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Harmonic Temperature Index of Certain Nanostructures

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Abstract –*In the study ofQSPR/QSAR, topological indices such as Zagreb index, Harmonic 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 Harmonic temperature index $HTI(G)$ 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 Harmonic temperature index $HTI(G)$of line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.*

Keywords– *Temperature of a vertex, HarmonicTemperature 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 numerousof topological descriptors that have found some applications in theoretical chemistry, especially in QSPR/QSAR research [2,3,4]. Within all topological indices, those 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 undergraph isomorphism.For a collection of recent results on topological indices, interested readers can refer the articles [5,6,7].

Let G be a connected graph of order$n$ and size m. 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 byd_u or $d(u)$.

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

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

whered_u is the degree of a vertex u, and n is order of graph G.

Harmonic index is defined for the first time by S. Fajtlowicz in [11]. The Harmonic index of a graph G is defined as:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}$$

Recently, Kishori P. N. and Dickson S. has introduced temperature index of a graph in [10] and is defined as $\sum_{uv \in E(G)}[T_u + T_v]$ and we extend this study for Harmonic temperature index.Inspired by the work on degree based topological indices and Harmonic index, we now define the Harmonic temperature index $HTI(G)$of a molecular graph G as follows.

$$HTI(G) = \sum_{uv \in E(G)} \frac{2}{T_u + T_v}$$

where$T_u$and $T_v$are the temperature of the vertex u and v, respectively.

II. On Chemical Applicability of the Harmonic Temperature Index

In this section we will discuss the regression analysis of entropy (S), acentric factor (AcentFac), enthalpy of vaporization (HVAP) and standard enthalpy of vaporization (DHVAP) of an octane isomers on the Harmonic