

## Jigsaw 2B

### Home Section 2.3. Origin of chemical shifts

1. The lowest energy electronic transitions in alkanes and alkenes are approximately 10 eV and 8 eV, respectively. Predict whether saturated ( $sp^3$ ) or unsaturated ( $sp^2$ )  $^{13}\text{C}$  nuclei have larger chemical shifts. Assume the paramagnetic contribution is the dominant contribution. Justify the assumptions made in this exercise.
  
2. [From lecture]  $^1\text{H}$  has a gyromagnetic ratio of  $2.68 \times 10^8 \text{ rad}\cdot\text{s}^{-1}\text{T}^{-1}$ .
  - a. What are the relative populations of the  $\alpha$  and  $\beta$  spin states of a proton in a 11.7 T spectrometer, at both room temperature and  $-150^\circ\text{C}$ ? The equation for the Boltzmann distribution is given below, where  $k = 1.381 \times 10^{-23} \text{ J/K}$ .  
Hint: Use the Larmor frequency to determine the energy difference.

$$\frac{N_\beta}{N_\alpha} = \exp\left(-\frac{\Delta E}{kT}\right)$$

- b. Based only on the answers to the previous question (i.e., ignoring changes in state of the sample, equipment logistics, etc.), which of these two temperatures would you choose to run an experiment? Why?