite frameworks, molecular descriptors, information entropies

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