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FULL PAPER

Cordial labelling of molecular structures and labelled topological indices of molecular graphs; a qspr model

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In the study of graph properties, topological indices and graph labelling are both enormous topics. In this paper, we connect the ideas of topological indices with graph labelling, resulting in a number of novel topological indices to study the labelled graphs. We present new topological indices for certain molecular graphs that admit cordial labelling in this article. Through topological indices, graph theory is playing an essential part in QSPR data analysis. In this paper, we consider the labelled square index SQI(G), labelled product Index PI(G), labelled sum Index SI(G), labelled Nirmala Index NI(G), labelled Sombor Index SOLI(G), labelled forgotten Index FI(G) and Cluster of all these Indices.

KEYWORDS

Chemical graph; molecular descriptor; labelled topological indices; cordial labeling; regression models; QSPR.

Introduction

Chemical graph theory is a branch of mathematics concerned with chemistry that blends mathematical design and graph theory to study chemical processes. It focuses on topological indices which have been closely connected with chemical molecules and molecular characteristics. Topological indices are frequently utilized in the structure-activity relationship/ quantitative structure-property (**QSAR/ QSPR**) design to predict the characteristics of a molecule or molecules.

Let $G(V,E)$ be a simple connected graph with $V(G)$ as the vertex set and E as the edge set $E(G)$. A molecular graph is a figure that used to represent synthesized good in addition to express the drug's chemical structure. We refer to [1] for any additional concepts or terms.

A molecular descriptor emphasizes in providing the most accurate numerical representation of potential molecule form. The most commonly used molecular descriptors are molecular connectivity indices. These molecular meters are often referred to it as topological indices because it describes the topology of a molecule. They are considered like graph invariants since their concepts are based on notions from graph theory. In theoretical chemistry, their specific features have been studied and have found with considerable form particularly in QSPR/QSAR/QSTR research [2-12].

A molecular graph depicts the unsaturated hydrocarbon skeletons of molecules and their compounds. Its edges indicate covalent links between non-hydrogen atoms, while its vertices represent non-hydrogen atoms. Molecular graphs have important functions in chemoinformatics [13], quantitative structure-property relationships(QSPR), quantitative structure-activity relationships (QSAR), virtual