Quantum Chemical Estimation of the Acidities of Compounds in Dimethyl Sulfoxide Solution

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Abstract. Most acidities and basicities of chemical compounds are measured in aqueous solution, since this solvent is generally most applicable to biochemical and environmental applications, but the acidities of compounds in other solvents can also be of interest. As a polar, aprotic solvent, dimethyl sulfoxide (DMSO) presents a different environment for acid dissociation, and this solvent offers informative comparisons with the vacuum environment. Here quantum chemical approaches previously used for the estimation of aqueous pK_a values are applied to the estimation of DMSO acidities for two series of compounds: alcohols/phenols and azoles. Calculations were performed using density functional theory (B3LYP/6-31+G*) with and without the SM8/DMSO solvent model. Good correlations are found between the calculated and experimental pK_a values for both series of compounds.

Keywords: Acidity, pK_a, DMSO, Alcohols, Azoles, Quantum Chemistry

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