

EDGE VERSION OF NEW JOIN GRAPHS AND THEIR INVARIANT

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Abstract: A molecular structure descriptor (topological descriptor) is numerical value associated with chemical construction for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. The topological descriptors are very important role in mathematical chemistry, especially, they are used in the studies of *QSAR/QSPR*. In this paper, we study the *H*-invariant of edge version of new join graphs.

Keywords and Phrases: Graph invariant, Degree, Topological descriptor.

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1. Introduction and Preliminaries

Quantitative structure-activity relationship models (QSAR models) are regression or classification models used in the chemical and biological sciences and control system engineering. One of the first historical QSAR chemical applications was to predict boiling points. Those numerical quantities which transform a chemical structure to a numerical number called the topological descriptors/indices. In QSAR study, chemical graph theory plays an important role in modelling of organic chemical structures to hydrogen depleted graphs in which vertices correspond to atoms and edges correspond the bonds in the underlying chemical compounds.

The Zagreb invariants have been introduced more than thirty years ago by Gutman and Trinajestić [4]. They are defined as $M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))$