

A. Given the force constants for N₂ and O₂ are 2287 and 1133 N/m, respectively, calculate their vibrational frequencies.

Solution: You will need to use the reduced mass that you calculated in part A. Recall that the classical relationship between the frequency and the force constant holds also in quantum mechanics.

$$\omega = \sqrt{\frac{k}{\mu}}$$

The quantity ω is the angular frequency, which is related to the frequency in Hz as $\omega = 2\pi\nu$. To obtain the answer in wavenumbers (cm⁻¹) we divide by c .

$$\tilde{\nu} = \frac{1}{2\pi c} \sqrt{\frac{k}{\mu}}$$

For nitrogen we have

$$\tilde{\nu} = \frac{1}{2(3.14159)(2.99 \times 10^{10} \text{ cm/s})} \sqrt{\frac{2287 \text{ N/m}}{1.162 \times 10^{-26} \text{ kg}}} = 2360 \text{ cm}^{-1}$$

For oxygen we have:

$$\tilde{\nu} = \frac{1}{2(3.14159)(2.99 \times 10^{10} \text{ cm/s})} \sqrt{\frac{1133 \text{ N/m}}{1.328 \times 10^{-26} \text{ kg}}} = 1554 \text{ cm}^{-1}$$

If you are given the vibrational wavenumbers you can obtain the force constants as follows:

$$\begin{aligned} \text{For oxygen } k &= \mu\omega^2 = 4\pi^2c^2\mu\tilde{\nu}^2 \\ &= 4(3.14159)^2(2.99 \times 10^{10} \text{ cm/s})^2(1.337 \times 10^{-26} \text{ kg})(1551 \text{ cm}^{-1})^2 \\ &= 1133 \text{ N/m} \end{aligned}$$

$$\begin{aligned} \text{For nitrogen } k &= \mu\omega^2 = 4\pi^2c^2\mu\tilde{\nu}^2 \\ &= 4(3.14159)^2(2.99 \times 10^{10} \text{ cm/s})^2(1.17 \times 10^{-26} \text{ kg})(2353 \text{ cm}^{-1})^2 \\ &= 2287 \text{ N/m} \end{aligned}$$

B. Calculate the infrared absorption intensity of the $v=0 \rightarrow v=1$ transition of O₂.

Solution: Neither N₂ nor O₂ has a dipole moment. Therefore, neither has a vibrational (infrared) absorption spectrum.

Infrared absorption intensity for oxygen = _____.