

Jigsaw 3E

General

1. True or false. Justify your answer.
 - a) Fourier transformation converts time domain to the frequency domain.
 - b) Fourier transformation converts frequency domain to the time domain.
 - c) Multiplet splitting patterns are caused by scalar couplings.
 - d) Reducing the magnetic field results in smaller separation of peaks within multiplets in ppm.
2. The international reference compound used in NMR to set up the chemical shift scale is tetramethylsilane, $\text{Si}(\text{CH}_3)_4$, commonly known as TMS. Consider a sample containing pure liquid TMS for analysis.

Isotope	Nuclear Spin	Natural Abundance	$\gamma / \text{rad}\cdot\text{s}^{-1}\cdot\text{T}^{-1}$
^1H	$\frac{1}{2}$	~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 $\geq 1\%$ natural abundance), the nuclear spin, the natural abundance, and the gyromagnetic ratio of each isotope. Which isotopes are NMR-active? Why?
- b. 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. Why is it not possible to detect this theoretical spectrum, i.e. to detect heteronuclei in one single experiment?