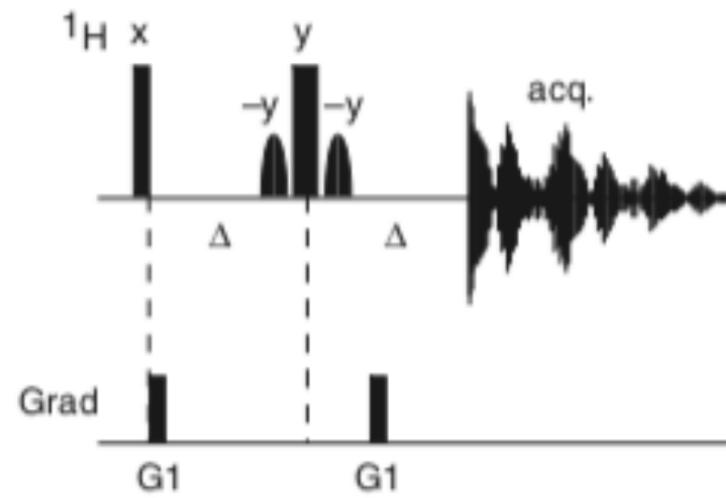


NMR structural analysis – seminar

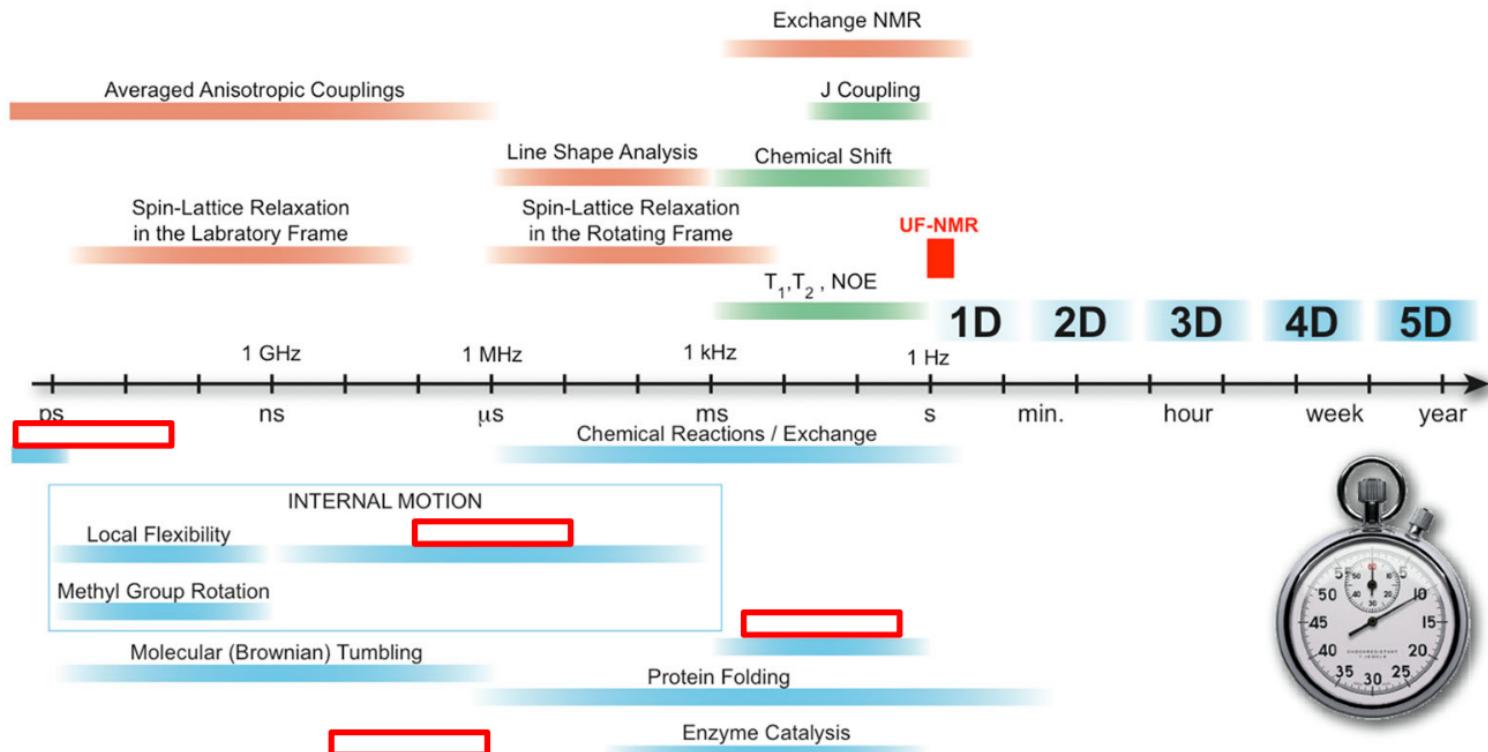
May 4, 2022

Water suppression



Soft-hard-soft: $90^\circ_{-\gamma} - 180^\circ_y - 90^\circ_{-\gamma}$

Localize dynamical processes: *domain motions, vibration, H-transfer, diffusion*



From A. Krushelnitsky, D. Reichert PNMR 47 (2005) 1–25

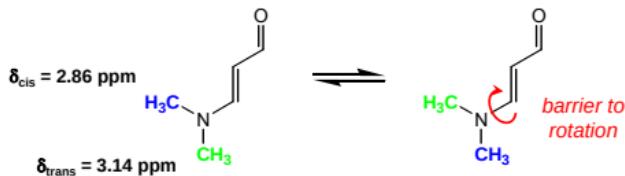
Kinetic data from T-dependent NMR experiments

Measuring Dynamics with NMR

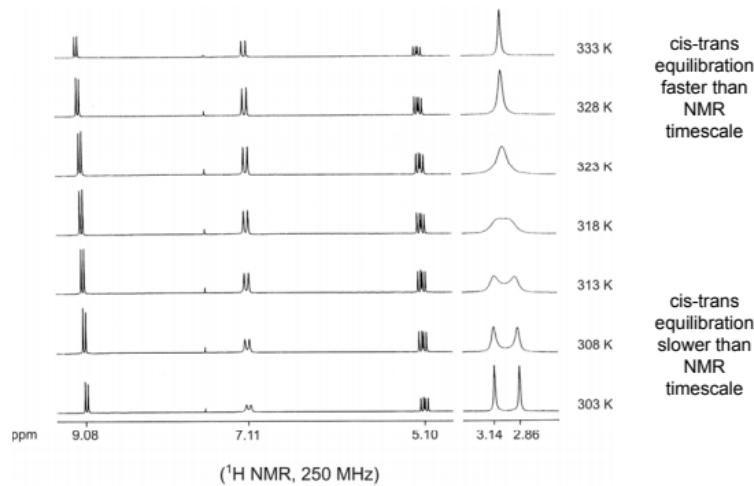
For nuclei that undergo chemical exchange:

- If chemical exchange is **slower** than NMR timescale, then all signals of components are observed.

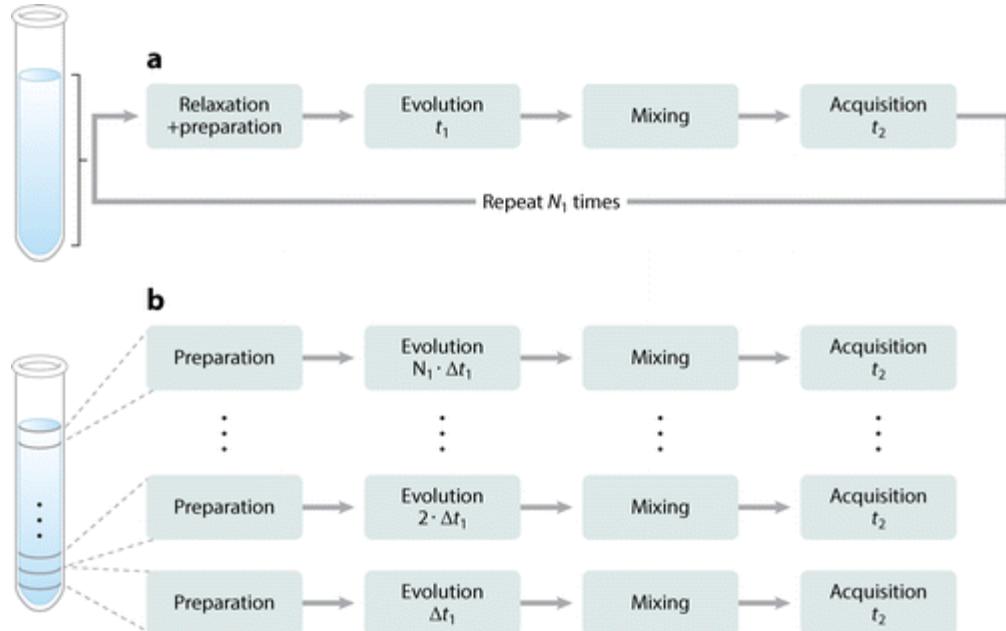
Example: Conformational equilibria.



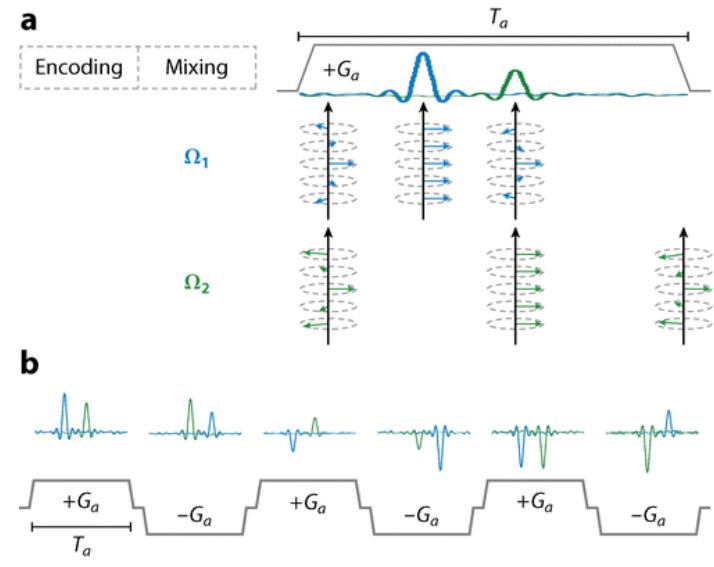
Measuring Dynamics with NMR



Ultra-fast NMR

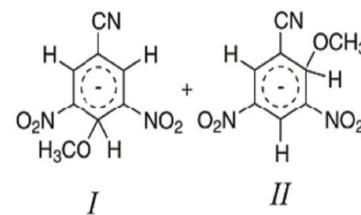
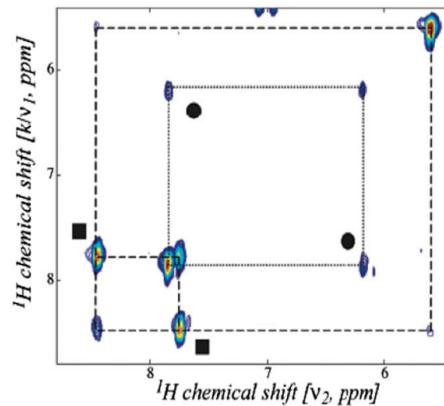
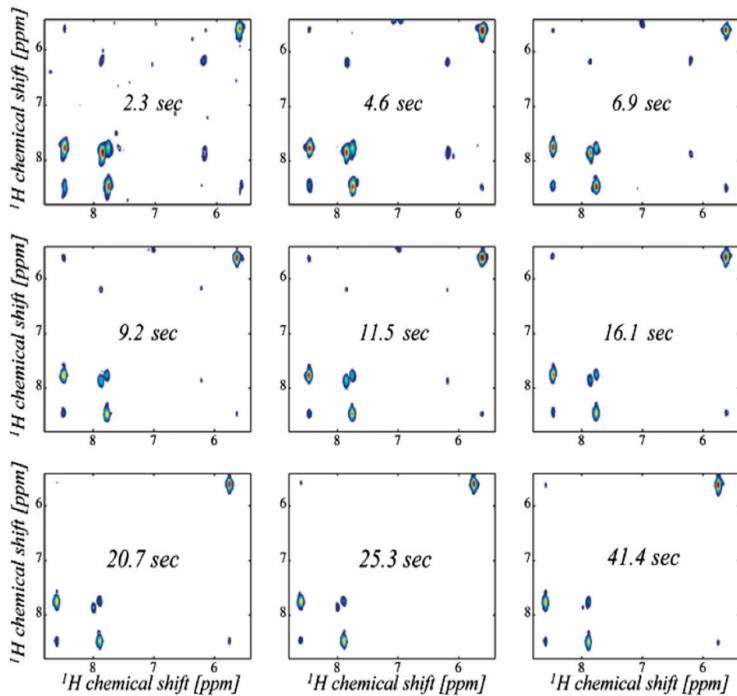
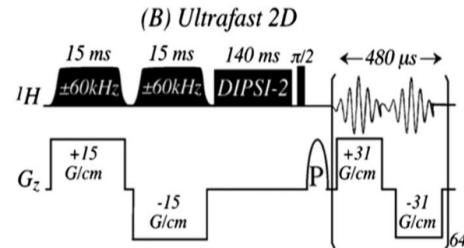
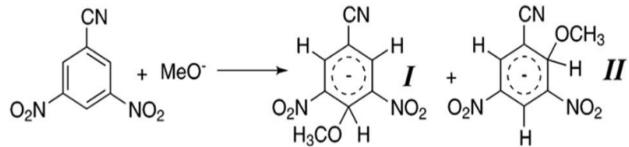


Giraudeau P, Frydman L. 2014.
 Annu. Rev. Anal. Chem. 7:129–61

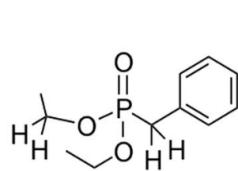


Giraudeau P, Frydman L. 2014.
 Annu. Rev. Anal. Chem. 7:129–61

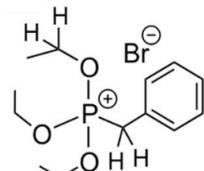
Monitoring chemical reaction



Monitoring chemical reaction

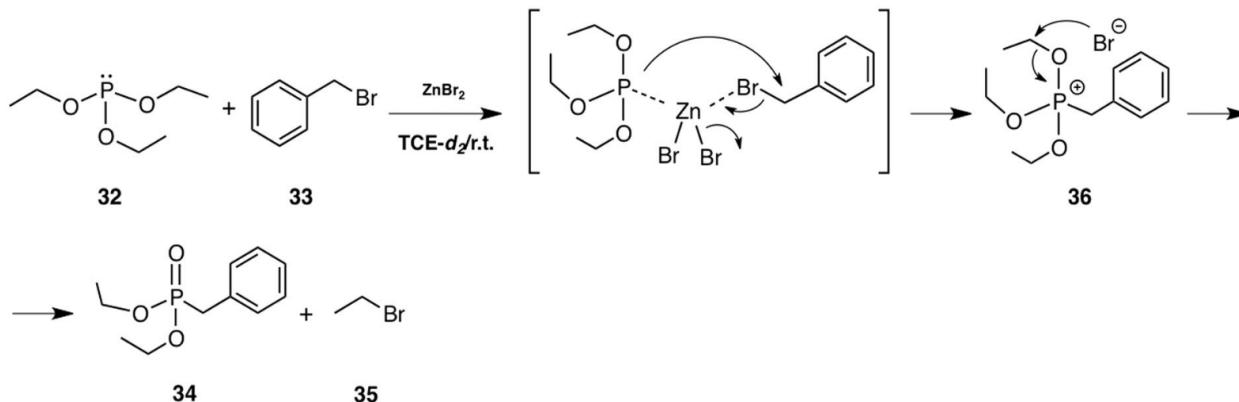
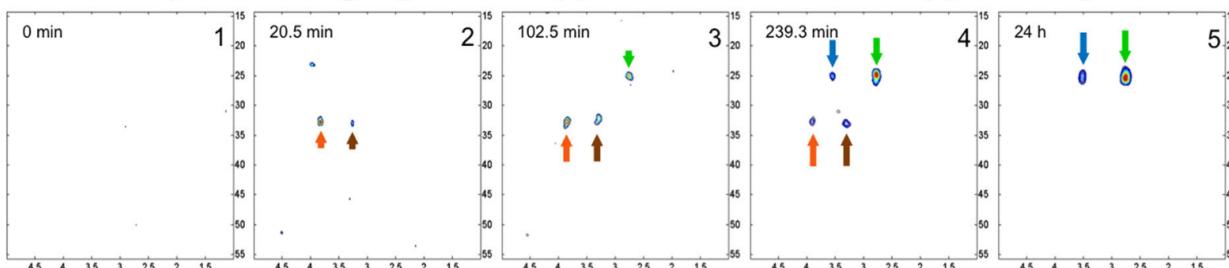


34



36

Spectral range: [1.00-5.00 ppm in ^1H and 14.3-55.7 ppm in ^{31}P]



Paramagnetic NMR – pseudocontact shift

