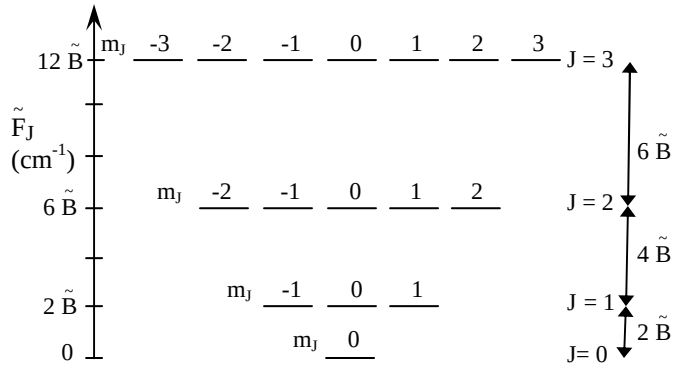
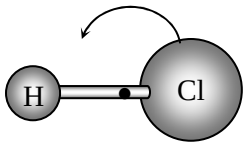
Rotational Spectroscopy - Diatomics





$$E_J = \frac{\hbar^2}{2I} J(J+1)$$

$$I = \mu R^2 \qquad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

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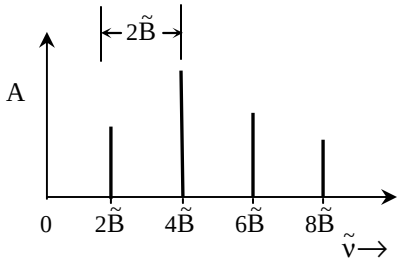
magnitude of the angular momentum = $\hbar\sqrt{J(J+1)}$ projection $J_z = m_J \hbar$

$$\tilde{F}_J = \frac{E_J}{hc} = \frac{\hbar}{4\pi Ic} J(J+1)$$

$$\tilde{B} = \frac{\hbar}{4\pi Ic}$$

$$\tilde{F}_J = \frac{E_J}{hc} = \tilde{B}J(J+1) \qquad E_J = \tilde{B}hc\, J(J+1)$$



transition : upper←lower J' ← J"

$$\tilde{\nu}_{J'} = \tilde{F}_{J'} - \tilde{F}_{J'-1} = \tilde{B}J'(J'+1) - \tilde{B}(J'-1)(J'-1+1)$$

$$= 2\tilde{B}J' \qquad J' \sim \text{upper level}$$

$$\tilde{\nu}_{J''} = \tilde{F}_{J''+1} - \tilde{F}_{J''} = 2\tilde{B}(J''+1) \qquad J'' \sim \text{lower level}$$

$H^{35}Cl$ spacing 20.880 cm^{-1} $\tilde{B} = 10.440\ cm^{-1} \frac{100cm}{1m} = 1044.0\ m^{-1}$

$\tilde{B} = 1044.0\ m^{-1} = \frac{\hbar}{4\pi\,\mu R^2 c}$ $\langle\tilde{B}\rangle \propto \langle 1/R^2\rangle$ averaged over $\upsilon = 0$ vibration

$\mu = \frac{1.0078 \times 34.9688}{1.0078+34.9688} \frac{1}{N_A} \frac{1\ kg}{1000g} = 1.62665 \times 10^{-27}$ kg isotope specific in SI units!

$I = 2.68135 \times 10^{-47}\ kg\ m^2$ $R_o = 1.28389 \times 10^{-10}\ m = 0.12840\ nm = 1.2840\ Å$

Centrifugal Distortion

$$\tilde{F}_J = \tilde{B}J(J+1) - \tilde{D}[J(J+1)]^2$$

HCl: $\tilde{D} = 0.00053\ cm^{-1}$

Model prediction: $\tilde{D} = \frac{4\tilde{B}^3}{\tilde{\nu}_o^2}$ $\tilde{D} = 4(10.44\ cm^{-1})^3/(2886\ cm^{-1})^2 = 0.00055\ cm^{-1}$