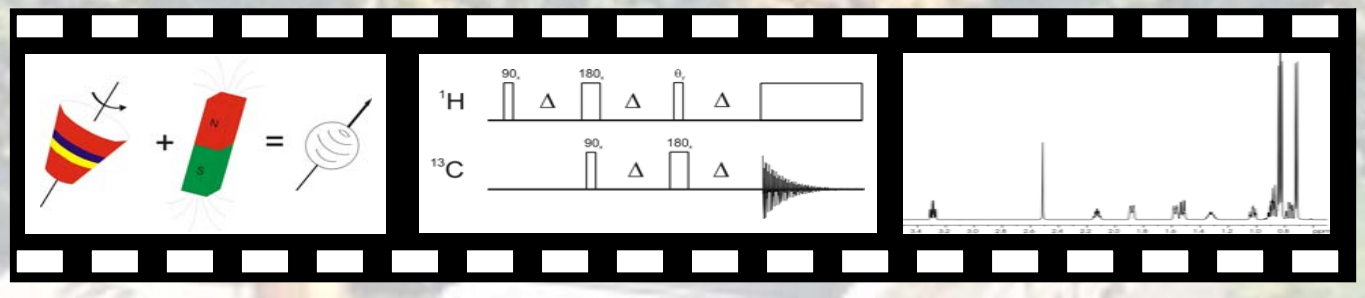
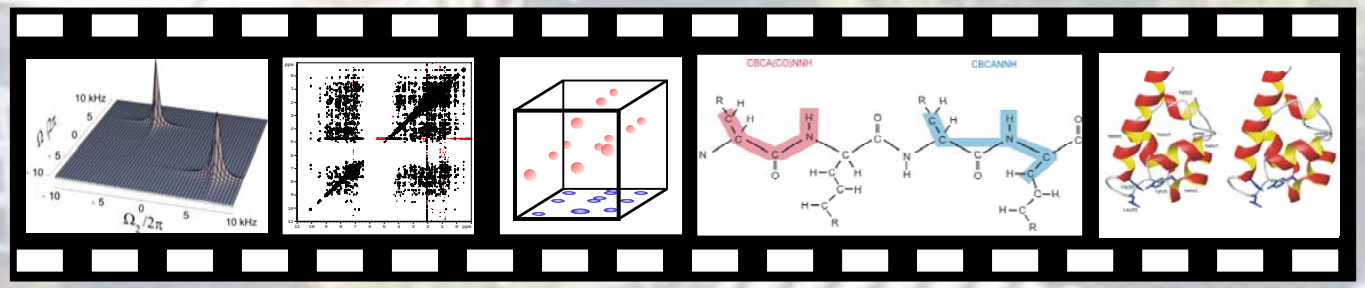


Veränderung der Linienbreite von NMR-Linien durch Austauschprozesse

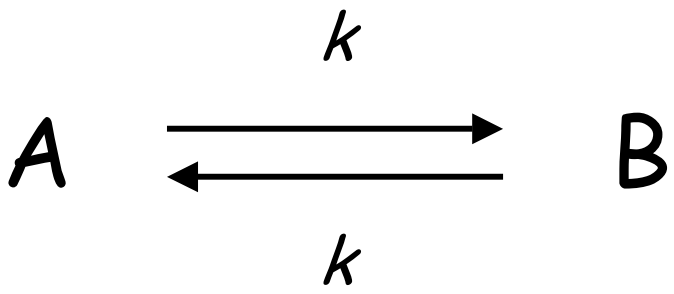
Gruppenseminar 07.01.2010

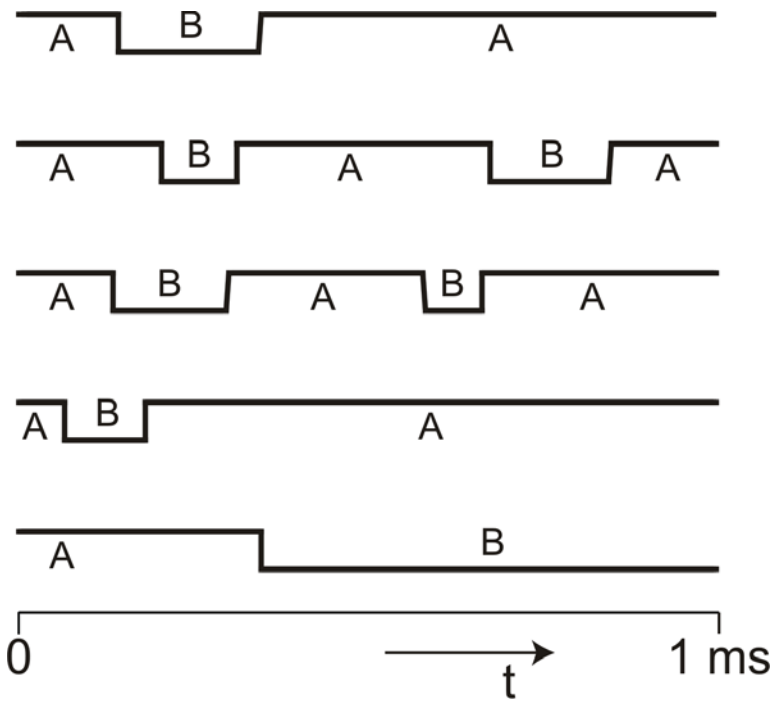


In vielen unserer Projekte spielt die Linienverbreiterung durch Austauschprozesse (leider) oft eine wichtige Rolle

z.B. Phytochrome oder B2705/9

Austausch ist aber auch bei Untersuchungen von Protein-Ligand-Wechselwirkungen von Bedeutung





$\Omega_\Delta = \Omega_A - \Omega_B$

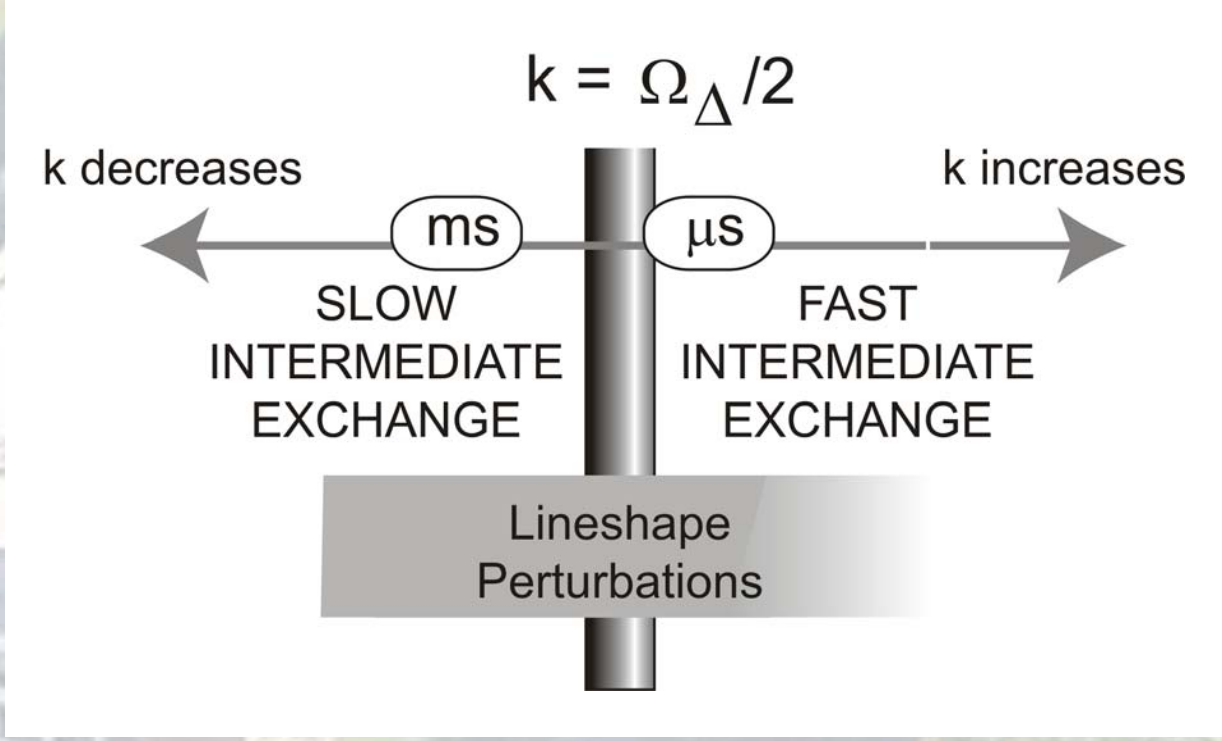
intermediate exchange:

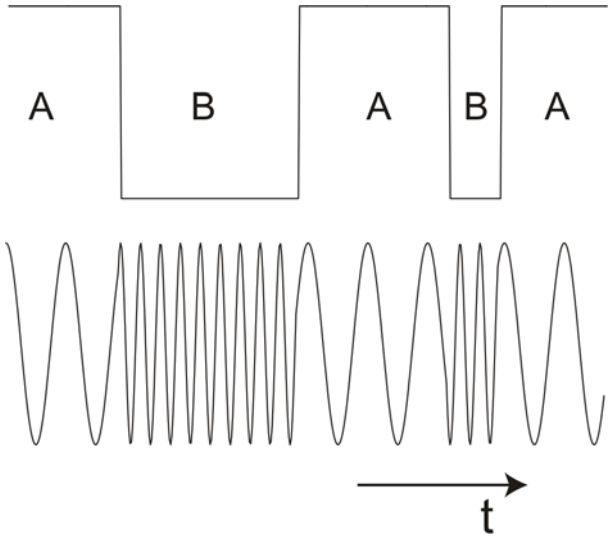
$k \sim |\Omega_\Delta / 2|$

slow intermediate exchange: $k < |\Omega_\Delta / 2|$

fast intermediate exchange: $k > |\Omega_\Delta / 2|$

cross over point (coalescence): $k = |\Omega_\Delta / 2|$

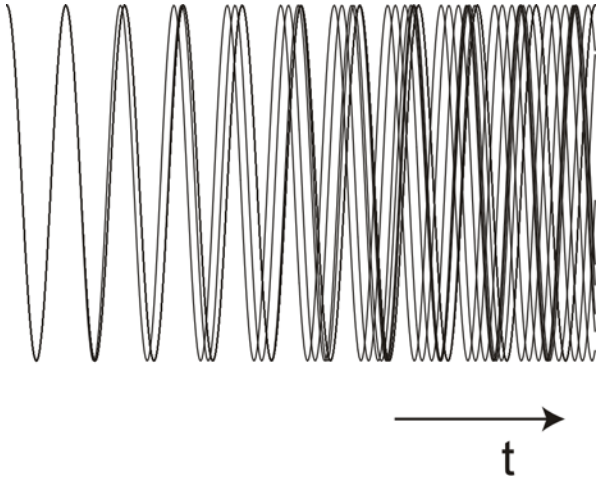




Ω_Δ = 20 kHz

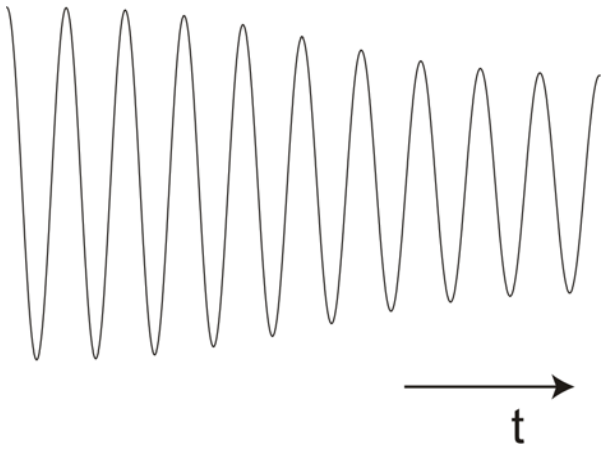
k = 3 kHz

20 Moleküle überlagert:



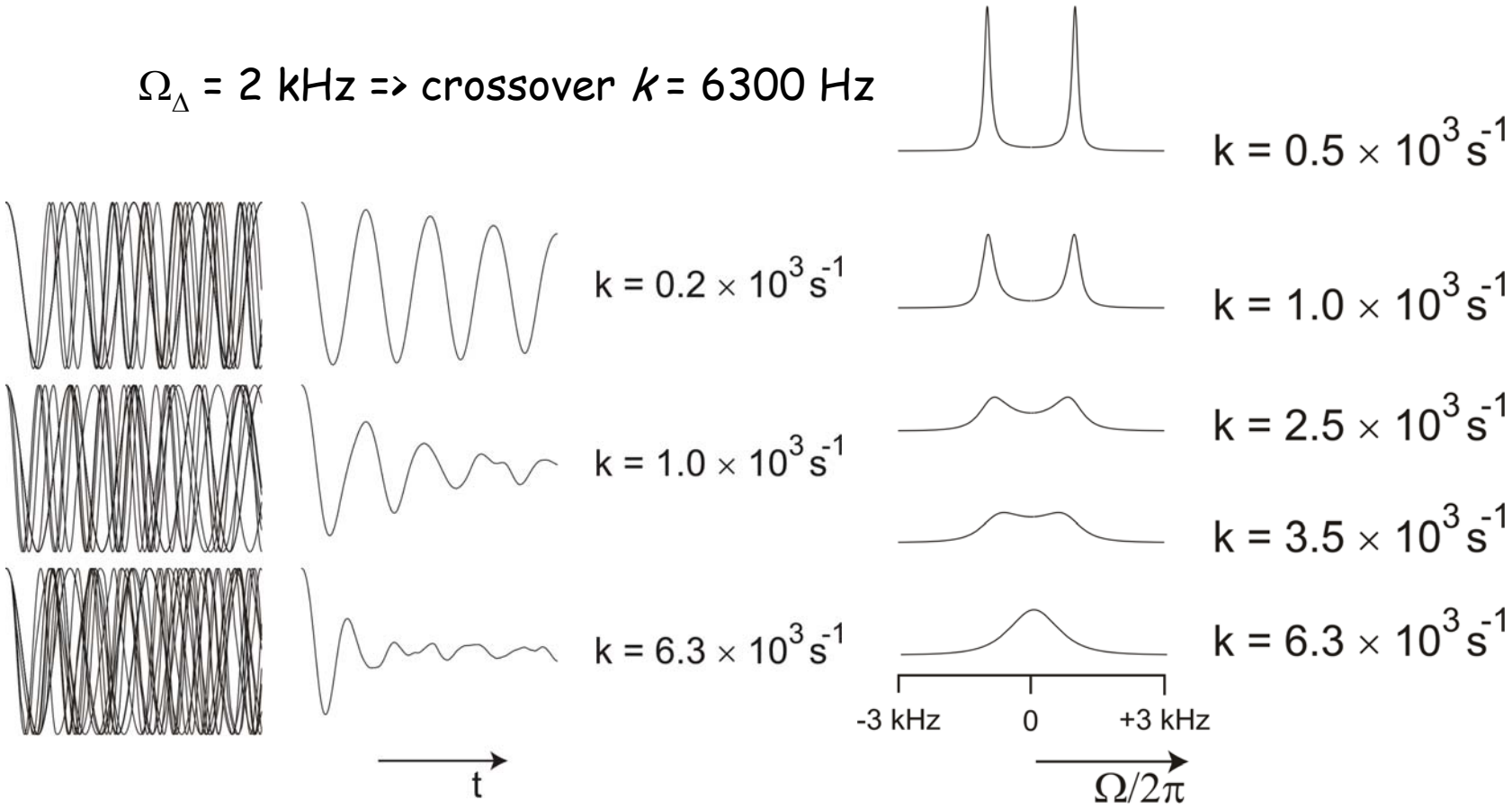
Ω_Δ = 1 kHz

k = 500 Hz



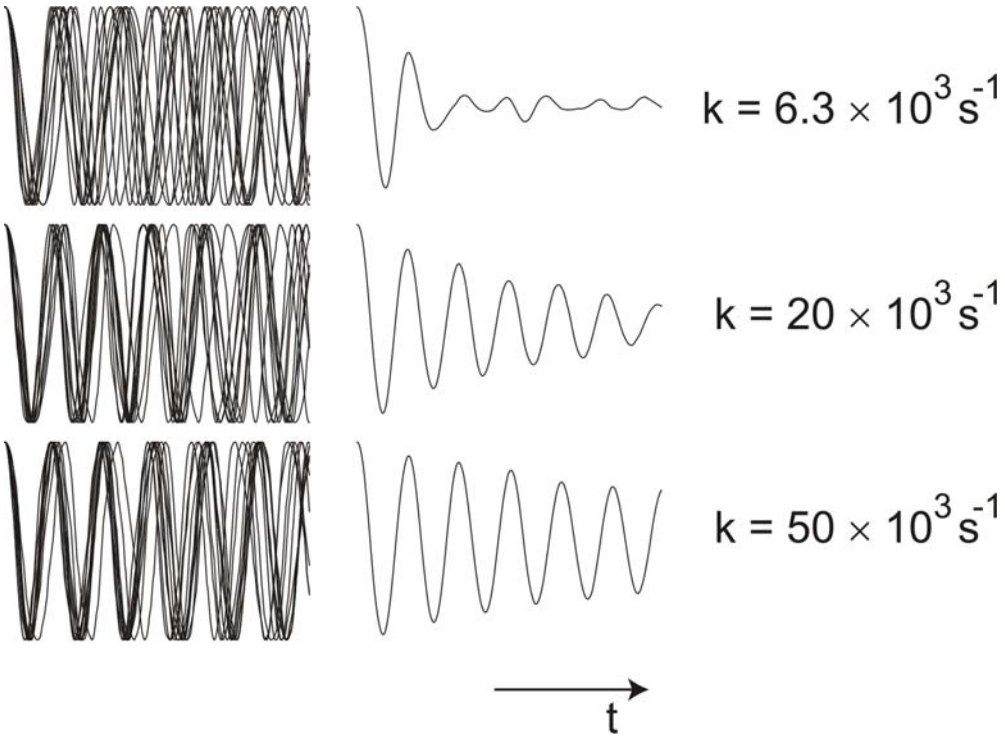
slow intermediate exchange: $k < |\Omega_\Delta / 2|$

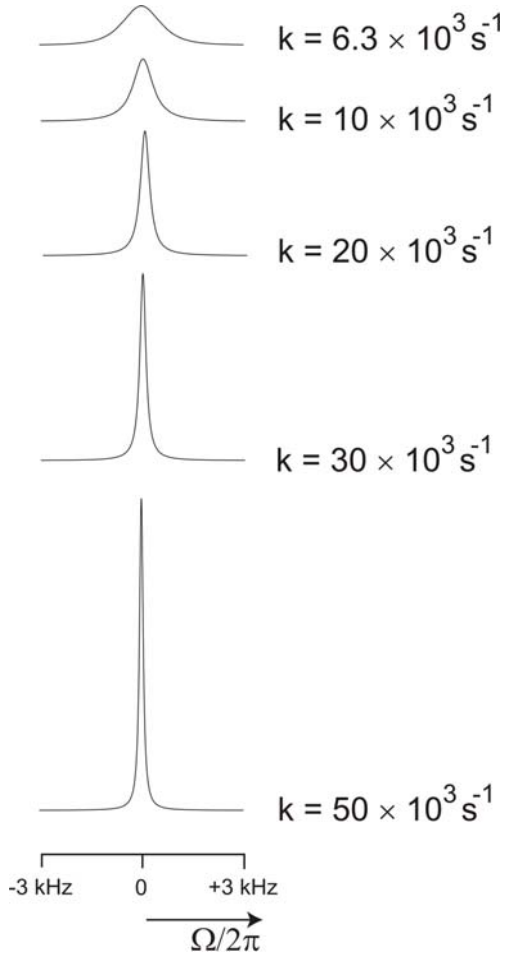
Ω_Δ = 2 kHz => crossover k = 6300 Hz

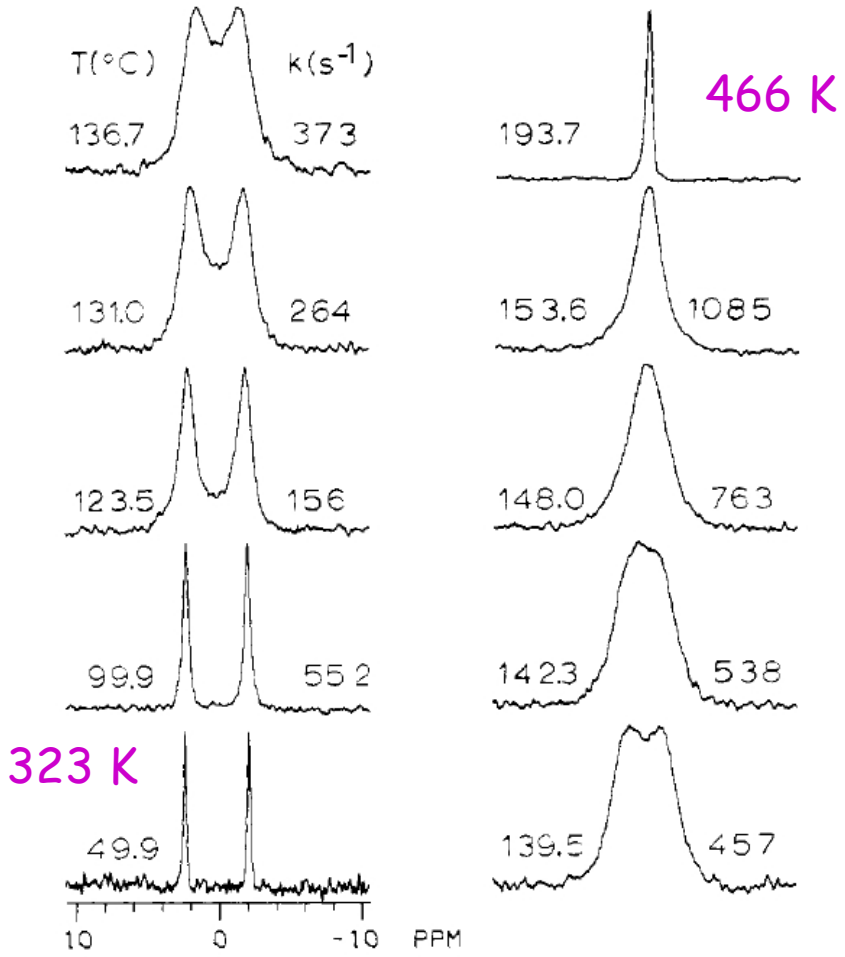


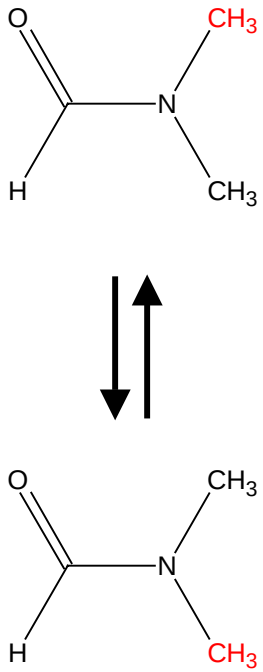
fast intermediate exchange: $k > |\Omega_\Delta / 2|$

Ω_Δ = 2 kHz => crossover k = 6300 Hz

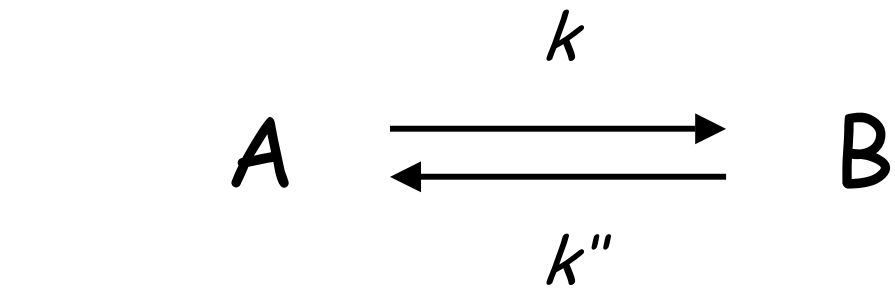


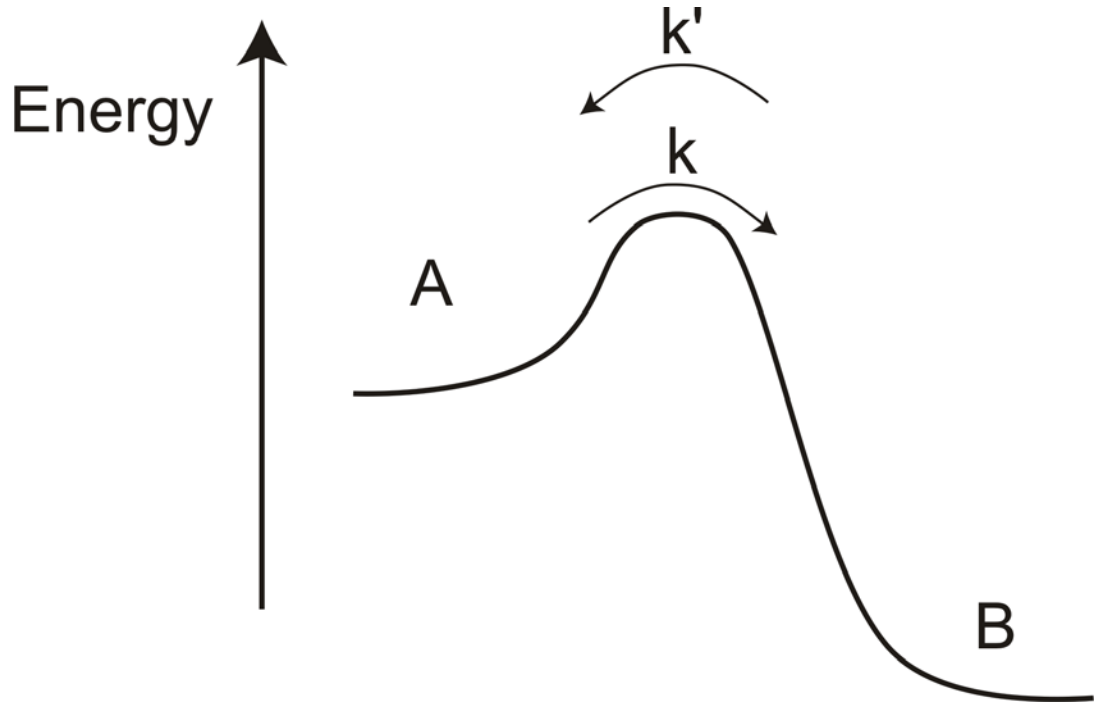


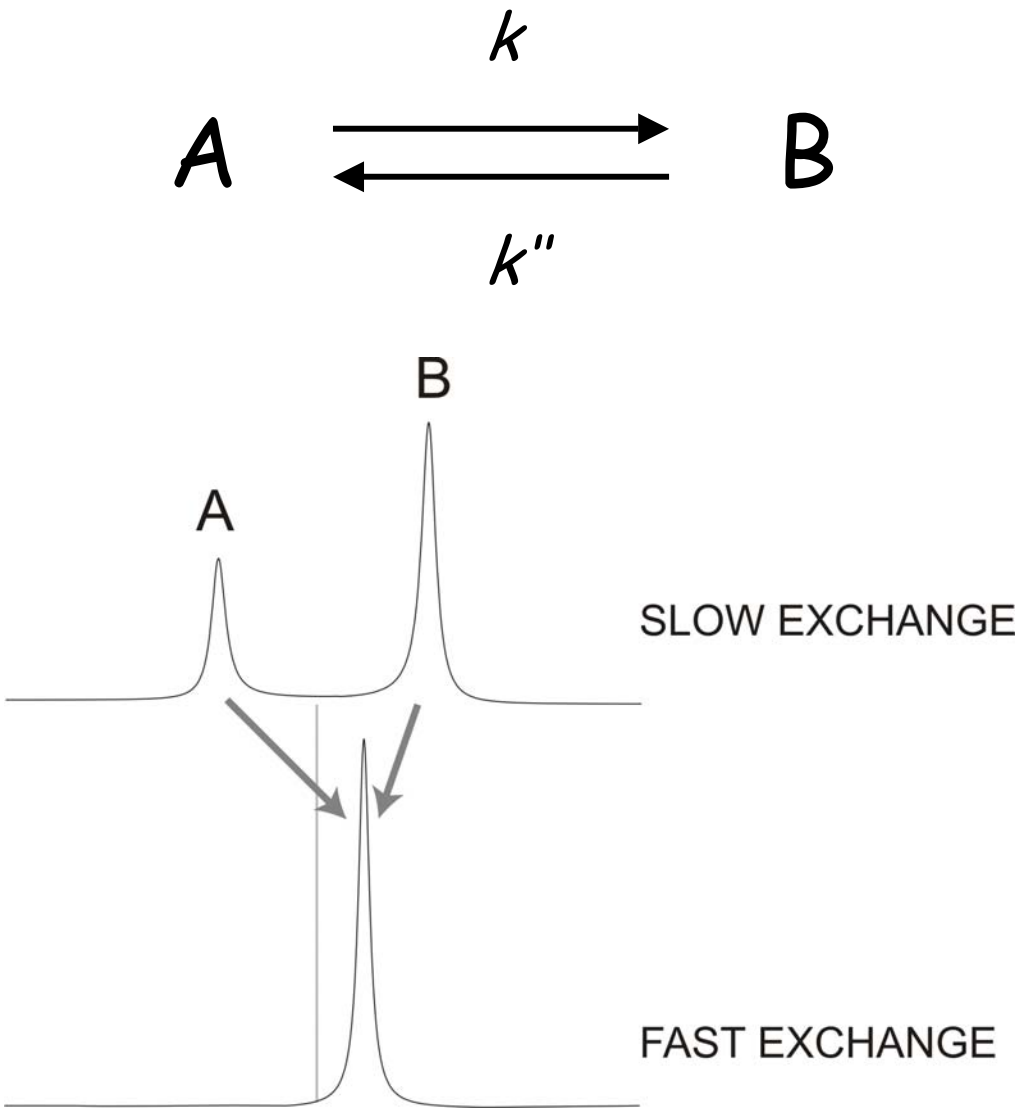




J. Am. Chem. Soc. **106**, 2451-2452 (1984)


k
A
B
k''


Energy
k'
k
A
B


k
A
B
k''
B
A
SLOW EXCHANGE
FAST EXCHANGE

Wichtig ist offensichtlich das Verhältnis von

k zu Ω_Δ

k wird durch die Temperatur beeinflußt, Ω_Δ durch die Magnetfeldstärke

Um vom cross-over-point, wo die Linien besonders breit sind, wegzukommen, lohnt also die Variation der beiden Parameter, was aber oft nicht so leicht möglich ist