NMR Resources

- Cantor and Schimmel, Chapter 9
  - Dated, but a good qualitative discussion of relaxation and signal strength
- Rule and Hitchens, *Fundamentals of Protein NMR Spectroscopy*
  - Hands down the best introductory text
- Cavanagh, *et al*., *Protein NMR Spectroscopy: Principles and Practice*
  - Detailed information for practitioners
- Abragam, *Principles of Nuclear Magnetism*
  - The “Bible” of NMR

Nuclear Spin

Table 12.1 Nuclei Commonly Used in Biochemical NMR

Isotope	Spin	Natural Abundance (%)	Gyromagnetic Ratio (10^7 rad/sec · T)	Relative[a] Sensitivity	Relative[b] Sensitivity in Natural Abundance	Relative NMR-Frequency
^{1}H	1/2	99.98	26.7522	1.00	1.00	100.000
^{2}H	1	1.5×10^{-2}	4.1066	9.65×10^{-3}	1.45×10^{-6}	15.351
^{13}C	1/2	1.108	6.7283	1.59×10^{-2}	1.76×10^{-4}	25.144
^{15}N	1/2	0.37	−2.7126	1.04×10^{-3}	3.85×10^{-6}	10.133
^{19}F	1/2	100	25.1815	0.83	0.83	94.077
^{31}P	1/2	100	10.8394	6.63×10^{-2}	6.62×10^{-2}	40.481
^{113}Cd	1/2	12.26	−5.9609	1.09×10^{-3}	1.33×10^{-3}	22.182

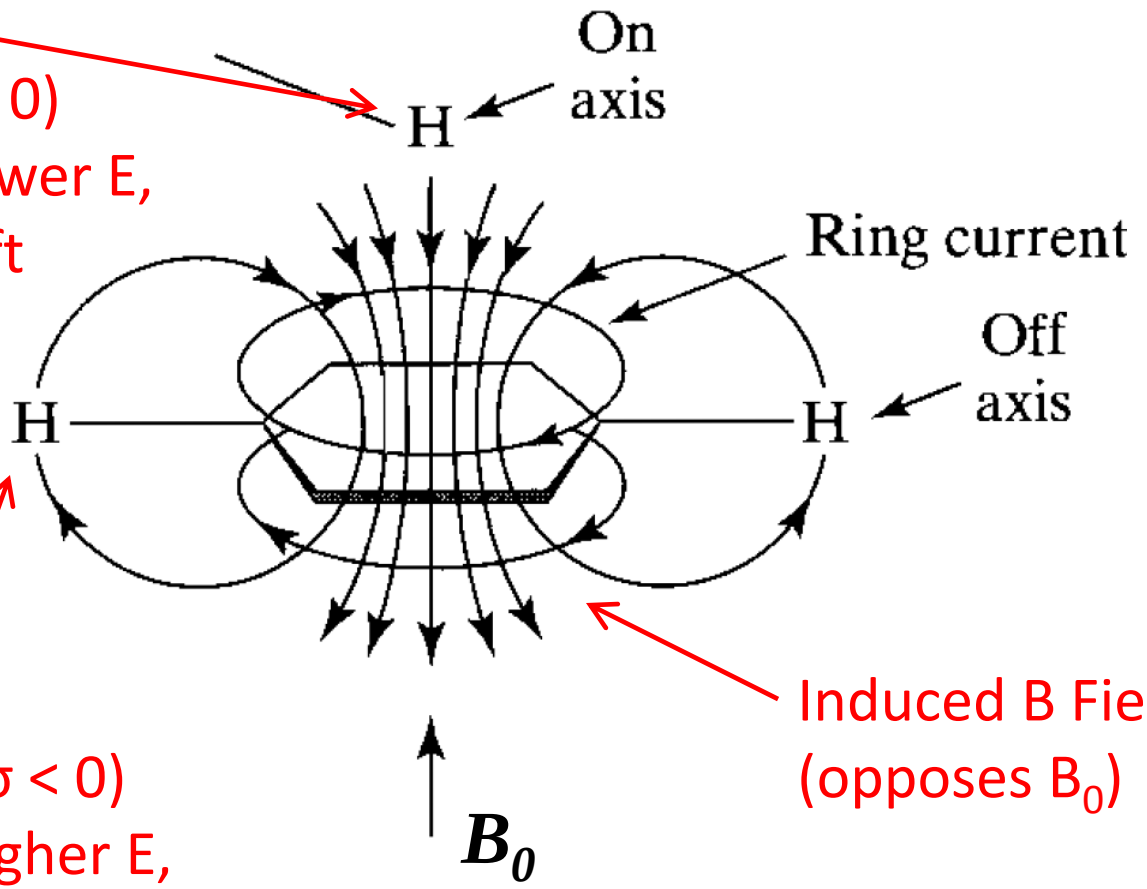
[a]At constant field for equal number of nuclei.

[b]Product of relative sensitivity and natural abundance.

From *Physical Biochemistry*
van Holde *et al*., Chapt. 12, p. 548

Shielding Constant: Benzene

Weaker B_{eff}
- shielded ($\sigma > 0$)
- absorbs at lower E,
- "upfield" shift



Stronger B_{eff}
- deshielded ($\sigma < 0$)
- absorbs at higher E,
- "downfield" shift

Induced B Field (opposes B_0)

Summary

- Nuclear spin is quantized; this results in energy splitting as $\vec{\mu}$ interacts with $\vec{B}_0$
- Energy splitting depends on the gyromagnetic ratio and the (local) magnetic field
- Splitting is << RT, so population differences are small
- Effective magnetic field is extremely sensitive to local environment; shielding creates different absorption energies