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 λ_1, the connectivity index χ, 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, λ_1, E, and Z, whereas the analogous problem for χ 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 λ_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 λ_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).