CHEM 221

Instrumental Analysis

Problem Set #6 – Solutions

Spring 2005

Chapter 19

#1. In a CW-NMR, *absorption* of EMR from an applied RF source is measured. This absorption signal is acquired as either the magnetic field strength or the RF frequency is varied. The signal is due to transitions from the ground state to the excited state, so saturation will adversely affect the signal.

In a pulsed FT-NMR, the analyte is in a fixed-strength magnetic field and I subjected to periodic pulses of RF EMR. Absorption of the RF during the pulse creates an excited state population that is at its maximum (ideally, the transition is saturated). After the pulse, the signal due to the decay to the ground state of the excited state species is measured as a function of time. This free induction decay (FID) signal is then transformed to the frequency domain via Fourier transform.

#2. Advantages of FT-NMR:

- Much greater sensitivity (decreased sample size requirements, and multi-nuclear capability)
- Increased analysis speed
- Higher resolution
- Improved S/N due to signal averaging capability

Disadvantages of FT-NMR: *cost!*

#3. Increased magnetic field:

- Increases sensitivity
- Improves resolution
- Spectra more likely to be 1^{st}-order (easier to interpret)

#4. Record spectra at two different magnetic fields. Spin-spin splitting is independent of magnetic field strength, while the absolute magnitude of the chemical shift (Hz or mG) will increase with increasing field.

Additional Problems

#1. Since $\nu \propto H$: $\nu_1/H_1 = \nu_2/H_2$

$$\frac{60.00\ \text{MHz}}{14{,}092\ \text{G}} = \frac{270.00\ \text{MHz}}{H_2}$$

H_2 = 63,414 Gauss = ***63,410 Gauss***

#2. Coupling constants (J, Hz): independent of magfield strength

Chemical Shifts (δ): The *absolute magnitude* (Hz) of the shift will increase with increasing magnetic field strength.. The *relative* shift (ppm) will remain unchanged due to the equivalent shift of the internal reference.