



Notice for the PhD Viva Voce Examination

Ms Ishita Sarkar (Registration Number: 2090225), 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, 22 July 2024 at 2.30 pm in Room No. 044, Ground Floor, R & D Block, CHRIST (Deemed to be University), Bengaluru - 560029.

Title of the Thesis	:	A Study on Certain Topological Indices and Related Polynomials in Graphs
Discipline	:	Mathematics
External Examiner (Outside Karnataka)	:	Dr R Sundareswaran Associate Professor Department of Mathematics Sri Sivasubramaniya Nadar College of Engineering Kelavakkam, Chennai – 603110 Tamil Nadu
External Examiner (Within Karnataka)	:	Dr Devadas Nayak C Associate Professor Department of Mathematics Manipal Institute of Technology Manipal, Uttara Karnataka District Karnataka
Supervisor	:	Dr Manjunath N Associate Professor Department of Sciences and Humanities School of Engineering and Technology CHRIST (Deemed to be University) Bangalore Kengeri Campus Bengaluru - 560074 Karnataka

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.

Place: Bengaluru
Date: 12 July 2024



Registrar

ABSTRACT

Topological indices are invariants of molecular graphs which are used for structure-property or structure-activity correlations. In this study, we have worked upon the bounds and exact expressions of certain specific topological indices related with some graph operations. Further, we have determined the formulations of certain topological indices and co-indices for the total transformation graph. In addition, we have worked upon the reformulated forgotten index and obtained its exact expressions with respect to the generalized transformation graphs and other graph product variants. We describe graph transformations, by means of which the reformulated forgotten index increases or decreases. Using these transformations, the trees, unicyclic and bicyclic graphs extremal with respect to the index are characterized.

We carried out the computation of equitable and non-equitable Zagreb and the relative equitable and non-equitable Zagreb indices of certain chemical compounds like the polycyclic aromatic hydrocarbons, the rhombus silicate and the rhombus oxide networks using the equitable Zagreb polynomial formulations. As to demonstrate the application of our study, we have carried out the quantitative structure property relationship analysis of the anti-HIV and anti-Covid drugs with respect to the physico-chemical drug characteristics using the notion of M-polynomial and topological indices, thus signifying the potency of the molecular descriptors and asserting that the indices taken under study are inherent units for the QSPR inspection of the drugs.

Keywords: Topological index, graph operation, transformation graph, M-polynomial, QSPR analysis.

Publications:

1. **Ishita Sarkar** and Manjunath Nanjappa, "QSPR Analysis of Certain Anti-HIV Drugs", South East Asian J. of Mathematics and Mathematical Sciences, 18(3) (2022), 283-306.
2. **Ishita Sarkar** and Manjunath Nanjappa, "On Second Hyper-Zagreb index of Corona Products Related to R-graphs", International Journal of Applied Mathematics, 36(3) (2023), 301-322.
3. **Ishita Sarkar**, Manjunath N. and B. Chaluvvaraju, "Bounds Related to Product Variants of Graphs", Palestine Journal of Mathematics, 12(2) (2023), 1-24.
4. **Ishita Sarkar**, Manjunath N. and K. Ramesha, "QSPR Analysis of Polycyclic Aromatic Hydrocarbons", Journal of Mines, Metals and Fuels, 70(8A) (2022), 49-55.
5. **Ishita Sarkar**, N. Manjunath, B. Chaluvvaraju and V. Lokesha, "Bounds of Sombor Index for F-Sum Operation", Palestine Journal of Mathematics, 12(2) (2023), 504-516.
6. **Ishita Sarkar**, Manjunath Nanjappa and Ivan Gutman, "Bounds on Sombor Index for Corona Products on R-Graphs", Communications in Combinatorics and Optimization, 9(1) (2024), 101-117.
7. **Ishita Sarkar**, Manjunath Nanjappa and Ivan Gutman, "On Transformed Graphs", South East Asian J. of Mathematics and Mathematical Sciences, 19(2) (2023), 179-202.
8. **Ishita Sarkar**, Manjunath Nanjappa and Ivan Gutman, "Extremal Reformulated Forgotten Index of Trees, Unicyclic and Bicyclic Graphs", Filomat, 38(1) (2024).