Nuclear Magnetic Resonance

NMR spectrum

- NMR spectrum of 1,1,2 trichloroethane
- Two different types of H
- Signals from both alkanes are split
- Integrals are in 2:1 ratio

Spin-spin coupling

- Spin-spin coupling responsible for multiple signals.
- For example, the single H atom experiences three different magnetic fields

- Add a term to the Hamiltonian.

Wavefunction

- Distinguishable protons.
- Four different eigenstates for the nuclear Zeeman portion of Hamiltonian.

- Operate on the respective wavefunction with the Hamiltonian to determine state energies.

Energies (1)

Energies (2)

Energies (3)

Spin-spin coupling

- Spin-spin hamiltonian
  - $\hat{H}_{ss} = hJ_{12}/hbar^2 * I_1 * I_2$
  - J_{12} spin coupling constant
- Wavefunctions are not eigenstates of $\hat{H}_{ss}$ so they are treated using perturbation theory

Spin-spin coupling (1)

Spin-spin coupling (2)

Spin-spin coupling (3)

Spin-spin coupling

- Energy level diagram with spin-spin coupling.

- Only four different transitions are allowed.

Indistinguishable protons

- Why do indistinguishable protons not show a splitting?
- Consider dichloromethane.

- Need symmetric and antisymmetric wavefunctions

Indistinguishable protons (1)

- Apply same Hamiltonian to the system

Indistinguishable protons (2)

- Apply same Hamiltonian to the system

Indistinguishable protons (3)

- Spin-spin coupling

Indistinguishable protons (4)

- Spin-spin coupling