CH-314 Structural Analysis
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Jigsaw 1C

Introduction to Nuclear Magnetic Resonance

1. * [Keeler Sections 2.1 and 3.2] The international reference compound used in NMR to set up the chemical shift scale is tetramethylsilane, $Si(CH_3)_4$, commonly known as TMS. Consider a sample containing pure liquid TMS for analysis. *See also: Jigsaw 1B.1*

Isotope	**Nuclear Spin**	**Natural Abundance**	**γ / rad·s^{-1}·T^{-1}**
^{1}H	½	~100%	2.675×10^8

   a. Complete the table above by filling in the most common isotope(s) present in the sample (list all isotopes with ≥ 1% natural abundance), the nuclear spin, the natural abundance, and the gyromagnetic ratio of each isotope. Which isotopes are NMR-active? Why?

   b. [Keeler Section 3.3] Consider a magnetic field strength (B_0) of 11.7467 T. What are the resonance frequencies of the active nuclei (in MHz)?

   c. Considering the high symmetry of the molecule and neglecting all couplings, each nucleus gives rise to a single peak in the spectrum at the resonance frequency. Draw the spectrum, using an absolute frequency axis (in MHz).

d. * [Keeler Section 2.4] Why is it not possible to detect this theoretical spectrum, i.e. to detect heteronuclei in one single experiment?

2. * [Keeler Section 2.3] The following ^{1}H spectrum is of a molecule with the chemical formula $C_4H_{10}O$. Predict the structure of the molecule, assign the spectrum, and give the relative intensities of the signals.