

Alkanes with Greatest Estrada Index

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If $\lambda_1 > \lambda_2 \geq \lambda_3 \geq \dots \geq \lambda_n$ are the eigenvalues of the molecular graph, then the Estrada index, a recently conceived molecular structure-descriptor is $EE = \sum_{i=1}^n e^{\lambda_i}$. The same alkanes, whose molecular graphs have extremal Wiener indices and λ_1 , are shown to be also extremal with regard to the Estrada index.

Key words: Estrada Index; Alkanes; Extremally Branched Alkanes; Molecular Graph; Volkmann Tree.