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DEGREE-BASED GRAPHICAL DESCRIPTORS OF RANDOM CYCLOOCTANE CHAINS

Veena Mathad[1], Patil Manjula Shankargouda[2] and Puneeth S.[3]

[1]Department of Studies in Mathematics, University of Mysore, Manasagangotri, Mysuru, India (E-mail: veena_mathad@rediffmail.com) ORCID: 0000-0002-6621-9596

[2]Department of Mathematics, Government-First Grade College & P.G. Centre, Dharwad, India (E-mail: manjulapatil2010@gmail.com) ORCID: 0009-0007-2727-9696

[3]Department of Advanced Computing, St Joseph's University, Bangalore, India (E-mail: puneethprajwal@gmail.com) ORCID: 0000-0002-5532-696X

Abstract. A random cyclooctane chain is a molecular graph of a saturated hydrocarbon with at least two rings. All rings are cyclooctane, each ring joins with no more than two other rings through a single bond, and two rings join with one other ring. This article aims to find the expected values of degree-based graphical descriptors namely, Harmoic index, Redefined First Zagreb index, Redefined Second Zagreb index, Inverse Degree index, Agumented Zagreb index and Symmetric division degree index for random cyclooctane chains. The primary objective is to provide explicit analytical formulae for these indices, offering a theoretical method to predict the physicochemical properties of random cyclooctane chains. By utilizing recurrence relations and branching probabilities, the study established a consistent numerical hierarchy as $\mathbb{E}_p^{ID} < \mathbb{E}_p^{H} < \mathbb{E}_p^{R_1Z} < \mathbb{E}_p^{R_2Z} < \mathbb{E}_p^{SD} < \mathbb{E}_p^{AZ}$.

Keywords: Chemical Graph Theory, Cyclooctane Chains, Degree-based Graphical indices.

AMS (MOS) subject classification: 05C09, 05C92, 92E10.

1 Introduction

Chemical graph theory, a branch of mathematics which deals with the mathematical modelling of graphs is also an essential branch of theoretical chemistry. Initial chemical research introduced the theory of chemical graphs. Chemists have confirmed that the physicochemical properties of a compound have been associated with molecular arrangement, with results derived from an enormous number of investigational data [3]. Cyclooctane, an eight-membered cyclic hydrocarbon, has emerged as a focal point within the computational chemistry domain over recent decades. Cyclooctane chains play a key role in computational chemistry as macrocyclic aromatic hydrocarbons. The unique features and shape-shifting abilities of cyclooctanes have led to their widespread use in chemical and biological industries [1, 4].