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Topological Indices of Molecular Graphs Under Specific Chemical Reactions

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Abstract

Molecular graph serves as a convenient model for any real or abstract chemical compound. A topological index is the graph invariant number calculated from the graph representing the molecule. The advantage of topological indices is that it may be used directly as simple numerical descriptors in QSPR/QSAR models. Most of the topological descriptors are based either on atom-atom connectivity or on topological distances. A chemical reaction can be represented as the transformation of the chemical (Molecular) graph representing the reaction's substrate into another chemical graph representing the product. The type of chemical reaction where two substrates combine to form a single product (combination reaction) motivated us to study the effect of topological indices when a bridge is introduced between the respective vertices (of degree i, i=1, 2, 3) of two copies of the same graph. The graph obtained in this manner may or may not exist in reality, but it is the interest of the chemist to check the stability of the so obtained structure of the product. In this paper we present an algorithm to calculate the distance matrix of the resultant graph obtained after each iteration and thereby tabulate various topological indices. We also give the explicit formula for calculating Wiener index of the graph representing the resulting product.