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Notice for the PhD Viva Voce Examination

Ms Anjusha Asok (Registration Number: 1881504), PhD scholar at the School of Sciences, CHRIST (Deemed to be University), Bangalore will defend her PhD thesis at the public viva-voce examination on Monday, 1 April 2024 at 11.00 am in Room No. 044, Ground Floor, R & D Block, CHRIST (Deemed to be University), Bengaluru - 560029.

Title of the Thesis	:	**QSPR Studies of Chemical Compounds Using Topological Indices**
Discipline	:	**Mathematics**
External Examiner (Outside Karnataka)	:	**Dr R Sundara Rajan** Professor Department of Mathematics Hindustan Institute of Technology and Science Rajiv Gandhi Salai Padur, Chennai – 603103 Tamil Nadu
External Examiner (Within Karnataka)	:	**Dr Raghavendra A** Professor Department of Mathematics Poornaprajna College Udupi - 576101 Karnataka
Supervisor	:	**Dr Joseph Varghese** Professor Department of Mathematics School of Sciences CHRIST (Deemed to be University) Bengaluru – 560029 Karnataka

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The members of the Research Advisory Committee of the Scholar, the faculty members of the Department and the School, interested experts and research scholars of all the branches of research are cordially invited to attend this open viva-voce examination.

Registrar

Place: Bengaluru
Date: 23 March 2024

ABSTRACT

Graph theory is an important branch of mathematics and chemistry in which graphs allow the modelling of the relationship between objects, which are addressed by the vertices of a graph. In this context, graph theory has gained extensive recognition not only from the mathematical society but also from the various scientific fields. One of the exciting fields of mathematics, which has a wide range of applications in chemistry, is graph theory, which further resulted in chemical graph theory. In Chemical graph theory, we treat the atoms of the compounds as vertices and the bond between the atoms as an edge between the corresponding vertices of the graph. A topological graph index, a molecular descriptor, is a mathematical formula that can be applied to any graph that models a quantitative structural property (QSPR) between the physiochemical properties and the molecular descriptors of chemical compounds. These days, the topological indices receive great attention among chemists and graph theorists as they theoretically allow the prediction of physio-chemical properties of chemical compounds, reducing the cost and the consumption of time. This engrossed the idea of the relevance of the study of topological indices.

In our research, we include the investigation of 30 topological indices, which incorporate Harary, Wiener, Zagreb and connectivity indices, along with some physiochemical properties of a set of 18 octane isomers and 209 polychloro biphenyls to develop a QSPR model. We found that the physiochemical properties of octane isomers such as BP, HVAP, DHVAP, HFORM, AcenFac, and TSA and physiochemical properties of polychlorobiphenyls such as RRT are associated with at least one of the topological indices of our concern with a significant level of regression. Also, we develop a regression model for predicting BP, HVAP, DHVAP, HFORM, AcenFac, RRT and TSA for octane isomers and polychlorobiphenyls. The study also includes identifying trees and unicyclic graphs with given values of forgotten and hype Zagreb indices, which resulted in the characterization of trees and unicyclic graphs for hyper and forgotten Zagreb indices. The characterization of reformulated Zagreb indices for trees is also studied, which in turn stirs up the inverse problem for entire Zagreb indices for trees. Further, we introduce Python programs to find certain degrees, distances, and eccentricity-based topological indices for any molecular graph.

Keywords: QSPR, Chemical compounds, Molecular graphs, Topological indices, Zagreb indices, Eccentricity indices, Connectivity indices, Python programming.

Publications:

1. **A. Asok**, J. V. Kureethara, "Characterization of the Forgotten Topological Index and the Hyper Zagreb index for Unicyclicgraphs", MATCH Commun. Math. Comput. Chem., 84(3),739 – 751, 2020.
2. J. V. Kureethara, **A. Asok** and I. N. Cangul, "Inverse Problem for the Forgotten and the Hyper agreb Indices of Trees", Communications in combinatorics and Optimization, 7(2), 203-209, 2021.
3. **A. Asok**, J. V. Kureethara, "Extremal trees of Reformulated and the Entire Zagreb Indices", International Conference on Artificial Intelligence on Textile and Apparel, 389-403, 2023.