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Bi-Distance Approach to Determine the Topological Invariants of Silicon Carbide

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Abstract:

The use of silicon carbide is increasing significantly in the fields of research and technology. Topological indices enable data gathering on algebraic graphs and provide a mathematical framework for analyzing the chemical structural characteristics. In this paper, well-known degree-based topological indices are used to analyze the chemical structures of silicon carbides. To evaluate the features of various chemical or non-chemical networks, a variety of topological indices are defined. In this paper, a new concept related to the degree of the graph called "bi-distance" is introduced, which is used to calculate all the additive as well as multiplicative degree-based indices for the isomer of silicon carbide, Si_2C_3-1[t, h]. The term "bi-distance" is derived from the concepts of degree and distance in such a way that second distance can be used to calculate degree-based topological indices.

Keywords: Bi-distance edges, Molecular graph, Randic index, Silicon Carbide Si_2C_3-1[t, h], Topological index, Zagreb index.

Introduction:

Leonhard Euler **(1702–1782)** originated the term "graph" in graph theory in the eighteenth century. He was a mathematician from Switzerland. He used graph manipulation to solve Konigsberg Bridge problems [1].

The subject of mathematics termed "graph theory" deals with structures of vertices represented by a series. Graph theory has evolved into an important field of mathematical research with relevance in chemistry, operations research, the social sciences, and computer science. All of the graphs in this paper are simple, connected, and planar. A graph is formed of vertices, nodes, or points that are connected by edges, arcs, or lines. "Graph theory" is the word used in mathematics to describe the analysis of graphs, which are mathematical patterns used to express pair-wise relationships among variables.

Graphs are one of the major aspects of discrete mathematics, and they have diverse applications in our daily life. The implementation of graph theory can be seen in nano-chemistry, computer networks, Google maps, and molecular graphs. Chemical graph theory is a sub-field of mathematical chemistry that uses graph theory to mathematically model chemical structures. It integrates chemistry and graph theory to investigate the physical and chemical properties of substances in more depth [2].

According to the IUPAC terminology[3], a "topological index" is a numerical number associated with a chemical composition that is used to correlate the chemical structure with numerous physical attributes, chemical reactivity, or bioactivities. In the recent two decades, it has become very widespread to investigate the physicochemical and structural features of molecular graphs, which are vital to chemical engineering and pharmaceutical research, using graph-theoretical methods. The T-indices are a