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SOME INVARIANTS OF SPECIAL GRAPHS

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Abstract: The topological invariants are very important role in mathematical chemistry, especially, they are used in the studies of QSAR/QSPR. In this paper, we study the some topological invariants of special types of graphs.

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

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1. Introduction and Preliminaries

Chemical graph theory is the topological branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena. A topological descriptor is a map f from G to R in which G is a set of simple finite graphs. The Zagreb invariants have been introduced more than thirty years ago by Gutman and Trinajestić [1]. They are defined as $M_1(G) = \sum_{u \in V(G)} d_G(u)^2$ and $M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v)$, where $d_G(u)$ is the degree of u in G.

Furtula and Gutman in [4] recently investigated this invariant and named this invariant as F-invariant and showed that the predictive ability of this invariant is almost similar to that of first Zagreb invariant and for the entropy and acetic factor, both of them yield correlation coefficients greater than 0.95. The F-invariant of a graph G is defined as $F(G) = \sum_{u \in V(G)} d_G^3(u) = \sum_{uv \in E(G)} (d_G^2(u) + d_G^2(v))$. The inverse degree invariant of a connected graph G is defined as $ID(G) = \sum_{u \in V(G)} \frac{1}{d_G(u)}$.