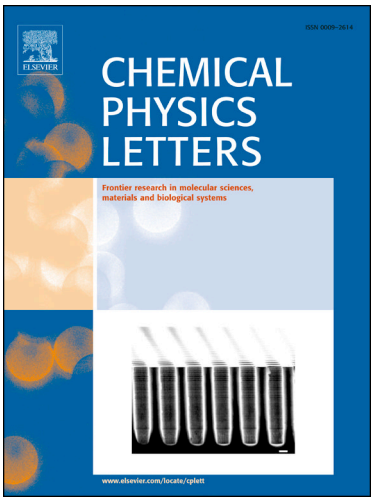

Computing distance-based topological descriptors of complex chemical networks: New theoretical techniques

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Computing distance-based topological descriptors of complex chemical networks: New theoretical techniques*

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Abstract

Structure-based topological descriptors/indices of complex chemical networks enable prediction of physico-chemical properties and the bioactivities of these compounds through QSAR/QSPR methods. In this paper, we have developed a rigorous computational and theoretical technique to compute various distance-based topological indices of complex chemical networks. A fullerene is called the IPR (Isolated-Pentagon-Rule) fullerene, if every pentagon in it is surrounded by hexagons only. To ensure the applicability of our technique, we compute certain distance-based indices of an infinite family of IPR fullerenes. Our results show that the proposed technique is more diverse and bears less algorithmic and combinatorial complexity.

Keywords: Combinatorial algorithms; Distance-based topological descriptors; Chemical networks; IPR fullerenes; QSAR of fullerenes.

1 Introduction

For undefined notations and terminologies, we refer to next section.

A broad spectrum of physico-chemical characteristics, specifically, the characterization and modelling of molecular structures has found graph theory, especially distance-based numerical graph descriptors/indices, significantly useful. The fact that the underlying activities and properties of molecules are closely related to their connectivities in its chemical graph is actually the platform where the graph-theoretic applications in chemistry and drug research originate. The study of topological connectivity and characterization of a chemical structure finds a deep concern with graph theory. The exploration of relationships between graph-theoretic topological indices and physico-chemical properties of underlying chemical structures has been a focus of research over the years [1]. As certain physico-chemical characteristics can be derived from their chemical structures, the relation with the quantitative structure-activity (QSAR) and structure-property (QSPR) relationships are developed [2].

The integeration of concepts from chemistry, mathematics and information science forms an emerging field nowadays called *cheminformatics*. The quantification of the chemical structure is the key step in QSAR/QSPR study so as building a close correlation model between the physico-chemical and biological properties for the corresponding chemical structures of a wide range of chemical compounds [1, 2].

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