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Computation of Several Banhatti and Reven Invariants of Silicon Carbides

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Abstract

Expressions for the molecular topological features of silicon carbide compounds are essential for quantitative structure-property and structure-activity interactions. Chemical Graph Theory is a subfield of computational chemistry that investigates topological indices of molecular networks that correlate well with the chemical characteristics of chemical compounds. In the modern age, topological indices are extremely important in the study of graph theory. Topological indices are critical tools for understanding the core topology of chemical structures while examining chemical substances. In this article, compute the first and second k-Banhatti index, modified first and second k-Banhatti index, first and second k-hyper Banhatti index, first and second hyper Revan indices, first Revan vertex index, and third Revan index for Silicon Carbide SiC4-II [p, q] for all values of p and q.

Keywords: Banhatti Indices, Hyper Banhatti Indices, Hyper Revan indices, Silicon carbide SiC_4-II [p, q], Topological Indices.

Introduction

Mathematical chemistry is a field of theoretical chemistry that uses mathematical approaches to discuss molecule structure without necessarily using quantum mechanics. Graph theory can be used to represent a chemical structure, with vertices representing atoms and edges representing chemical bonds. Chemical graph theory is a field of mathematical chemistry that bridges the gap between mathematics, chemistry, and graph theory to solve chemical issues mathematically. If there is a connection between any two vertices in a network, it is said to be connected [1].

A molecular descriptor, also known as a topological graph index, is a mathematical formula that may be applied to any graph that describes a molecule structure. The topological index is used extensively in this field of research to investigate the topological features of various chemical structures. The topological index is a numerical parameter associated with a chemical compound's molecular network. Topological indices are numerical values that describe the entire structure of a graph [2]. The topological indices are effective in predicting the physicochemical characteristics and bioactivity of the chemical compound. In mathematical chemistry, molecular descriptors serve an important role, particularly in the quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies [3-6].

Silicon Carbide (SiC) was the first substance to exhibit covalent bonds between C and Si atoms, which were commonly found in diatomic layers. These layers combine to produce tetrahedral orientated C and Si atom molecules with a short bound length and high binding strength. Silicon carbide is the most extensively applicable material in