The atmosphere is made up of 79% N_2 and 20% O_2. To apply rotational or vibrational spectroscopy formulae to these diatomic molecules, you will need to use the reduced mass, given by:

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

A. Calculate the reduced mass for both N_2 and O_2 in kilograms.

Solution: for oxygen.

$$\mu = \frac{m_O m_O}{m_O + m_O} = \frac{m_O}{2} = \frac{16}{2}(1.660\ x\ 10^{-27}\ amu) = 1.328\ x\ 10^{-26}\ kg$$

and for nitrogen

$$\mu = \frac{m_N m_N}{m_N + m_N} = \frac{m_N}{2} = \frac{14}{2}(1.660\ x\ 10^{-27}\ amu) = 1.162\ x\ 10^{-26}\ kg$$

Reduced mass for oxygen = ______________________.

Reduced mass for nitrogen = ______________________.

B. Given the rotational constant $\widetilde{B}$ = 1.99 cm^{-1} for N_2 and 1.45 cm^{-1} for O_2 determine the bond length of each molecule.

Solution: If we solve for the rotational energy from the Schrodinger equation the energy levels are:

$$E = \frac{h^2}{8\pi^2 \mu R^2} J(J+1)$$

or

$$\tilde{\nu} = \frac{h}{8\pi^2 c \mu R^2} J(J+1)$$

Note that we used h and not h_bar above so there is an extra factor of $4\pi^2$ in the denominator. Recall that the difference between any two levels is two 2J so that the rotational spectrum is a progression of lines with a spacing that is equal to twice the rotational constant B.

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

If given $\widetilde{B}$ you can solve for the internuclear distance of a diatomic as follows.

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

For nitrogen

$$R = \sqrt{\frac{6.626\ x\ 10^{-34}\ Js}{8(3.141)^2\left(2.99\ x\ 10^{10}\frac{cm}{s}\right)(1.162\ x\ 10^{-26}\ kg)(1.99\ \mathrm{cm}^{-1})}} = 1.1\ \text{Å}$$

For oxygen

$$R = \sqrt{\frac{6.626\ x\ 10^{-34}\ Js}{8(3.141)^2\left(2.99\ x\ 10^{10}\frac{cm}{s}\right)(1.328\ x\ 10^{-26}\ kg)(1.45\ \mathrm{cm}^{-1})}} = 1.3\ \text{Å}$$

NOTE: In this problem all of the quantities are in MKS units except the speed of light. We cm/s because this way our answer is consistent with units of cm^{-1}.

Bond length for oxygen = _______________________.

Bond length for nitrogen = _______________________.

C. Calculate the intensity of the J=0 → J=1 transition in the rotational spectra of N_2.

Solution: Neither N_2 nor O_2 has a dipole moment. Therefore, neither has a pure rotational (microwave) absorption spectrum.

Microwave absorption intensity for nitrogen = _______________________.

D. Given the force constants for N_2 and O_2 are 2287 and 1133 N/m, respectively, calculate their vibrational frequencies.

Solution: Again 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 ω = 2πν. Therefore,

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

To obtain the answer in wavenumbers (cm^{-1}) we use the fact that

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

n_tilde is the answer in wavenumbers.

For nitrogen we have

$$\tilde{\nu} = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}} = \frac{1}{2(3.141)(2.99\ x\ 10^{10}\ cm/s)}\sqrt{\frac{2287\ N/m}{1.17\ x\ 10^{-26}\ kg}}$$

$$= 2354\ cm^{-1}$$

For oxygen we have:

$$\dot{\nu} = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}} = \frac{1}{2(3.141)(2.99\ x\ 10^{10}\ cm/s)}\sqrt{\frac{1133\ N/m}{1.337\ x\ 10^{-26}\ kg}}$$

$$= 1550\ cm^{-1}$$

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

For oxygen $k = \mu\omega^2 = 4\pi^2c^2\mu\cancel{\nu}^2$

$= \ 4(3.14159)^2(2.99\ x\ 10^{10}\ cm/s)^2(1.337\ x\ 10^{-26}\ kg)(1551\ cm^{-1})^2$

$= 1133$ N/m

For nitrogen $k = \mu\omega^2 = 4\pi^2c^2\mu\cancel{\nu}^2$

$= \ 4(3.14159)^2(2.99\ x\ 10^{10}\ cm/s)^2(1.17\ x\ 10^{-26}\ kg)(2353\ cm^{-1})^2$

$= 2287$ N/m

E. Calculate the infrared absorption intensity of the v=0 → v=1 transition of O_2.

Solution: Neither N_2 nor O_2 has a dipole moment. Therefore, neither has a vibrational (infrared) absorption spectrum.

Infrared absorption intensity for oxygen = ______________________.