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REVAN TOPOLOGICAL INDICES OF SUPRAMOLECULAR FUSHINE ACID USEFUL IN MEDICAL APPLICATIONS

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Abstract

Chemical graph theory plays a pivotal role in mathematical chemistry by representing chemical structures as graphs, with vertices denoting atoms and edges denoting chemical bonds. Topological indices, numerical invariants derived from such graphs, have been widely employed in quantitative structure property relationship ($QSPR$) and quantitative structure activity relationship ($QSAR$) studies. These indices correlate molecular structure with physicochemical and biological properties and have become crucial tools in drug design. Supramolecular chemistry, which studies entities formed bymolecular self-assembly through non-covalent interactions, offers an exciting avenue for designing complex molecular architectures. In this work, we investigate the supramolecular structure of Fuchsine ($C_{20}H_{19}N_3HCl$), a magenta dye of significant microbiological and histological importance. We construct a supramolecular sheet, denoted $[m, n]$, comprising $m \times n$ units of Fuchsine molecules. The corresponding chemical graph is simple, connected, and finite, consisting of $38mn + m + n$ vertices and $42mn$ edges, which are further classified by the Revan degrees of their end vertices. We derive closed-form expressions for several Revan degree-based topological indices of the supramolecular Fuchsine sheet, including the first and second Revan indices(R_1 and R_2), Atomic Bond Connectivity Revan index(*ABCR*), Geometric-Arithmetic Revan index(GAR), the first and second hyper Revan indices(HR_1 and HR_2), the first and second modified Revan indices(mR_1 and mR_2) , forgotten Revan index(FR). A detailed numerical and graphical analysis demonstrates that all these indices increase monotonically with the parameters m and n, reflecting the scaling behaviour of the supramolecular structure. Among the indices studied, the first hyper Reven index exhibits the highest values, whereas the first modified Revan index yields the lowest. Our findings provide a comprehensive mathematical characterization of the supramolecular Fuchsine graph, offering valuable insights for modelling and predicting the properties of complex chemical systems using topological descriptors.

Keywords*:* *Revan Indices, Supramolecular Fuchsine, QSPR/QSAR Studies*