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Thermochemistry of organometallic reactions in solution: joint ITC and DFT study

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The understanding of certain, still unknown, aspects of the chemical bond is made possible by new theoretical tools, particularly static DFT-D or DFT methods corrected for dispersion. These methods allow accounting for, in a physically relevant way, the effects of dispersion at medium and long distance [1]. For the further assessing the accuracy of static DFT-D calculations the providing of referential experimental data was found to be essential. It has been shown that Isothermal titration calorimetry (ITC) techniques can provide reliable thermodynamic parameters of reaction (enthalpy ΔHr, Gibbs free energy ΔGr and entropy ΔSr) [2], while some recent studies showed good agreement between experimental and theoretical results [2].

The study presented here sheds some light on the thermochemistry of reactions in solution by preforming ITC experiments in chlorobenzene and static DFT-D calculations. The study points out that, in cases where solvent molecules can interact significantly with molecules of reactants, an accounting for the explicit solvation is of crucial importance for agreement between experiment and theory. The results of various kinds of organometallic reactions will be presented in some details.

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