Estrada Index of Benzenoid Hydrocarbons

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A structure-descriptor EE, recently proposed by Estrada, is examined. If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the molecular graph, then $EE = \sum_{i=1}^{n} e^{\lambda_i}$. In the case of benzenoid hydrocarbons with n carbon atoms and m carbon-carbon bonds, EE is found to be accurately approximated by means of the formula $a_1 n \cosh\left(\sqrt{2m/n}\right) + a_2$, where $a_1 \approx 1.098$ and $a_2 = -0.64$ are empirically determined fitting constants. Within classes of benzenoid isomers (which all have equal n and m), the Estrada index is linearly proportional to the number of bay regions.

Key words: Estrada Index; Benzenoid Hydrocarbons; Molecular Graph; Spectrum (of Graph).