Superposition-additive approach: thermodynamic parameters of monosubstituted alkanes

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Abstract

The superposition-additive approach developed earlier was shown to be applicable for the calculations of the thermodynamic parameters of formation and atomisation of conjugate systems, their dipole polarisability, molecular diamagnetic susceptibility, π-electronic ring currents etc. In this publication, the applicability of this approach for the calculation of the thermodynamic parameters (enthalpy and Gibbs' energy of formation from elementary substances, and absolute entropy) of alkanes, fatty alcohols, thioalcohols, amines, nitriles, fatty carboxylic acids and nitriles with general composition $C_nH_{2n+1}X$ (X is the functional group) is studied. It is shown that the thermodynamic quantities determined using the proposed approach agree to within the satisfactory precision with the available calculated and experimental data.

Key words: superposition-additive approach, substituted alkanes, postulate of atoms in molecules, transferability, additivity, enthalpy, entropy, Gibbs energy.