NMR Spectroscopy of Organic Compounds

Lesson 6: Nuclear Overhauser effect



Martin Dračínský

Overview

- NOE principle
- NOE experiments

NOE – principle: cross relaxation



NOE

- Molecular reorientation correlation time τ_c
- $\omega \cdot \tau_c \ll 1 double-quantum relaxation is more effective, NOE is positive$
- $\omega \cdot \tau_c >> 1 zero-quantum relaxation is more effective, NOE is negative$
- $\omega \cdot \tau_c \approx 1 \text{NOE}$ is close to zero
- NOE efficiency $\eta = (I_{\text{NOE}} I_0) / I_0$
- $\eta_{MAX} = \gamma_{IRR} / 2\gamma_{OBS}$ ¹H 0.5 ¹³C 1.99 ¹⁵N -6.93

NOE



Spin diffusion



Distance measurement

- NOE decreases with sixth power of internuclear distance



$$r(H1,H3) = r(H1,H2) \cdot (\eta_{H1,H2} / \eta_{H1,H3})^{1/6}$$

1D NOE





2D experiments

- NOESY
- ROESY (Spinlock during mixing time)





2D experiments

















