Extremal Chemical Trees

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A variety of molecular-graph-based structure-descriptors were proposed, in particular the Wiener index $W$, the largest graph eigenvalue $\lambda_1$, the connectivity index $\chi$, the graph energy $E$ and the Hosoya index $Z$, capable of measuring the branching of the carbon-atom skeleton of organic compounds, and therefore suitable for describing several of their physico-chemical properties. We now determine the structure of the chemical trees (= the graph representation of acyclic saturated hydrocarbons) that are extremal with respect to $W$, $\lambda_1$, $E$, and $Z$, whereas the analogous problem for $\chi$ was solved earlier. Among chemical trees with $5$, $6$, $7$, and $3k + 2$ vertices, $k = 2, 3, \ldots$, one and the same tree has maximum $\lambda_1$ and minimum $W$, $E$, $Z$. Among chemical trees with $3k$ and $3k + 1$ vertices, $k = 3, 4, \ldots$, one tree has minimum $W$ and maximum $\lambda_1$ and another minimum $E$ and $Z$.

Key words: Chemical Tree; Branching; Wiener Index; Hosoya Index; Connectivity Index; Eigenvalue (of a graph); Energy (of a graph).