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On Topological Properties Of Dyck-56 Networks

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Abstract

In *QSAR/QSPR* study, physico-chemical properties and topological indices such as Randić, atom-bond connectivity (*ABC*) and geometric-arithmetic (*GA*) index are used to predict the bioactivity of chemical compounds. A topological index can be considered as a transformation of a chemical structure into a real number, these topological descriptors significantly correlate certain physico-chemical properties of the corresponding chemical compounds. Graph theory has found a considerable use in this area of research. In this paper, we derive analytical closed results for the general Randić index $R_\alpha(G)$ (for different values of α), first Zagreb, *ABC* and *GA* indices for the Dyck-56 chemical networks for the first time.

Key words: General Randić index, *ABC* index, *GA* index, Dyck-56 network

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1 Introduction

In theoretical chemistry, the graph theoretic models can be used to study the properties of molecules. Topological indices plays a vital role in *QSAR/QSPR* study. The application of molecular structure descriptors is nowadays a standard procedure in the study of structure-property relations, especially in *QSAR/QSPR* researches [1, 5, 7, 8, 9, 12, 13, 14, 16, 17, 18, 20, 21, 22, 23, 33, 35, 4, 24, 25]. In the last few years, the number of proposed molecular descriptors is rapidly growing, they correlate the certain physico-chemical properties of chemical compounds. A close correlation of Randić index to the boiling point and Kovats constants has been found. A good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes is provided by the atom-bond connectivity (*ABC*) index. For certain

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