

## **"Theoretical prediction and interpretation of NMR and EPR parameters"**

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Nowadays quantum chemical calculations of NMR parameters (chemical shift tensors, indirect nuclear spin-spin couplings, electric field gradients and contact and pseudo-contact shifts) become increasingly popular. Most of such calculations are performed using Density Functional Theory (DFT). Being a relatively inexpensive approach (in comparison with post-Hartree-Fock approaches), DFT however leads to quite accurate results due to (implicit) inclusion of electron correlation effects.

During the lecture, different computational aspects affecting the accuracy of the calculated results will be addressed. Examples demonstrating a typical accuracy in calculations of NMR and EPR parameters will be shown. Inclusion of environmental effects (solvent effects, interactions in crystals and similar) will be also considered.

Relativistic effects play an important role in chemistry and, especially, in the field of NMR and EPR spectroscopy. We will give a short excursion in the field of relativistic calculations of NMR and EPR parameters. Relativistic effects and paramagnetic NMR are two very closely related (from a theoretical point of view) issues. A short introduction to calculations of PNMR shifts will be included in the lecture.

While quantum-chemical calculations can often provide NMR parameters with useful accuracy, there is much more than just the numbers that can be gained from calculations. We will discuss a few approaches to interpretation of chemical shifts and spin-spin couplings with a stress on our recent development: visualization of indirect spin-spin coupling pathways and chemical shifts using a real space functions.