

TRANSIT ISOMORPHISM AND ITS STUDY ON OCTANE ISOMERS

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Abstract: Having defined and studied, the transit index and transit decomposition of a connected graph, we introduce the concept of transit isomorphism. In this paper we discuss the transit isomorphism between certain graphs and its line graphs. Construction of transit isomorphic graphs is also dealt with. Finally we discuss how transit isomorphism relates to chemical properties of octane isomers.

Keywords and Phrases: Transit index, Transit decomposition, Majorized Shortest Paths, Transit Isomorphism.

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1. Introduction

In mathematical chemistry, a molecule's properties are predicted based on its structure. Molecules are modeled as graphs, and their properties are studied using graph invariants. A graph invariant can be a polynomial, a set of values or a single value. A single value characterising the topology of a molecular graph has been termed a topological index by Hosoya. In the literature we come across many such topological indices.