Examples Week 3

1. *Calculate the bond length of CO from a rotational band line spacing of 3.86 cm^{-1}.*

The rotational constant is easily obtained from the rotational line spacing for a rigid rotator

$$\nu = 2B(J+1) \;\; \rightarrow \;\; \Delta\nu = 2B \quad B = 1.93\,\mathrm{cm}^{-1}$$

The rotational constant is related to the moment of inertia I by

$$B = \frac{h}{8\pi^2 cI}$$

The moment of inertia around the symmetry axis is

$$I = m_r r^2 \qquad m_r = \frac{m_C m_O}{m_C + m_O}$$

where r is the bond length (distance between C and O) and m_r is the reduced mass,

$$m_r = \frac{12(16)}{12+16} 1.66 \times 10^{-27}\,\mathrm{kg} \; = 1.14 \times 10^{-26}\,\mathrm{kg}$$

Therefore the bond length is

$$r^2 = \frac{h}{8\pi^2 cBm_r}$$

$$r^2 = \frac{6.626 \times 10^{-34}\,\mathrm{J\,s}}{79.0(3.00 \times 10^8\,\mathrm{m/s})(193\,\mathrm{m}^{-1})(1.14 \times 10^{-26}\,\mathrm{kg})} \; = 1.27{\times}10^{-20}\,\mathrm{m}^2$$

$$r = 1.13\mathrm{A}$$