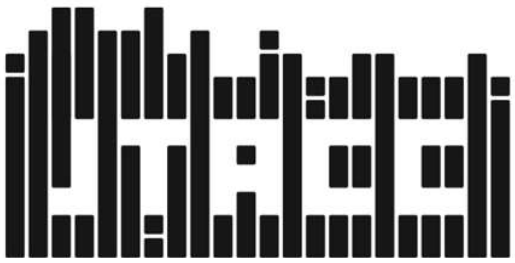

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BOOK OF ABSTRACTS

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15

BENCHMARKING TO DFT-D CALCULATIONS BY ITC EXPERIMENTAL DATA

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The London forces [1–3], or dispersion, are omnipresent in the nature. It constitutes an important part of the energy contribution to the stabilization of the tertiary structure of peptides, other natural polymers and the spontaneous coalescence of atomic aggregates or apolar molecules. The specificity of the force of London is that it acts at long distances and it is always attractive, and it is therefore effective intramolecularly and determines in many situations the conformational behaviour of organic molecules and organometallics as well. It plays an essential role in chiral recognition and discrimination processes.

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 allow to account for in a physically relevant way the effects of dispersion at medium and long distance [4]. For the further assessing the accuracy of static DFT-D calculations providing a referential of experimental data was found essential.

It has been shown that ITC techniques can provide reliable reaction enthalpy ΔH_r, Gibbs free energy of reaction ΔG_r and reaction entropy ΔS_r as well [5].

Some recent studies showed good agreement between experimental and theoretical results [6–8].

This study will shed some light on the thermochemistry of the reactions in solution by preforming ITC experiments in chlorobenzene, from one side, and static DFT-D calculations at different levels of theory, from another side *(Fig. 1)*. By comparison of obtained results one could conclude on the excellent agreement between experimental and theoretical data, which could be promising for the further development and application of static DFT-D computational methods.

As examples, the results of various organometallic reactions will be presented in some details [9].

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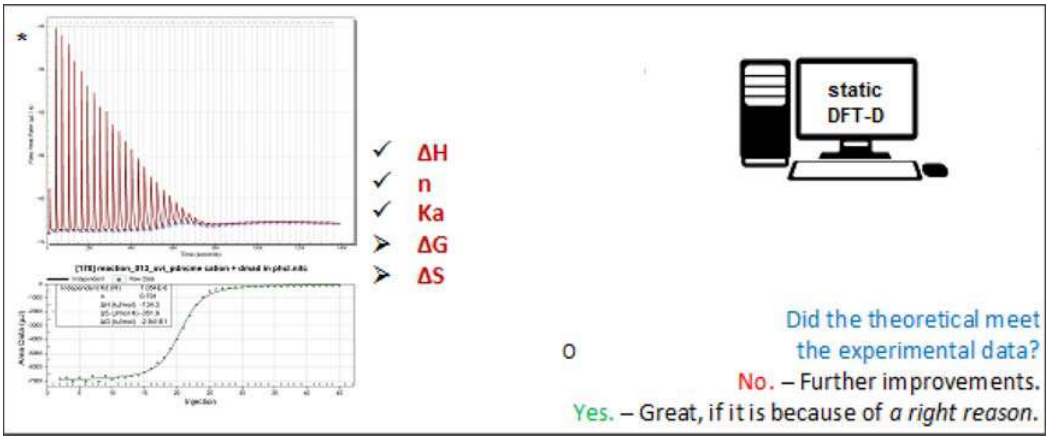

Fig.1. ➢ Example of ITC thermogram, ✓ results that could be obtained by ITC and ○ general conclusion of the work