CH-314 Structural Analysis
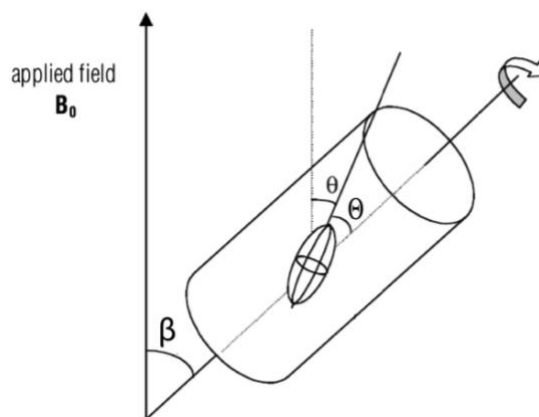ruben.rodriguezmadrid@epfl.ch
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Jigsaw 5D

1. [Week 4 Slides 47-50] The diagram shows the schematic sample setup for a magic-angle spinning experiment.

   a. Define the angles β, θ and Θ.

   b. Name three interactions which are averaged or partially averaged by sample spinning.

   c. For a nucleus with a chemical shielding tensor with axial symmetry, we can write the chemical shift as the sum of isotropic and anisotropic terms:

   $$\delta = \delta_{iso} + (\delta_{zz} - \delta_{iso})\left(\frac{3\cos^2\beta - 1}{2}\right)$$

   For which angle β does the anisotropic part average to 0?

   d. What is the effect of spinning at β = 90°?

2. [From Past Exam] [Keeler Section 9.8] The rate constant (in s⁻¹) for a symmetrical two-site exchange has the temperature dependence $k = 10^{13}\exp[-2500/T]$. The rate constant in Hz for which the two peaks merge together is $k_{merge} = \frac{\pi\delta v}{\sqrt{2}}$, where δv is the chemical shift difference in Hz. Consider a chemical shift difference of 1.0 ppm. Determine the number of peaks in the 400 MHz spectra at the following temperatures:

   a. 98 K

   b. 108 K

   c. 150 K