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Atom bond connectivity temperature index

Afework Teka Kahasy *, Kishori Narayankar , Dickson Selvan

Department of Mathematics, Mangalore University, Mangalagangothri-574199, India.

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Abstract. In the study of QSPR/QSAR, topological indices such as Zagreb index, Randic index, atom-bond connectivity index are exploited to estimate the bioactivity of chemical compounds. Inspired by many degree based topological indices, we propose here a new topological index, called the atom bond connectivity temperature index $ABCT(G)$ of a molecular graph G which shows good correlation with entropy, acentric factor, enthalpy of vaporization and standard enthalpy of vaporization of an octane isomers. In this paper, we compute the atom bond connectivity temperature index $ABCT(G)$ of line graphs of subdivision graphs of $2D-$lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.

Key words and phrases : temperature of a vertex, atom bond connectivity temperature index, nanostructures.

1 Introduction

Molecular descriptors are playing significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [13]. There are numerous of topological descriptors that have found some applications in theoretical chemistry, especially in $QSPR/QSAR$research [2, 6, 7]. Within all topological indices one of the most investigated are the descriptors based on the valences of atoms in molecules (in graph-theoretical notions degrees *of vertices of graph*) [11].
Topological indices are numerical parameters of a graph which are invariant undergraph isomorphism. For a collection of recent results on topological indices, we refer the interested reader to the articles [1, 3, 5].

*Corresponding author (Email address: kafew17@gmail.com).
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