



GEOMETRIC ARITHMETIC TEMPERATURE INDEX OF CERTAIN NANOSTRUCTURES

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Abstract: In the study of QSPR/QSAR, topological indices such as Zagreb index, geometric arithmetic 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 geometric arithmetic temperature index $GATI(G)$ 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 geometric arithmetic temperature index $GATI(G)$ of line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p, q]$.

Keywords: Temperature of a vertex, geometric arithmetic temperature index, nanostructures.

I. INTRODUCTION

Molecular descriptors are playing significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [1]. There are numerous of topological descriptors that have found some applications in theoretical chemistry, especially in QSPR/QSAR research [2,3,4]. 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*).

Topological indices are numerical parameters of a graph which are invariant under graph isomorphisms. For a collection of recent results on topological indices, we refer the interested reader to the articles [5,6,7].

Let G be a connected graph with n vertices and m edges. Let $V(G)$ and $E(G)$ be its vertex and edge sets, respectively. The edge joining the vertices u and v is denoted by uv . The *degree* of a vertex u in a graph G is the number of edges incidence to u and is denoted by d_u or $d(u)$.

The temperature of a vertex u of a connected graph G is defined by Siemion Fajtlowicz as [8].

$$T(u) = \frac{d_u}{n - d_u}$$

where d_u is the degree of a vertex u , and n is the number of vertices of a graph G .

... [9], Vukičević et al. defined a new topological index “geometric arithmetic index” of a graph G denoted by $GA(G)$ and is defined by,

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$