

## **Area of interest in Research: Chemical Graph Theory**

### **Title of Research Work: A STUDY ON THE DEGREE BASED TOPOLOGICAL INDICES AND ENERGY OF SOME CLASSES OF GRAPHS**

#### **ABSTRACT**

Branch of Mathematics which combines graph theory and chemistry is called chemical graph theory. A topological index is a numerical descriptor of the molecular structure derived from the corresponding molecular graph, which can be used to characterize the chemical compound and predict certain physico chemical properties like boiling point, molecular weight, density, refractive index, and so forth [1]. Degree-based and distance-based topological indices are the two most important categories of topological indices for graphs. Wiener index, which is based on the topological distance between vertices in the corresponding graph, is the most well-known and often used topological index. It was defined and used by Harold Wiener in 1947 which helped him to investigate the boiling point of Paraffins[2].

The general form of degree based topological index is given by

$$TI(G) = \sum_{xy \in E(G)} F(d(x), d(y))$$

Where  $G = (V(G), E(G))$  is a simple, undirected, and connected graph,  $d(x)$  denotes the degree of the vertex  $x$ ,  $d(y)$  denotes the degree of the vertex  $y$  and  $F(d(x), d(y))$  is a function appropriately chosen for the computation.

#### **Research Gap**

- Not all topological indices (Reduced Sombor, Dharward and SK group of indices etc.) are calculated for graphs and graph operations. So, it is an area of study.
- Several researchers computed  $M$  – polynomial for various simple and connected graphs. However, no one has paid more attention to the  $M$  – polynomial of numerous graph operations on graphs (Nazari et al., 2022). So, to calculate such  $M$  – polynomial is an area of research.

#### **Objectives of Study**

- Computation of degree based Topological Indices for classes of Graphs, line graphs, subdivision graphs and Nanostructures.
- Determine topological indices of graph operations
- Identify relationship between different topological indices
- Calculation of energy of classes of graphs using topological indices
- Try to identify bounds for topological indices for classes of graphs
- Computation of  $M$ -polynomials for classes of graphs and of graph operations

#### **Research Methodology**

- Data collection through Journals and academic documents.
- Preparation of summaries of the work that have already been done relating to proposed area
- Topological indices, index relations,  $M$ -Polynomials are to be found for various classes of graphs
- Graphical representation of topological indices for comparison.
- Establish and publish new results

## References

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- [3] Deutsch, E., & Klavžar, S. (2015). IJMC M-Polynomial and Degree-Based Topological Indices. In *Iranian Journal of Mathematical Chemistry* (Vol. 6, Issue2).
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