Question

Rotational Energy Levels: The rotational spectrum of HCl contains the following wavelengths:

$$12.03 \times 10^{-5}\, m$$
$$9.60 \times 10^{-5}\, m$$
$$8.04 \times 10^{-5}\, m$$
$$6.89 \times 10^{-5}\, m$$
$$6.04 \times 10^{-5}\, m$$

If the isotopes involved are ^{1}H and ^{35}Cl, find the distance between the hydrogen and chlorine nuclei in an HCl molecule.

Solution

Given the selection rule $\Delta J = \pm 1$, the wavelengths in the spectrum correspond to differences in consecutive energy levels, ΔE

$\lambda = 12.03 \times 10^{-5}$

$$\Delta E = hc/\lambda = hc(8.313 \times 10^3) = 4hc(2.078 \times 10^3)$$

$\lambda = 9.60 \times 10^{-5}$

$$\Delta E = hc(10.42 \times 10^3) = 5hc(2.083 \times 10^3)$$

$\lambda = 8.04 \times 10^{-5}$

$$\Delta E = hc(12.44 \times 10^3) = 6hc(2.073 \times 10^3)$$

$\lambda = 6.89 \times 10^{-5}$

$$\Delta E = hc(14.51 \times 10^3) = 7hc(2.073 \times 10^3)$$

$\lambda = 6.04 \times 10^{-5}$

$$\Delta E = hc(16.56 \times 10^3) = 8hc(2.070 \times 10^3)$$

The theoretical values of ΔE are $\dfrac{(J+1)\hbar^2}{I}$ hence the spectrum results from $J = 3, 4, 5, 6$ and 7

Equating the theoretical values with the average of those observed (for any J)

$$\frac{\hbar^2}{I} = hc(2.075 \times 10^3) \qquad \text{or} \qquad I = \frac{\hbar}{2\pi c(2.075 \times 10^3)} = 2.70 \times 10^{-47}\, kg\, m^2$$

The moment of inertia $I = m'R^2$ where m' is the reduced mass, R the distance between the nuclei

$$m' = \frac{m_1 m_2}{m_1 + m_2} = \frac{35}{36}(1.66 \times 10^{-27}) = 1.61 \times 10^{-27}\, kg$$

$$I = m'R^2$$
$$R^2 = \frac{2.70 \times 10^{-47}}{1.61 \times 10^{-27}} = 1.67 \times 10^{-20}$$
$$R = 1.29 \times 10^{-10}\, m$$

The distance between the hydrogen and chlorine nuclei in the HCl molecule is $0.129\, nm$.