Abstract

This study thoroughly examines topological indices by utilising algebraic polynomials in various chemical networks. The inquiry encompasses a diverse range of molecular structures, including complex hexagonal cages, adaptable metal-organic frameworks, promising niobium dioxide, and fundamental alkanes and alkenes. By utilising sophisticated mathematical methods like M-polynomials, Forgotten polynomials, and other algebraic tools, new closed equations are created to reveal the intricate structural importance of these networks.

The work enhances our comprehension of diverse topological indices, such as the General Randić index, Zagreb indices, modified Zagreb indices, Atom-Bond connectivity, and Hyper Zagreb index, through meticulous computer analysis. These indices are important markers of the chemical, physical, and mathematical characteristics that are inherent in the networks being studied. The process of obtaining complete equations and drawing conclusions for these indices provides essential understanding of the complex relationship between molecule structures and their topological features.

This work focuses on developing advanced techniques for accurately calculating and comparing topological indices, enabling a more comprehensive understanding of molecular structures and their quantitative characteristics. The study employs a comprehensive approach that encompasses mathematical, visual, and computer analyses. The software utilises numerical tables, 3D displays, line graphs, and statistical tools to analyse the intricate connections between structural features and topological indices. This study represents a significant milestone in the exploration of topological indices and their use in molecular analysis. The study integrates sophisticated mathematical techniques, computational simulations, and visual depictions to offer a thorough comprehension of molecular networks. This strategy has the capacity to propel future advancements in multidisciplinary scientific study.

The results of this study go beyond only understanding the theory and have practical applications in various scientific domains. The examination of topological indices has the potential to bring about significant breakthroughs in various fields, including chemistry, physics, materials science, and pharmacology. This research establishes

the foundation for the creation of safer medications, more efficient materials, and creative scientific procedures by enhancing our comprehension of molecular structures and their quantitative characteristics.