

On Structure Descriptors Related with Intramolecular Energy of Alkanes

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In an earlier work it was demonstrated that the Zenkevich index U provides a measure of the intramolecular energy of an organic molecule, and that – in the case of alkanes – it is related to the Wiener index. We now show that U is much closer related to the recently introduced variable Wiener index W_λ : Within sets of isomeric alkanes, the relation between U and W_λ is linear, the (U, W_λ) -points forming several, mutually parallel, lines. Each such line pertains to a group of isomers possessing a fixed number of methyl groups. There exists a critical value of the parameter λ for which all the (U, W_λ) -lines coalesce, in which case the relation between U and W_λ becomes independent of the number of methyl groups. Approximate analytical expressions for the (U, W_λ) -dependence are deduced.

Key words: Wiener Index; Variable Wiener Index; Zenkevich Index; Intramolecular Energy; Alkanes.