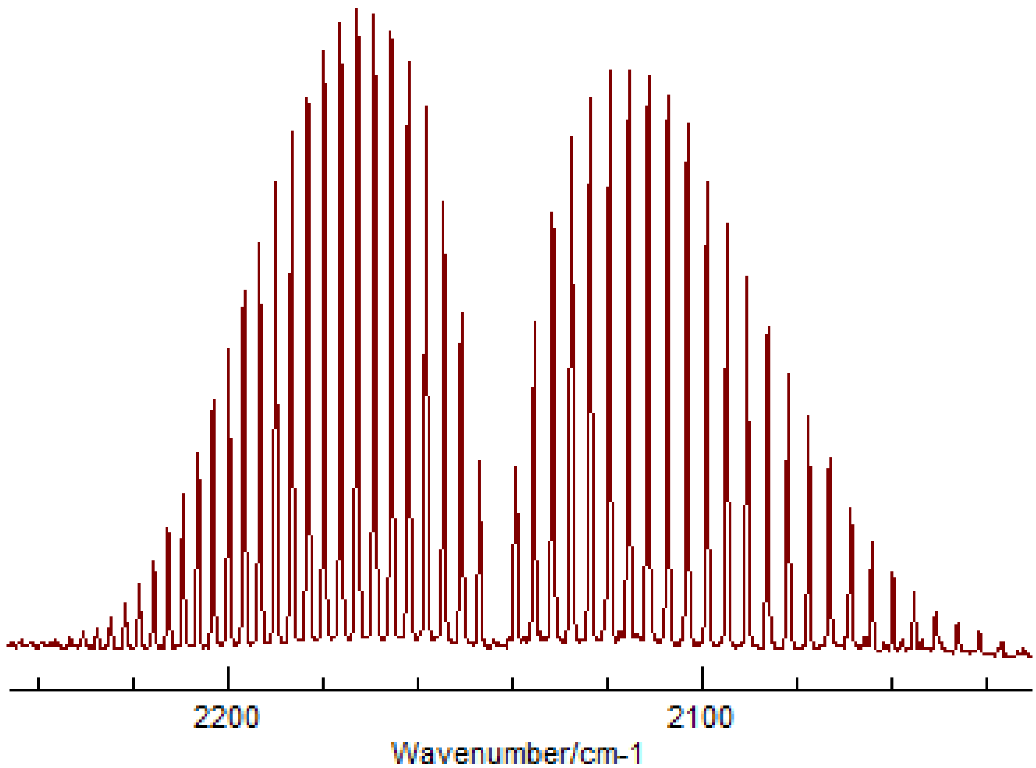
The rovibrational spectrum of CO is shown below.



A. Estimate the vibrational wavenumber of the stretching mode of CO from this spectrum.

The Q band is not observed since the rotational transition has ΔJ = 0. However, it is located at the mid-point between the first transitions of the P and R branches. Here it is:

$$\tilde{\nu} = 2143\ cm^{-1}$$

B. Based on this wavenumber calculate the force constant of the CO bond.

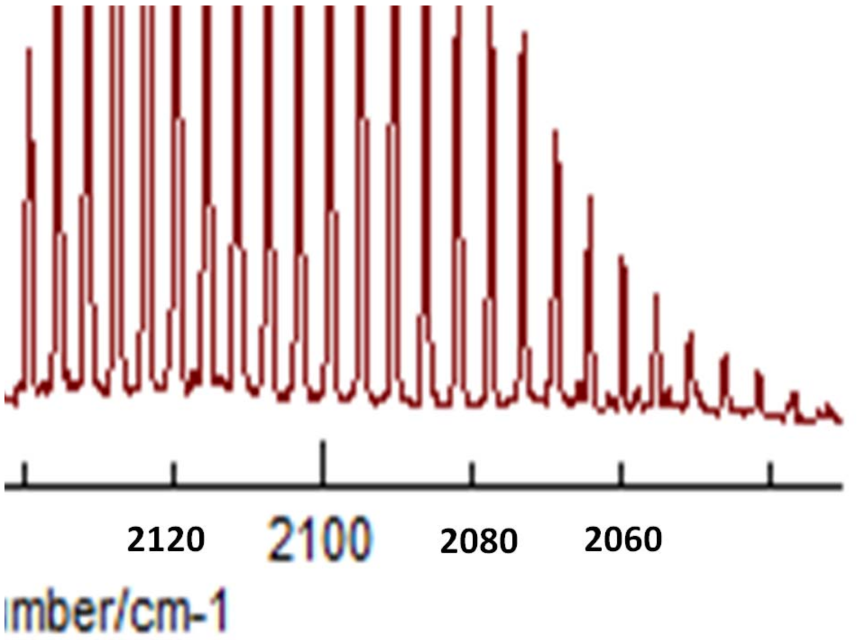
$$\mu = \frac{m_C m_0}{m_C + m_O} = \frac{12\ x\ 16}{28}(1.660\ x\ 10^{-27}\ amu) = 1.138\ x\ 10^{-26}\ kg$$

$$k = \mu\omega^2 = \mu 4\pi^2 c^2 \tilde{\nu}^2$$

$$k = (1.138\ x\ 10^{-26}\ kg)4(3.141)^2\left(2.99\ x\ 10^{10}\frac{cm}{s}\right)^2(2143\ cm^{-1})^2$$

$$k = 1844\ N/m$$

C. Estimate the rotational constant from the expansion of the figure shown below. The progression of lines has wave numbers 2146.8, 2150.7, 2154.6, 2158.4 cm^{-1} and so on.



Based on the fact that the line spacing is equal to two times the rotational constant, we conclude that the rotational constant is 1.93 cm^{-1}.

D. Based on this wavenumber calculate the bond length of CO.

$$R = \sqrt{\frac{h}{8\pi^2 c\mu\tilde{B}}}$$

For CO

$$R = \sqrt{\frac{6.626\ x\ 10^{-34}\ Js}{8(3.141)^2\left(2.99\ x\ 10^{10}\frac{cm}{s}\right)(1.138\ x\ 10^{-26}\ kg)(1.93\ \text{cm}^{-1})}} = 1.13\ \text{Å}$$