Chemical exchange

What happens if the ^{1}H spin changes its chemical environments during and NMR experiment?

Limiting cases

- Slow exchange
  Spectra are the superposition of sub-spectra from each of the species present

  Condition: $k < \Delta$ $\Delta = \Delta\delta$ or J

  k is the exchange rate

- Fast exchange
  "Single" species NMR spectrum with averaged NMR parameters weighted by the relative populations

  Condition: $k > 15\Delta$ $\Delta = \Delta\delta$ or J

Between these limits

- Intermediate exchange
- Complex lineshape changes

Chemical exchange

- NMR timescale
  - rate of a process compared with an NMR parameter

- Simplifies NMR spectra
  - cyclohexane: axial/equatorial exchange

    high temperature – single resonance
    low temperature – complex AA'A"..BB'B"..

- Broadening as a consequence of uncertainty in the energy

  If lifetime τ_A, energy uncertainty $\hbar\ \tau_A^{-1}$

  Since $E = h\nu$

  Lines will be broadened by $(\pi\tau_A^{-1})$

Intermediate lineshapes