

Name: _____

Break-out 3: Maxwell-Boltzmann Distribution

A proton in a magnetic field can only be in one of two energy levels (corresponding to spin +1/2 and spin -1/2). The energy spacing, ΔE , corresponds to a transition frequency ν of 600 MHz (in our biggest magnet!). Use the equation $\Delta E = h\nu$, ($h = \text{Planck's constant, } 6.6261 \times 10^{-34} \text{ Js}$). Use the Boltzmann distribution to calculate the following. Recall that Boltzmann's constant $k_B = 1.381 \times 10^{-23} \text{ J/K}$, and $1 \text{ MHz} = 10^6 \text{ s}^{-1}$.

(a) the absolute temperature when the proton is in the lower state *only*. $\boxed{T=0}$

Let the two different energy states be 1 = lower state and 2 = upper state

$$\frac{N_2}{N_1} = e^{-\Delta E/k_B T} \Rightarrow \text{want } N_2 = 0 \therefore N_2 = 0 = N_1 \underbrace{e^{-\Delta E/k_B T}}_{\text{for } e^{-x} \rightarrow 0, x \rightarrow \infty \therefore T \rightarrow 0 \text{ b/c}}$$

(b) the absolute temperature when the probability of finding the proton in either level is equal. $\frac{y}{0} = \infty$

If the probability of finding the proton in either level is equal,

$$\text{then } N_2 = N_1 \text{ and } \therefore \frac{N_2}{N_1} = 1 = e^{-\Delta E/k_B T} \quad \text{for } e^{-x} = 1, \text{ then } x \rightarrow 0 \text{ (b/c } e^0 = 1)$$

$$\text{for } x \rightarrow 0, \text{ then } \boxed{T \rightarrow \infty}$$

(c) the ratio of populations at ambient temperature (25 °C).

$$\frac{N_2}{N_1} = e^{-\Delta E/k_B T} = e^{-\frac{(6.6261 \times 10^{-34} \text{ Js} \times 600 \times 10^6 \text{ s}^{-1})}{(1.381 \times 10^{-23} \text{ J/K})(25 + 273 \text{ K})}}$$

$$= e^{-9.66 \times 10^{-5}} = 0.9999$$

(d) The transition between these two energy levels gives rise to an NMR signal. The magnitude of the signal depends on the difference in populations between the two energy states. What does this mean for NMR spectroscopists?

At room temperature, the ratio of populations is $\frac{0.9999}{1}$

\therefore there's not much difference $\hat{=}$ the NMR signal will be very small. However if you lower the temperature, you preferentially populate the lower energy level (as seen in (a)) $\hat{=}$ \therefore the signal will increase.