

# Bond length of HF and HCl

We would like to find the bond lengths of HF and HCl. 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 HF and HCl in kilograms.
- B. Given the rotational constant  $\tilde{B} = 19.5 \text{ cm}^{-1}$  for HF and  $17.9 \text{ cm}^{-1}$  for HCl determine the bond length of each molecule.

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A. Calculate the reduced mass for both HF and HCl in kilograms.

Solution: for HF.

$$\mu = \frac{m_H m_F}{m_H + m_F} = 0.95(1.660 \times 10^{-27} \text{ kg}) = 1.577 \times 10^{-27} \text{ kg}$$

and for HCl

$$\mu = \frac{m_H m_{Cl}}{m_H + m_{Cl}} = 0.972(1.660 \times 10^{-27} \text{ kg}) = 1.613 \times 10^{-27} \text{ kg}$$

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B. Given the rotational constant  $\tilde{B} = 19.5 \text{ cm}^{-1}$  for HF and  $17.9 \text{ cm}^{-1}$  for HCl 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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For HF

$$R = \sqrt{\frac{6.626 \times 10^{-34} \text{ Js}}{8(3.141)^2 \left(2.99 \times 10^{10} \frac{\text{cm}}{\text{s}}\right) (1.577 \times 10^{-27} \text{ kg})(19.5 \text{ cm}^{-1})}}$$
$$= 0.955 \text{ \AA}$$

For HCl

$$R = \sqrt{\frac{6.626 \times 10^{-34} \text{ Js}}{8(3.141)^2 \left(2.99 \times 10^{10} \frac{\text{cm}}{\text{s}}\right) (1.613 \times 10^{-26} \text{ kg})(17.9 \text{ cm}^{-1})}}$$
$$= 0.985 \text{ \AA}$$