4.1: Rudiments of Atomic Spectroscopy Using Mathcad

Planck's constant: $h = 6.6260810^{-34}$ Speed of light: $c = 2.997910^{8}\ \frac{m}{sec}$

Conversion factors: $nm = 10^{-9}m$ $pm = 10^{-12}m$ $aJ = 10^{-18}\text{Joule}$

Energy of a photon: $E_{photon} = h\nu = \frac{hc}{\lambda}$

Energy of the hydrogen atom: where n is a quantum number and can have integer values.

$$E_{atom} = \frac{-2.178aJ}{n^2}$$

Emission Spectroscopy

In emission spectroscopy a photon is created as the electron undergoes a transition from a higher to a lower energy state. Energy conservation requires

$$E_{atom}{}^{initial} = E_{atom}{}^{final} + E_{photon}$$

Example: Calculate the frequency, wavelength, and energy of the photon emitted when an electron undergoes a transition from the n=2 to the n=1 state.

$$n_i = 2 \quad n_f = 1 \quad \nu = \frac{-2.178aJ}{n_i^2} = \frac{-2.178aJ}{n_f^2} + h\nu \quad \left| \begin{matrix} solve, \nu \\ float, 4 \end{matrix} \right. \rightarrow \frac{0.2465e16}{sec}$$

Calculate the wavelength of the photon: $\lambda = \frac{c}{\nu}$ $\lambda = 121.619nm$

Calculate the energy of the photon: $h\nu = 1.633aJ$

Absorption Spectroscopy

In absorption spectroscopy a photon is absorbed and an electron is promoted to a higher energy level. Energy conservation requires

$$E_{atom}{}^{initial} = E_{atom}{}^{final} + E_{photon}$$

Example: Calculate the frequency, wavelength, and energy of the photon required to promote the electron from the n=1 to the n=3 level.

$$\nu = \nu \quad n_i = 1 \quad n_f = 3 \quad \nu = \frac{-2.178aJ}{n_i^2} + h\nu = \frac{-2.178aJ}{n_f^2} \quad \left| \begin{matrix} solve, \nu \\ float, 4 \end{matrix} \right. \rightarrow \frac{0.2922e16}{sec}$$

Calculate the wavelength of the photon: $\lambda = \frac{c}{\nu}$ $\lambda = 102.598nm$

Calculate the energy of the photon: $h\nu = 1.936aJ$