ON THE KCD INDICES AND EXTREMAL GRAPHS

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Abstract: In this article, we present results on KCD indices related to extremal graphs of unicyclic graphs and characterize them in terms of diameter of graphs.

Keywords and Phrases: Extremal graphs, unicyclic graphs, KCD indices.

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1. Introduction

Graph theory, a very important part of chemical graph theory is used to model the properties of molecular structures. Cheminformatics, a merger of chemistry, mathematics and information science deals with the quantitative structure property relationships (QSPR) which has emerged as a tool in the medical and chemical field as it helps to predict the physico-chemical properties of compounds. In particular, this branch studies the physical and chemical properties of chemical compounds. These molecular structures are studied using a tool from graph theory. This affordable tool is the topological index. It is used to mathematically compute the value for a graph to characterize its topology. It forms a very important part of graph theory and is widely used in the fields of mathematical chemistry and chemical graph theory. Thus, topological indices of graph theory have gained wide acceptance as a tool to perform the analysis of molecular structures. A rich theory