

## Self- and transport diffusion coefficients from NMR experiments

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Self-diffusion coefficients give insight into the mobility of molecular species and serve as benchmark variables for molecular modeling. Nuclear magnetic resonance (NMR) spectroscopy is an excellent method for the measurement of self-diffusion coefficients: In the present work, a pulsed gradient stimulated echo (PGSTE) pulse sequence was employed for their determination in binary and ternary liquid systems at 298 K and 1 bar. To ensure a high quality of the measurements, a preliminary gradient mapping was carried out. The experimental results are compared to molecular simulation data by Guevara-Carrion et al. [1] for binary systems (acetone/toluene, acetone/ethanol and acetone/cyclohexane) and to molecular simulation data that was determined in the present work for the ternary system acetone/toluene/cyclohexane.

Data on the self-diffusion coefficient was also extrapolated to infinite dilution, where the self-diffusion coefficient is equal to the transport diffusion coefficient. Furthermore, transport diffusion coefficients were determined from measurements with field gradient NMR, which yields quantitative spatially- and time-resolved information on the concentrations.

### References

- [1] G. Guevara-Carrion, T. Janzen, Y. M. Muñoz-Muñoz, J. Vrabec: *Mutual diffusion of binary liquid mixtures containing methanol, ethanol, acetone, benzene, cyclohexane, toluene, and carbon tetrachloride*. The Journal of Chemical Physics **144**, 124501 (2016).

