

Bond length of O₂ and N₂

The atmosphere is made up of 79% N₂ and 20% O₂. 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 N₂ and O₂ in kilograms.
- B. Given the rotational constant $\tilde{B} = 1.99 \text{ cm}^{-1}$ for N₂ and 1.45 cm^{-1} for O₂ determine the bond length of each molecule.
- C. Calculate the intensity of the J=0 → J=1 transition in the rotational spectra of N₂.

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A. Calculate the reduced mass for both N₂ and O₂ in kilograms.

Solution: for oxygen.

$$\mu = \frac{m_o m_o}{m_o + m_o} = \frac{m_o}{2} = \frac{16}{2} (1.660 \times 10^{-27} \text{ kg}) = 1.328 \times 10^{-26} \text{ kg}$$

and for nitrogen

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

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B. Given the rotational constant $\tilde{B} = 1.99 \text{ cm}^{-1}$ for N₂ and 1.45 cm^{-1} for O₂ determine the bond length of each molecule

The rotational constant \tilde{B} is:

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

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

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

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B. Given the rotational constant $\tilde{B} = 1.99 \text{ cm}^{-1}$ for N₂ and 1.45 cm^{-1} for O₂ determine the bond length of each molecule

For nitrogen

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

For oxygen

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

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C. Calculate the intensity of the $J=0 \rightarrow J=1$ transition in the rotational spectrum of N₂.

Solution: Neither N₂ nor O₂ has a dipole moment. Therefore, neither has a pure rotational (microwave) absorption spectrum.