
NMR Spectroscopy of Organic Compounds

Lesson 2: Selective decoupling, populations

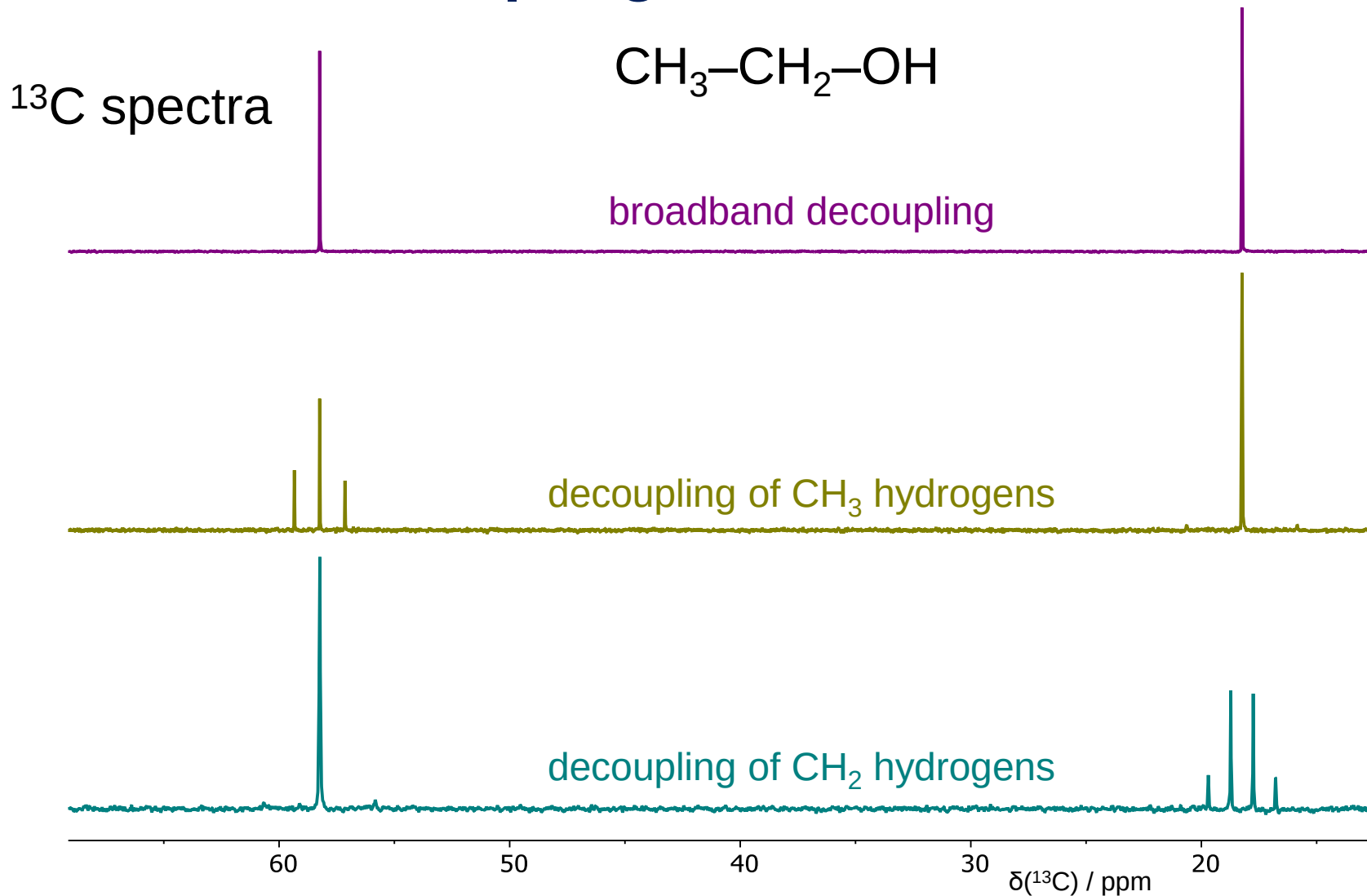


Martin Dračinský

Overview

- Selective decoupling
- Populations of spin states
- Polarization transfer

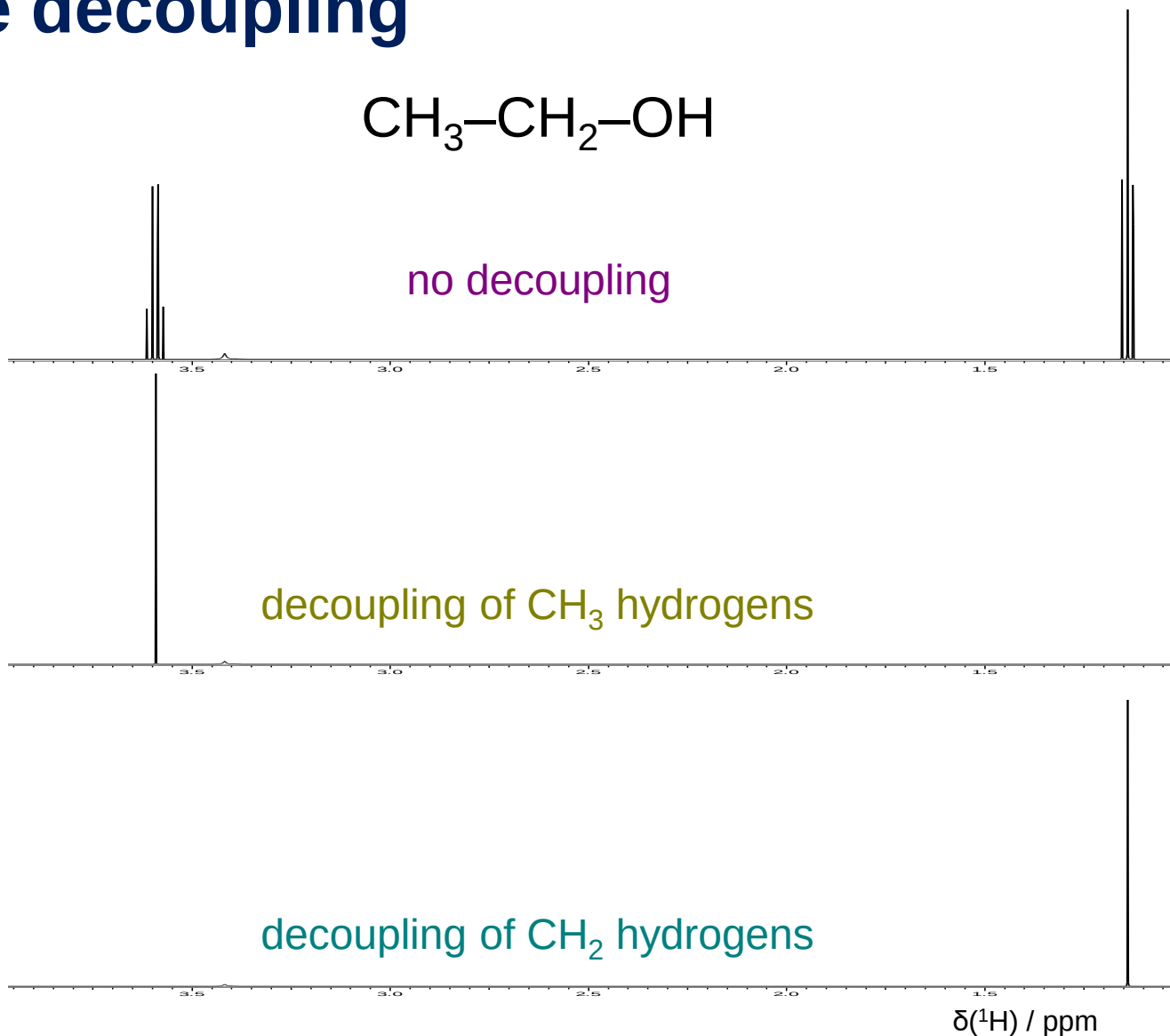
Selective decoupling



Selective decoupling

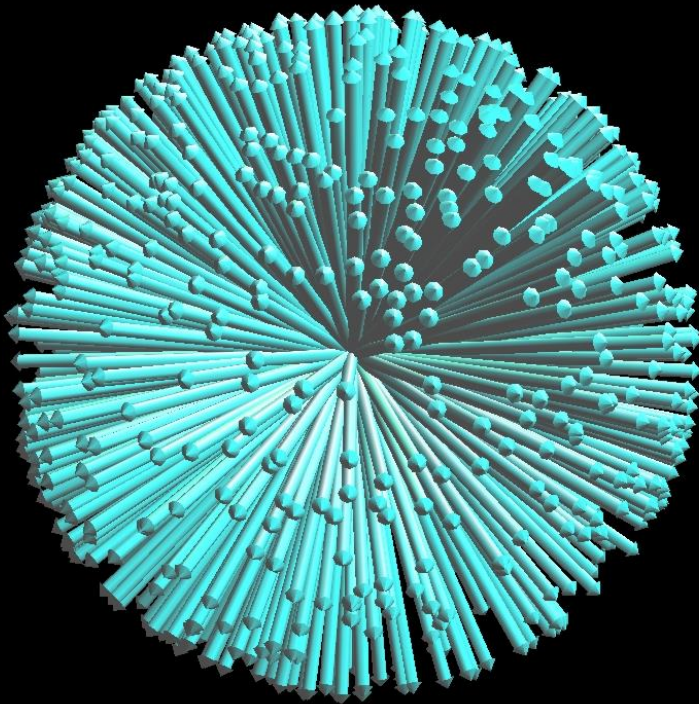


^1H spectra



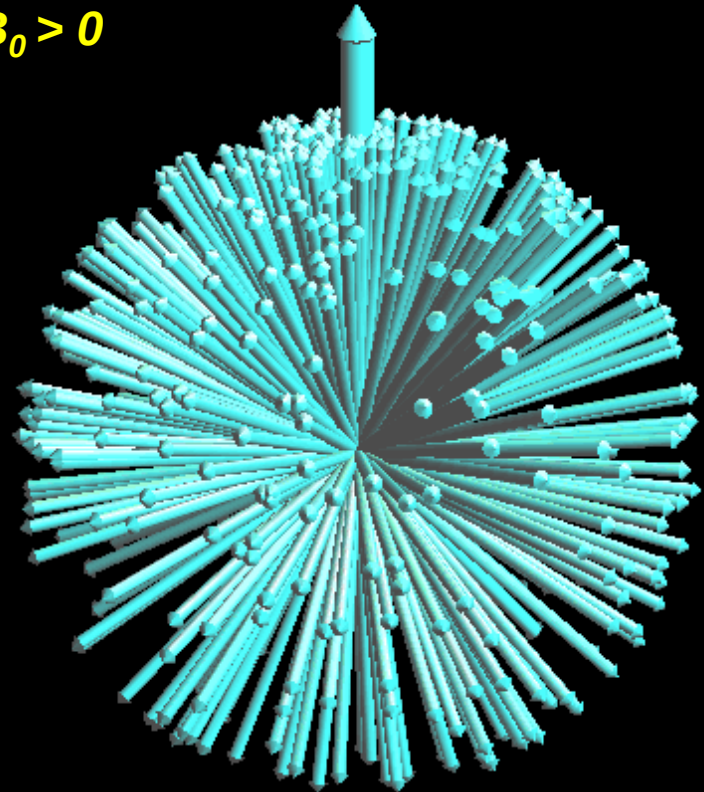
Populations of energy levels

$B_0 = 0$



$$\vec{M} = 0$$

$B_0 > 0$



$$\vec{M} = (0, 0, M_0)$$

Populations of energy levels

Boltzmann law

$$N_{\alpha} / N_{\beta} = e^{-\Delta E / k_b T}$$

$$\Delta E = \gamma \hbar B_0 / 2 \pi$$

Example: $T = 300 \text{ K}$, $B_0 = 7.05 \text{ T}$ (300 MHz)

$$N_{\beta} = 0.99995 N_{\alpha}$$

- Sensitivity

Populations of energy levels

Equilibrium



Saturation



Population inversion



90° pulse

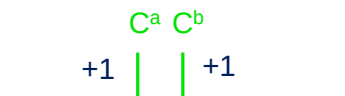
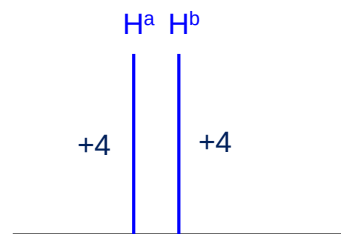
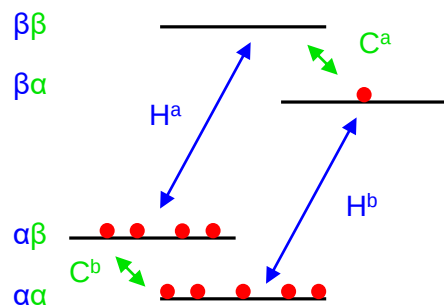
180° pulse



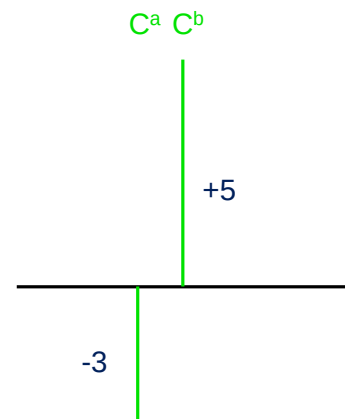
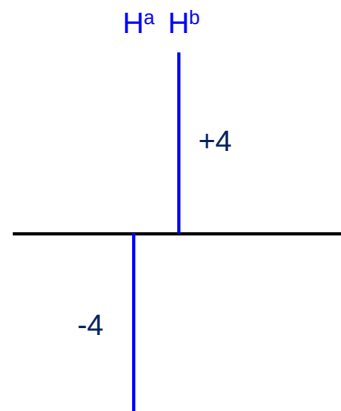
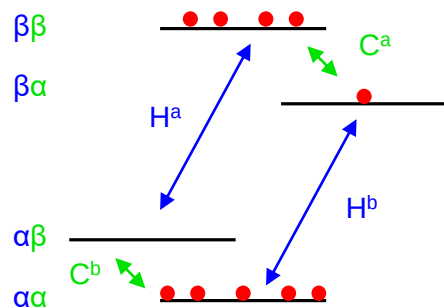
Polarization transfer



thermal equilibrium

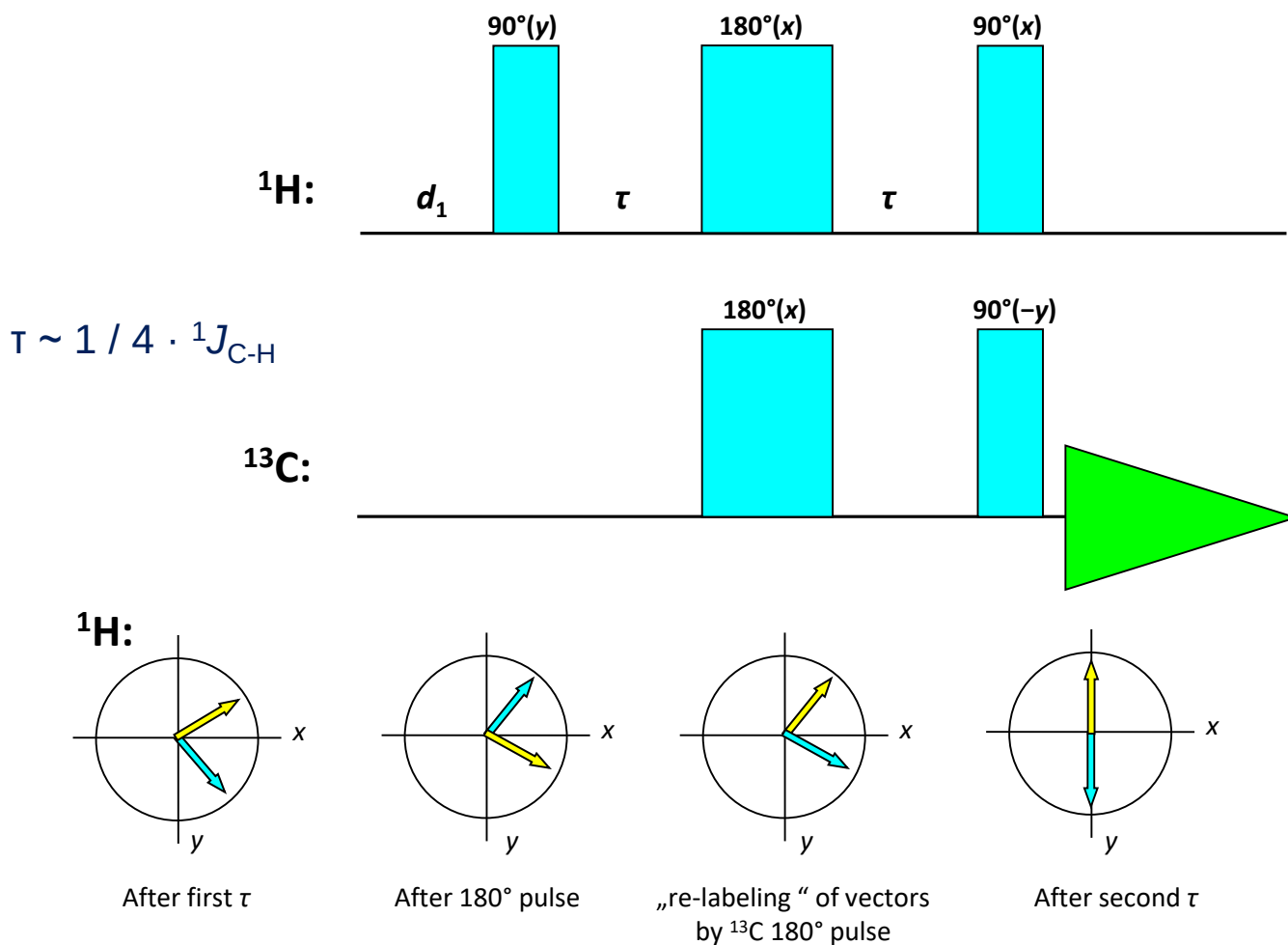


selective inversion of H^a line

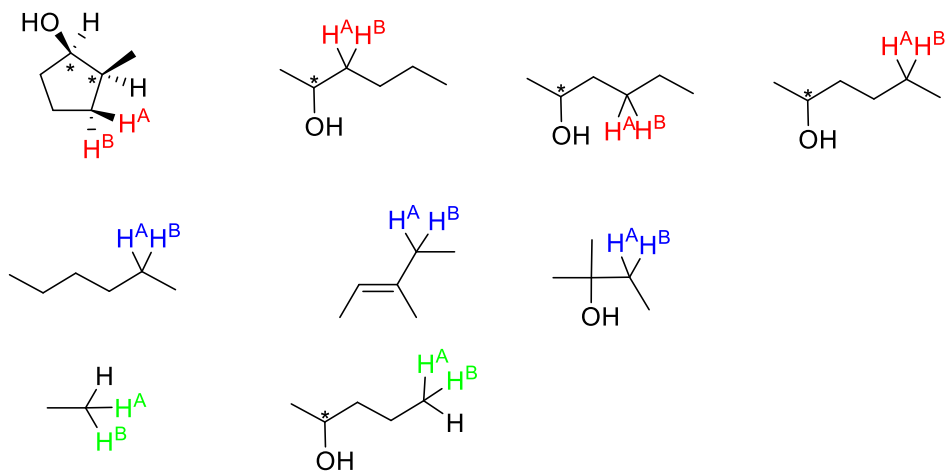


INEPT

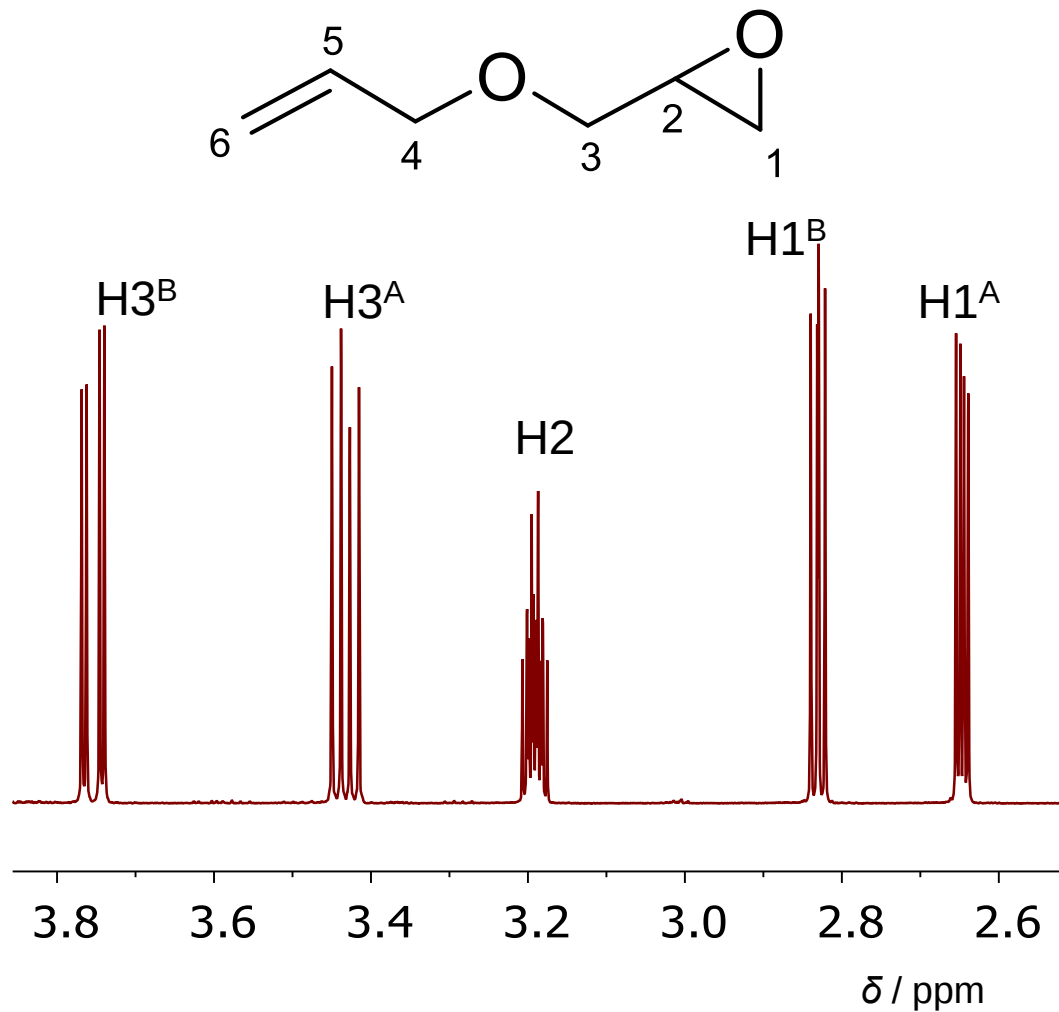
- Insensitive nuclei enhancement by polarization transfer



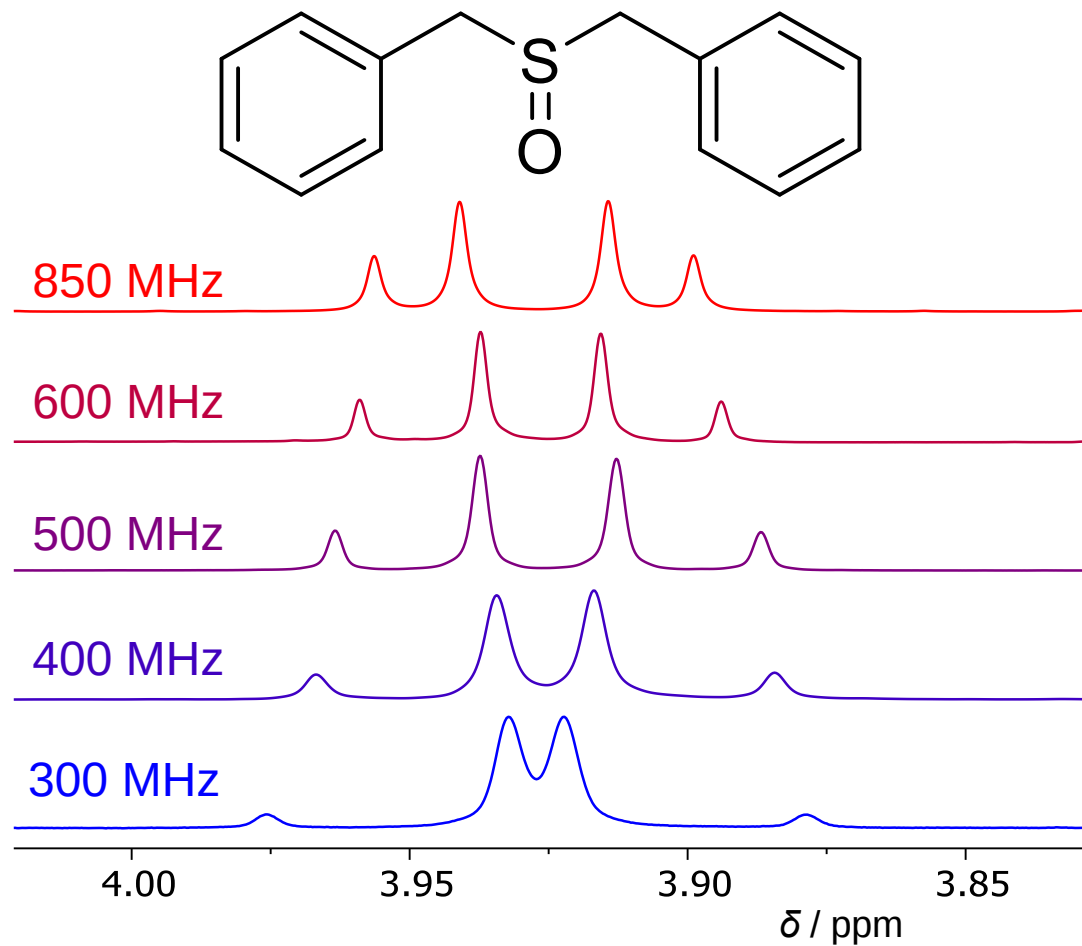
Homotopic, enantiotopic, diastereotopic



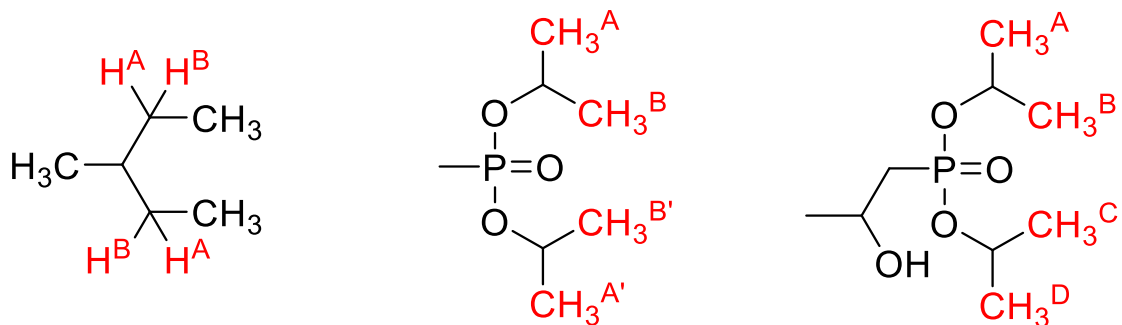
Homotopic, enantiotopic, diastereotopic



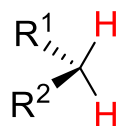
Homotopic, enantiotopic, diastereotopic



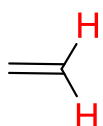
Homotopic, enantiotopic, diastereotopic



Geminal coupling



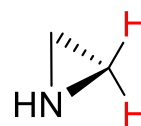
-12 Hz



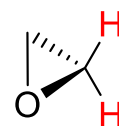
-3 to +3 Hz



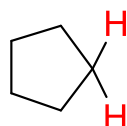
-4 Hz



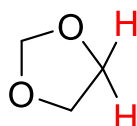
+2 Hz



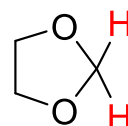
+5 Hz



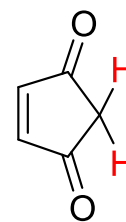
-13 Hz



-8 Hz

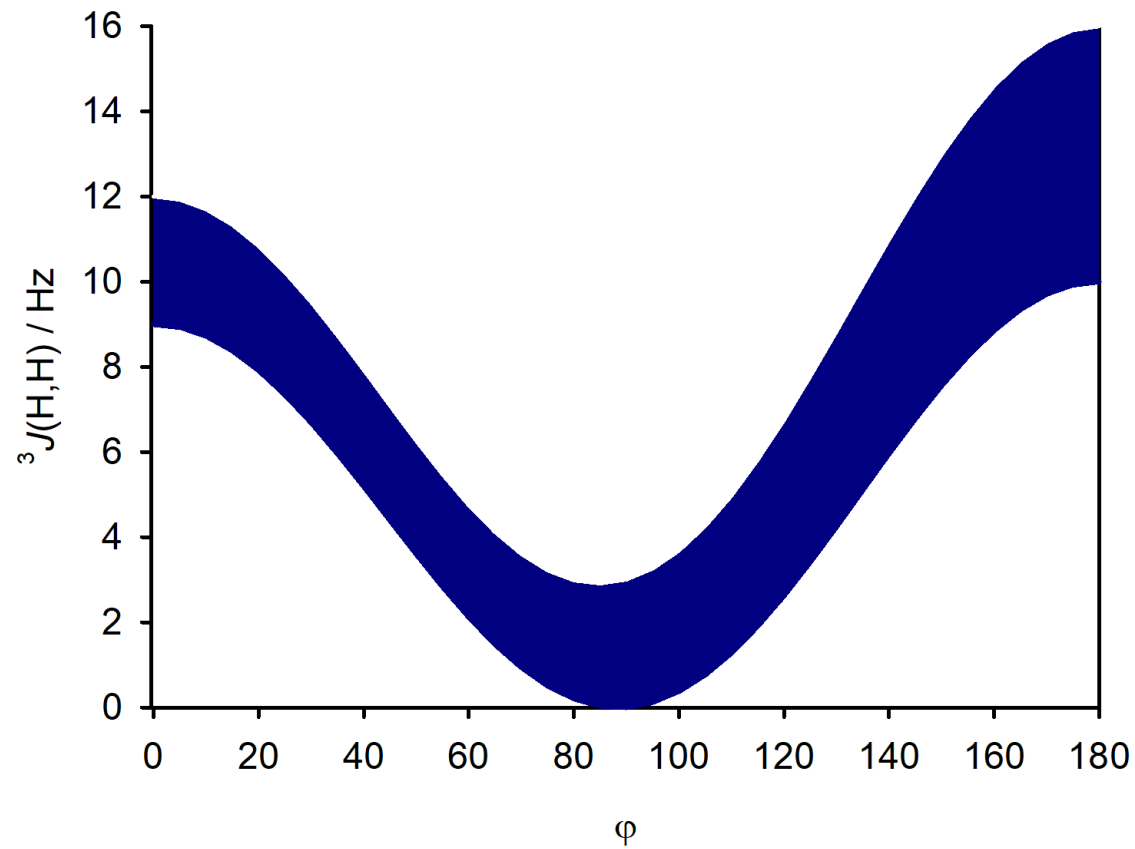


0 Hz

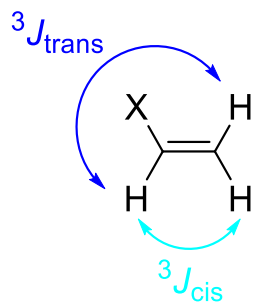
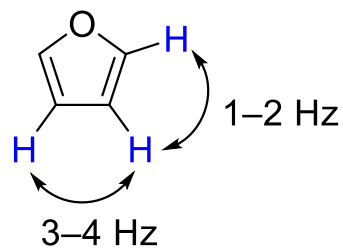
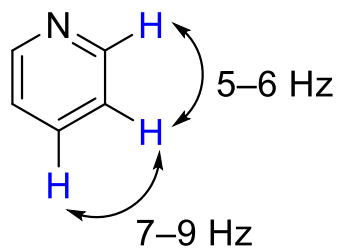
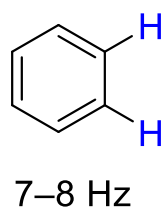
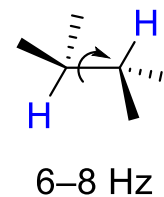
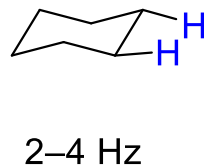
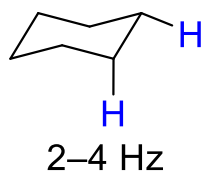
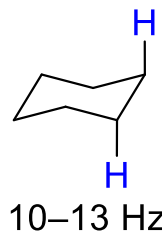


-21 Hz

Vicinal coupling

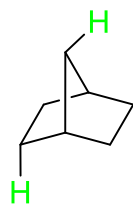


Vicinal coupling

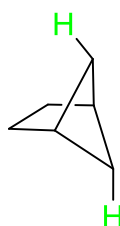


X	Li	H	Cl	OCH ₃	F
$^3J_{cis}$	19.3	11.6	7.3	7.1	4.7
$^3J_{trans}$	23.9	19.1	14.6	15.2	12.8

Long-range coupling



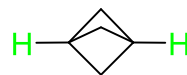
3-4 Hz



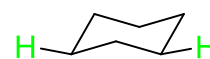
7-8 Hz



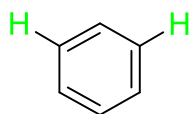
10 Hz



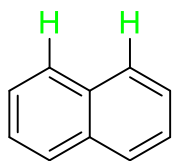
18 Hz



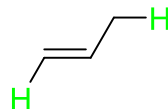
1-3 Hz



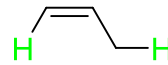
1-3 Hz



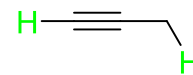
0.7 Hz



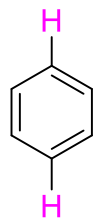
1-3 Hz



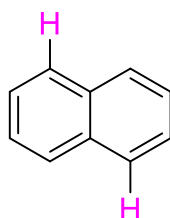
1-3 Hz



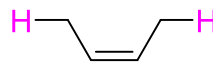
2-3 Hz



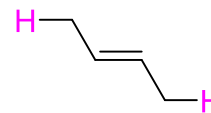
0.7 Hz



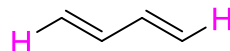
0.8 Hz



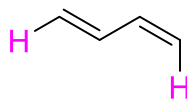
1-3 Hz



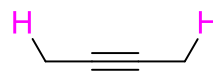
1-3 Hz



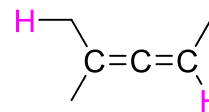
1.3 Hz



0.6 Hz



2-3 Hz



3 Hz