

(3.6) When the rotational quantum number n_r goes from 0 to 1 in H^{35}Cl , it is accompanied by the absorption of light with a wave number of 20.6 cm^{-1} . From this it is possible to calculate the interatomic distance between hydrogen and chlorine in the molecule. What is this distance?

First we need to define the atomic mass unit, u , the electron volt, eV , the Boltzmann constant, k , and the Planck constant, h (values from Appendix III):

$$u := 1.660540 \cdot 10^{-27} \cdot \text{kg} \quad eV := 1.6021773 \cdot 10^{-19} \cdot \text{joule} \quad nm := 10^{-9} \cdot m$$

$$k := 1.23980 \cdot 10^{-4} \cdot eV \cdot \text{cm} \quad h := 4.135669 \cdot 10^{-15} \cdot eV \cdot \text{sec}$$

Furthermore, we need to define the atomic masses of H- and Cl-atoms (data from Table 3.1):

$$M_H := 1.007825 \quad M_{Cl} := 34.968853 \quad \text{hence:} \quad m_H := M_H u \quad m_{Cl} := M_{Cl} u$$

The wave number is stated as:

$$\nu := 20.6 \cdot \text{cm}^{-1}$$

Using eqn. (3.40) and the statement that the rotational quantum number changed from 0 to 1 we can write:

$$I_{rot} := \frac{h^2 \cdot 1 \cdot (1 + 1)}{8 \cdot \pi^2 \cdot k \cdot \nu}$$

This rotational moment of inertia is valid for a reduced mass, m_{red} , calculated from the expression below eqn. (3.39):

$$m_{red} := \frac{1}{\left(\frac{1}{m_H} + \frac{1}{m_{Cl}} \right)}$$

Then we finally obtain the separation distance between the mass centra, r , from eqn. (3.39) as follows:

$$r := \sqrt{\frac{I_{rot}}{m_{red}}} \quad r = 1.293 \cdot 10^{-10} \cdot m \quad r = 0.1293 \cdot nm$$