

Jigsaw 5B

1. [Week 1 Slides 18-25] The complete NMR Hamiltonian for a molecule in a diamagnetic condensed sample is:

$$\mathcal{H}_{NMR} = \mathcal{H}_Z + \mathcal{H}_Q + \mathcal{H}_D + \mathcal{H}_{CS} + \mathcal{H}_J$$

- a. Name all the terms. For each term, determine if it will be observable in solid state NMR, in liquid state NMR, or in both. Justify your answers. Also state which units the corresponding values are usually reported in (e.g., Hz, MHz, ppm, etc.).
- b. Explain the main differences between scalar couplings and dipolar couplings. Why does one produce splittings in NMR spectra of liquids and the other one does not?
2. [From Past Exam] [Hore Section 3.7] The ^1H - ^1H J-coupling in $\text{CHX}_2\text{--CHY}_2$ is measured to be 3.27 Hz. If $J_g = 2.0$ Hz and $J_t = 8.7$ Hz, determine the population fractions of the two rotamers. J_g and J_t are the ^1H - ^1H coupling constants for the gauche and trans conformations, respectively.