

Jigsaw 5E

The NMR Hamiltonian

[Week 1 Slides 18–29] The complete NMR Hamiltonian for a molecule in a diamagnetic condensed sample is:

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

1. 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.).
2. How is each term of the Hamiltonian influenced by the magnetic field strength?
3. 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?
4. [Week 4 Slides 40–43] What is the main difference, in terms of molecular dynamics, between a liquid and a solid sample?