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Quantum-Chemical Model for Description of Solvation Effect in Proton-Transfer Reactions. Prediction of Gas-Phase Acidities of Organic Compounds

Antipin I., Mushkin V., Konovalov A.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Electrostatic solvation effects in proton-transfer reactions were described in terms of the AM1 and MNDO energies of electrostatic interaction between a unit positive charge with organic anions. These values were then used to estimate the gas-phase acidities of organic compounds from the ionic acidities in dimethyl sulfoxide. For 35 CH, NH, OH, and SH acids, the difference between the calculated and experimental gas-phase acidities does not exceed 15 kJ/mol (standard deviation 8.3 kJ/mol).