Modern Physics

Rotational and vibrational states

Problem 1.- Calculate the wavelength of a photon emitted during the transition from the l=3 to the l=2 rotational level of the HF molecule.

[For the HF molecule, $B = \frac{\hbar^2}{2I} = 4.158\times10^{-22}\,J$]

Solution: For the HF molecule, $B = 4.158\times10^{-22}\,J$, so the levels involved in the transition are:

$$E_2 = \frac{2(2+1)\hbar^2}{2I} = 6B = 2.495\times10^{-21}\,J$$

$$E_3 = \frac{3(3+1)\hbar^2}{2I} = 12B = 4.990\times10^{-21}\,J$$

A transition from l=3 to l=2 will produce a photon of wavelength:

$$\frac{hc}{\lambda} = E_3 - E_2 = \frac{12\hbar^2}{2I} - \frac{6\hbar^2}{2I} = 6B \rightarrow \lambda = \frac{hc}{6B} = \frac{6.62\times10^{-34}\,Js(3\times10^8\,m/s)}{6(4.158\times10^{-22}\,J)} = \textbf{79.6 μm}$$

Problem 1a.- Calculate the first five rotational energy levels of the HF molecule and find the wavelength of a photon emitted from a transition from the l=4 to the l=3 levels.

Solution: Recall that the rotational kinetic energy can be written as:

$$K.E._{rotational} = \frac{1}{2}I\omega^2 = \frac{(I\omega)^2}{2I} = \frac{L^2}{2I}$$

But in quantum mechanics the angular momentum L is quantized, so:

$$K.E._{rotational} = \frac{l(l+1)\hbar^2}{2I} = l(l+1)\frac{\hbar^2}{2I} = l(l+1)B \text{ , where } B = \frac{\hbar^2}{2I}$$

For the HF molecule $B = 4.158\times10^{-22}\,J$, so the first five levels are:

$$E_o = 0$$

$$E_1 = \frac{1(1+1)\hbar^2}{2I} = 2B = 8.317\times10^{-22}\,J$$

$$E_2 = \frac{2(2+1)\hbar^2}{2I} = 6B = 2.495\times10^{-21}\,J$$

$$E_3 = \frac{3(3+1)\hbar^2}{2I} = 12B = 4.990\times10^{-21}\,J$$

$$E_4 = \frac{4(4+1)\hbar^2}{2I} = 20B = 8.317\times10^{-21}\,J$$

A transition from *l*=4 to *l*=3 will produce a photon of wavelength:

$$\frac{hc}{\lambda} = E_4 - E_3 = \frac{20\hbar^2}{2I} - \frac{12\hbar^2}{2I} = 8B \rightarrow \lambda = \frac{hc}{8B} = \frac{6.62\times10^{-34}\,Js(3\times10^{8}\,m/s)}{8(4.158\times10^{-22}\,J)} = \mathbf{59.7\mu m}$$

Problem 2.- Calculate the first five vibrational energy levels of the HF molecule and find the wavelength of a photon emitted from a transition from the *n*=2 to *n*=1 levels ignoring any rotational effect.

Solution: The vibrational levels are quantized with energies given by $(n+1/2)\hbar\omega$ [where $\omega = 4.091\times10^{14}\,rad/s$ for the HF molecule], so the first five levels are:

$$E_o = 1/2\hbar\omega$$
$$E_1 = 3/2\hbar\omega$$
$$E_2 = 5/2\hbar\omega$$
$$E_3 = 7/2\hbar\omega$$
$$E_4 = 9/2\hbar\omega$$

A transition from *n*=2 to the *n*=1 level will produce a photon of wavelength:

$$\frac{hc}{\lambda} = E_2 - E_1 = 5/2\hbar\omega - 3/2\hbar\omega = \hbar\omega \rightarrow \lambda = \frac{hc}{\hbar\omega} = \mathbf{2.42\ \mu m}$$