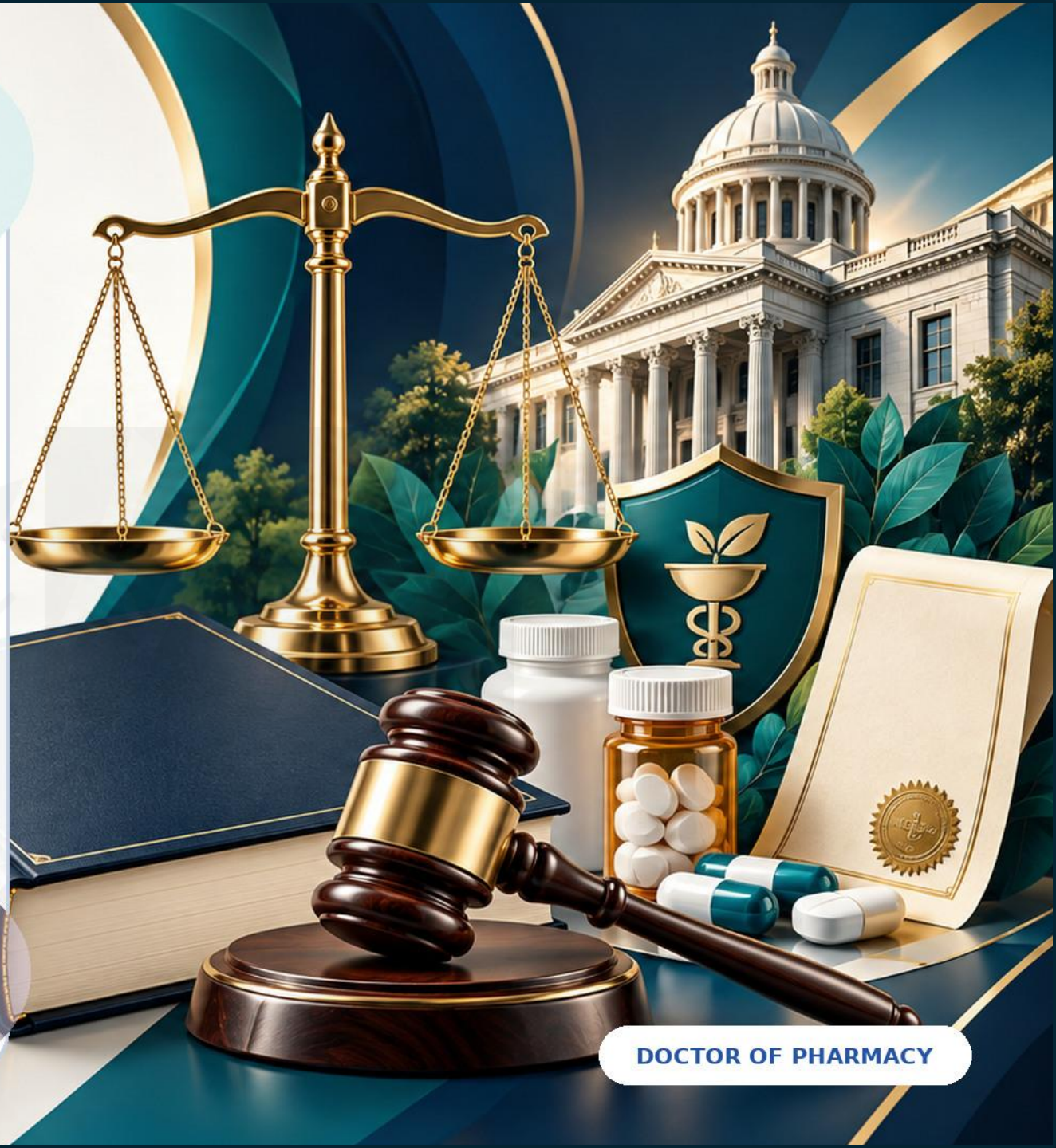
PHARM.D • YEAR 3

Pharmaceutical Analysis

CHAPTER 4.7

NMR and ESR

PPT CHAPTER COVER

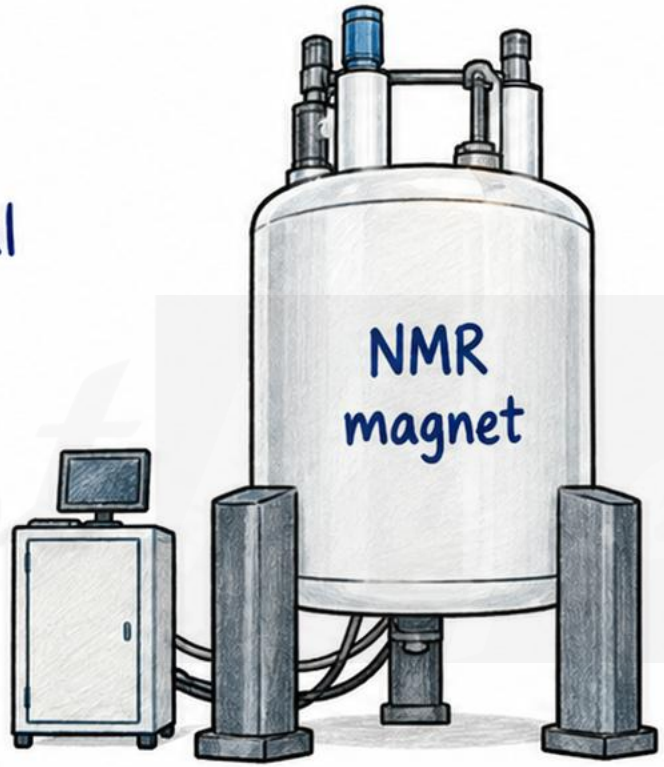


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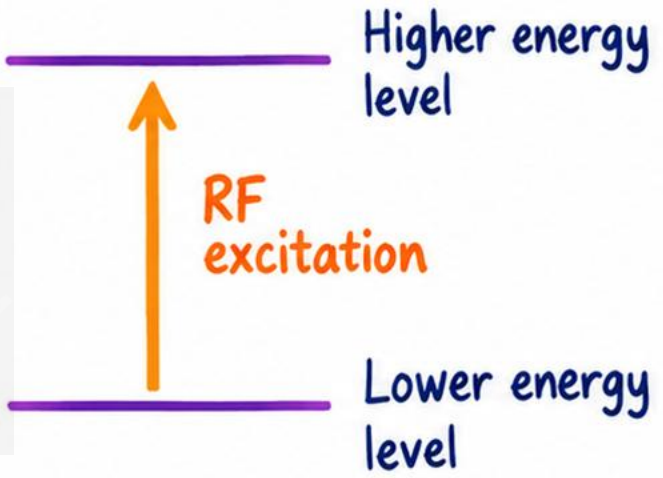
NMR: NUCLEAR SPIN IN A MAGNETIC FIELD

What is NMR?

- Nuclear magnetic resonance examines nuclei with non-zero spin in an external magnetic field.
- Examples include ^{1}H, ^{13}C, ^{19}F and ^{31}P.
- Appropriate radiofrequency excitation produces a measurable response that depends on nuclear environment.



Nuclear energy levels at a fixed magnetic field



Not atomic absorption spectroscopy (AAS)

- NMR is not atomic absorption spectroscopy: the PDF's opening AAS paragraph is a copied-topic error.

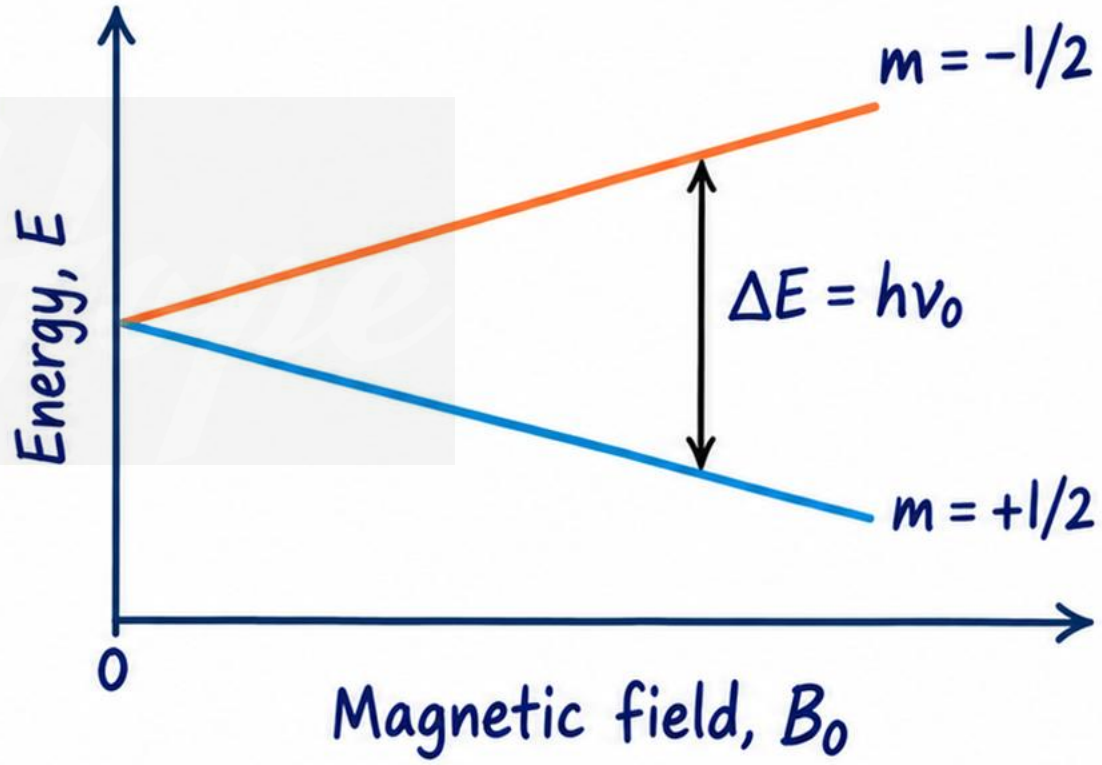
Value of NMR

- NMR is valuable for molecular structure and interactions rather than routine optical metal absorption.

MAGNETIC SPLITTING AND RESONANCE

- For a spin-½ nucleus, an applied field B_0 produces two energy levels.
- The resonance frequency is $\nu_0 = \gamma B_0/(2\pi)$, and the energy separation is $\Delta E = h\nu_0$.
- γ is the nucleus's gyromagnetic ratio.
- Different nuclei and electronic environments respond at different frequencies.
- The simple two-state picture applies to spin-½ nuclei; nuclei with larger spin have more than two magnetic substates.

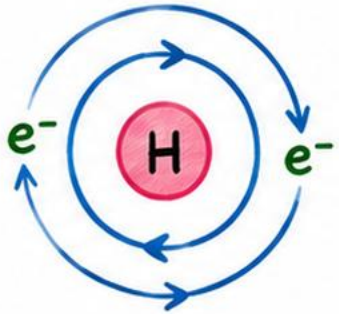
Zeeman splitting for a spin-½ nucleus (with positive gyromagnetic ratio)



$$\nu_0 = \gamma B_0/(2\pi)$$

CHEMICAL SHIFT

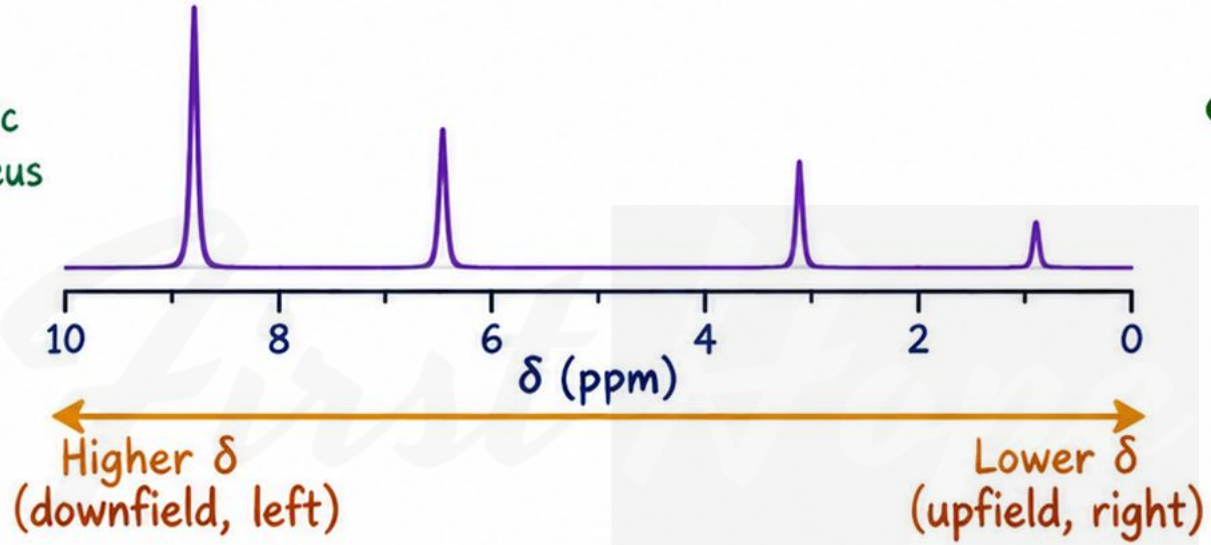
Shielded (upfield)



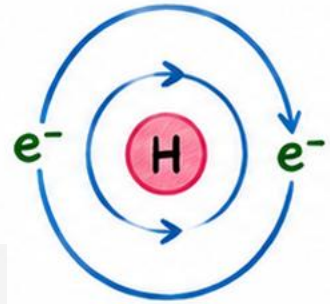
Higher electron density reduces the local magnetic field at the nucleus (shielding).

Appears at lower δ (upfield, right)

^{1}H NMR spectrum (schematic)



Deshielded (downfield)



Lower electron density increases the local magnetic field at the nucleus (deshielding).

Appears at higher δ (downfield, left)

Key points

- Electrons alter the local magnetic field experienced by a nucleus, shifting its resonance.
- Chemical shift is commonly reported in ppm: $\delta = (\nu_{sample} - \nu_{reference}) / \nu_{spectrometer} \times 10^6$, using consistent frequency units. This makes shifts comparable across field strengths.
- Signal positions help identify chemical environments, but depend on solvent, temperature and reference convention.
- A single shift does not uniquely identify a full molecule.

SPIN–SPIN COUPLING

Key concept

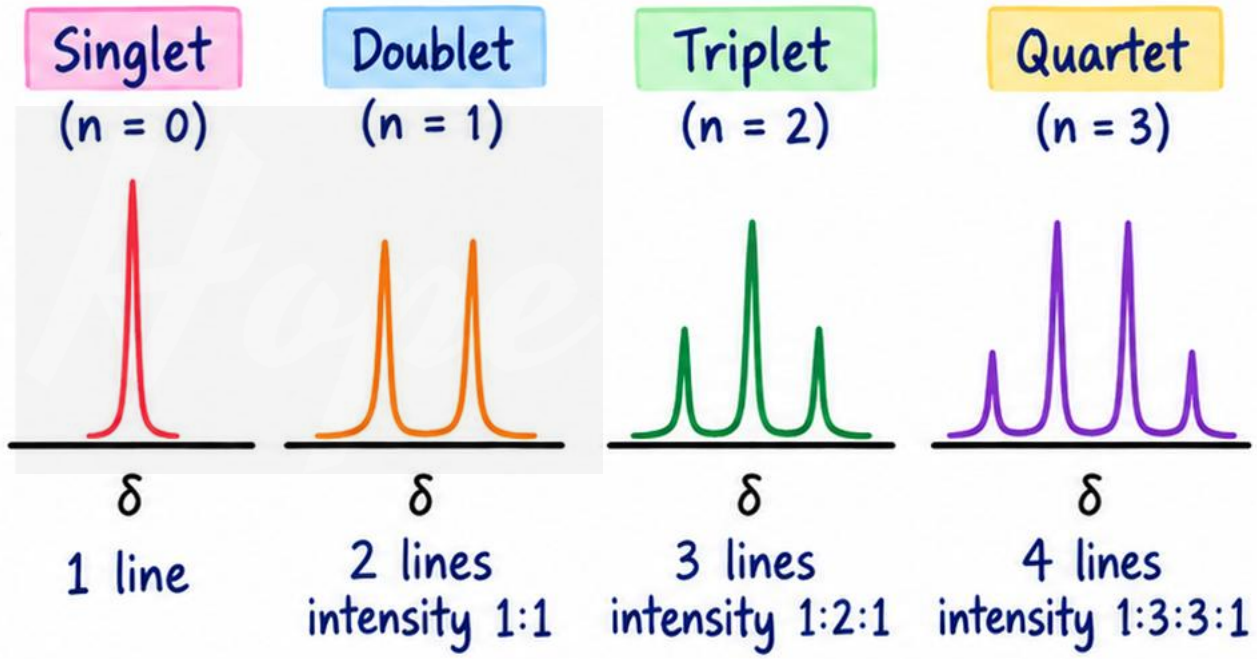
Interactions between nuclear spins can split signals into multiplets.

For simple first-order coupling to n equivalent spin-½ neighbours, a signal may form n + 1 lines with characteristic intensities.

This rule is conditional: nonequivalent neighbours, strong coupling and other spins give more complex patterns.

Coupling constants are reported in hertz.

Examples of first-order multiplets



Interpretation

Interpret multiplicity together with chemical shifts and other structural information rather than simply counting adjacent atoms.

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