Entropy Descriptors on Predictive QSAPR Modelling of Zeolite Structures

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ABSTRACT

Zeolites are microporous minerals with consistent pore holes, cages, and channels made of tetrahedral atoms (T atoms) connected by bridging oxygen atoms. Most zeolites have T atoms of aluminium and silicon, although phosphorus, germanium, titanium, boron, gallium, and lithium can also be present. Zeolites are useful as ion exchangers, catalysts, and adsorbents because they have various structures and compositions. A topological index, also known as a connectivity index, is a molecular descriptor derived from a chemical compound's molecular graph in chemical graph theory, molecular topology and mathematical chemistry. Degree-based and distance-based topological indices are significant classes. Topological indices can be used to predict various physiochemical properties, and this is a crucial component of QSAR/QSPR research. Graph entropy is an information-theoretic quantity and a distant derivative of thermodynamic entropy, another method for measuring a molecule's information content. The Shannon's entropy inspired graph entropies with topological indices which calculating the structure information of chemical graphs and complicated networks. In this paper, we compute a various number of degree and degree sum based information entropies for the zeolite with the aid of the information function and their correlation to the potential energy. The results have the ability to predict physicochemical characteristics including potential energy, atomic charges, phase transformation, NMR signal patterns, morphological, and stability analysis of the zeolite structures.

Keywords: Topological indices, Information entropies, Potential energies

DOI: 10.21467/abstracts.158 ISBN: 978-81-965621-0-6 (eBook)