DEGREE-BASED TOPOLOGICAL INDICES IN RANDOM POLYGONAL AND SPIRO CHAINS

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Abstract: A topological descriptors is a numerical quantity associated with the chemical structures which play an essential role in the chemical graph theory. In this work, we state and prove the expected values of the degree- based topological indices and generalized $ISI_{(\alpha,\beta)}$ index for the random l-polygonal chain and random l-polygonal spiro chain. Based on the results above, we present the average values of the TIs with respect to the set of all polygonal and spiro polygonal chains with n polygons. As applications, we apply the affiliated formulae to obtain the expected values of the TIs of some special polygonal chains and spiro polygonal chains. Furthermore, we present diverse representations of graph that highlights the correlations between expected mean of indices and structural parameters.

Keywords and Phrases: Topological indices, Generalized ISI index, Random polygonal chain, Random polygonal spiro chain, Expected value, Average value.

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1. Introduction

Chemical graph theory [32] is an essential branch of mathematics and theoretical chemistry which model graphs mathematically. A topological index or molecular descriptor [14, 25, 31] correlate each molecular structure with a numerical value. It helps to predict different kind of physico-chemical properties and biological activity associated with the structure of the compounds. These indices are extensively used