Abstract

Now a days graph theory is one of the prime objects of study in discrete mathematics. It has applications in diverse fields which include chemistry, linguistics, computer science, natural science, operations research and electrical engineering. A topological index is a numerical descriptor of a molecule, based on a certain topological feature of the corresponding molecular graph. The advantage of topological indices is in that they may be used directly as simple numerical descriptors in a comparison with physical, chemical or biological parameters of molecules in Quantitative Structure Property Relationships (QSPR) and in Quantitative Structure Activity Relationships (QSAR). Zagreb indices, were introduced 43 years ago by I. Gutman and N. Trinajstić [21]. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure-descriptors [3, 49]. In 1975, Randić proposed a structural descriptor called branching index [43] that later became the well-known Randić index (product-connectivity index), which is the most used molecular descriptor in QSPR and QSAR studies[49, 29]. The sum-connectivity index was proposed in [63] and it was found that the sum-connectivity index and the product-connectivity index correlate well among themselves and with the π-electronic energy of benzenoid hydrocarbons [36]. Many applications of the sum-connectivity index may be found in [37]. Recently, this concept was extended to the general sum-connectivity index in [64].

Chapter one of this dissertation briefly describes some basic definitions and notations of graph theory which we used in our research.

In chapter two we briefly introduce elements of chemical graph theory and some topological indices whose extremal properties we discuss in next chapters.

In chapter 3, using a graph transformation and several inequalities, in the class of n-vertex connected bicyclic graphs G with $n \geq 4$, we determine the unique graph minimizing the general sum-connectivity index for $-1 \leq \alpha < 0$.

In chapter 4 we deduced upper and lower bounds of $M_1(G)$ and an upper bound

of $M_2(G)$ in k-apex trees. We proved that in the class of k-apex trees ($k \geq 1$) of order $n \geq 5$, the graph $K_k + S_{n-k}$ maximizes the first and second Zagreb indices. We also proved that in the class of k-apex trees ($k \geq 1$) of order $n \geq 3k$ the graph G that has $n - 2k + 2$ vertices of degree 2 and $2k - 2$ vertices of degree 3 minimizes the first Zagreb index.

In chapter 5 we obtained explicit expressions for minimal first general Zagreb index $Z_p(G)$ for $p > 1$, which directly can be extended for $\gamma > 2$, where γ is the cyclomatic number of G.

In chapter 6 we determined the extremal values of the Narumi-Katayama, first Zagreb and second Zagreb indices of connected (n, n_1)-graphs with fixed cyclomatic number and showed that these bounds are tight.