

***** Useful formulas and constants to be attached to the final examination *****

Planck constant, $h = 6.626 \times 10^{-34}$ J s, Speed of light, $c = 3 \times 10^8$ m s⁻¹

Boltzmann constant, $k = 1.38 \times 10^{-23}$ J K⁻¹, $1 \text{ \AA} = 10^{-10}$ m

Atomic mass unit = 1.66×10^{-23} kg

Rotational constant in cm⁻¹, $B = h/(8\pi^2 c I)$ where $I = [m_1 m_2 / (m_1 + m_2)] r^2$

Rotational energy (in cm⁻¹): $E_J = BJ(J+1) - DJ^2(J+1)^2$

Vibrational energy (in cm⁻¹): $E_v = (v + 1/2)\omega_e - (v + 1/2)^2 \omega_e x_e$

Boltzmann distribution: $P_i/P_j = \exp[-(E_i - E_j)/kT]$

$N_J/N_{J=0} = (2J+1)\exp[-hcBJ(J+1)/kT]$

Nuclear spin Zeeman energy (in Hz), $E_Z = -m (\gamma/2\pi) B_0$

Chemical shielding energy (in Hz), $E_{CS} = \sigma m (\gamma/2\pi) B_0$

Indirect spin-spin (J) coupling energy (in Hz), $E_J = J m_1 m_2$

Boltzmann Law, $P_i \propto \exp(-E_i/kT)$

Selection rules: Raman spectroscopy, $\Delta J = 0, \pm 2$; NMR spectroscopy, $\Delta m = \pm 1$.

At 9.4 T, the Larmor frequencies of ¹H and ¹³C nuclei are 400 and 100 MHz, respectively.

In an AB spectrum, spectral line positions and relative intensities are determined by

Frequency	Relative intensity	
$\nu_1 = \frac{1}{2}(\nu_A + \nu_B + D + J)$	$1 - J/D$	$D = \sqrt{(\nu_A - \nu_B)^2 + J^2}$
$\nu_2 = \frac{1}{2}(\nu_A + \nu_B + D - J)$	$1 + J/D$	
$\nu_3 = \frac{1}{2}(\nu_A + \nu_B - D + J)$	$1 + J/D$	
$\nu_4 = \frac{1}{2}(\nu_A + \nu_B - D - J)$	$1 - J/D$	

The spectral density: $J(\omega) = 2\tau_C/(1+\omega^2\tau_C^2)$ where τ_C is the molecular rotational correlation time.

$$R_1 = \frac{1}{T_1} = \frac{1}{2}\gamma^2 [B_{xL}^2] J(\omega_0) + \frac{1}{2}\gamma^2 [B_{yL}^2] J(\omega_0)$$

$$R_2 = \frac{1}{T_2} = \frac{R_1}{2} + \frac{1}{2}\gamma^2 [B_{zL}^2] J(0)$$

where B_{xL} , B_{yL} , and B_{zL} are the individual components of the local magnetic field and ω_0 is the Larmor frequency for the nucleus under observation.