

FROM THEORETICALLY PREDICTED PROTON ISOTROPIC SHIELDINGS TO NMR EXPERIMENT IN THE GAS PHASE

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For years theoretically predicted NMR data including nuclear isotropic shieldings, and indirect nuclear spin-spin coupling constants of small, volatile molecules have been tested and verified using reliable gas phase experimental data. Obviously, such results do not depend on solute-solute and solute-solvent interactions. Unfortunately, due to technical problems, there exist relatively few NMR works in the gas phase.

The presented paper discusses an attempt to use a typical experimental setup for high-resolution NMR spectrometer for liquids to obtain 400 MHz proton NMR spectra of simple molecules in the gas phase using TMS as internal reference. Additionally, the proton spectra of methanol in deuteriochloroform, resembling quasi-gas phase conditions, were recorded and analyzed.

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