5.111 Principles of Chemical Science: Week 1

Logan Pachulski

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Progress Update

Over the past week I have been introduced to:

1. Additional notes on wave-particle duality,
2. Energies of orbitals in hydrogen.
3. The emission spectra of hydrogen.
4. The quantum numbers.
5. Wave-functions and nodes.

De Broglie wavelength.

Real quick: the de Broglie wavelength of a physical object is defined

$$\lambda = \frac{h}{mv}. \tag{1}$$

Hydrogen orbitals

The energy of an electron, in an atom with only 1 electron (and atomic number Z), is found to be

$$\frac{-Z^2 hcR}{n^2}. \tag{2}$$

The emission spectra of hydrogen.

The emission spectra of hydrogen is found to perfectly match the output V of the equation

$$V = hR\left(\frac{1}{n_1^1} - \frac{1}{n_2^2}\right). \tag{3}$$

Where $n_1 = 1, 2, 3, \cdots$ and $n_2 = n_1 + 1, n_1 + 2, \cdots$.

Quantum numbers.

Three quantum numbers describe the position of an electron within an atoms orbitals:

1. n - tells you the energy of the wave-function; principal quantum number
2. L - tells you the shape of the wave-function; orbital quantum number
3. m_L - tells what part of l the electron is found in.

Wave-functions and nodes.

Every combination of n and L has an associated multiplication of radial and angular components that make up the wave-function.

$$\Psi(r, \theta, \phi) = (\text{radial component}) \cdot (\text{angular component}) \tag{4}$$

And then every wave-functions have points in the radius or angles that have $\Psi = 0$ known as nodes; each wave-function has:

1. Radial nodes: n - 1 - L
2. Angular nodes: L.

Example lecture problem.

Problem: What is the energy of the light absorbed when an electron in a hydrogen atom makes the following transitions: (a) n = 1 to n = 4; (b) n = 3 to n = 8; (c) n = 2 to n = 4.

Solution: Recall

$$E_n = \frac{-hcR}{n^2} \implies \Delta E_{n_1 \to n_2} = |-hcR\left(\frac{1}{n_1^1} - \frac{1}{n_2^2}\right)| \tag{5}$$

Thus,

1. (a) $= |-hcR\left(\frac{1}{1^2} - \frac{1}{4^2}\right)| = 2.04 \cdot 10^{-18}$
2. (b) $= |-hcR\left(\frac{1}{3^2} - \frac{1}{8^2}\right)| = 2.08 \cdot 10^{-19}$
3. (c) $= |-hcR\left(\frac{1}{2^2} - \frac{1}{4^2}\right)| = 4.09 \cdot 10^{-19}$

Olympiad problem.

Problem: How many electrons in a ground-state As atom in the gas phase have quantum numbers $n = 3$ and $l = 1$?
Solution: Since $n = 3$ and $L = 1$, we are looking at the 3p block for astatine; it has 3 electrons in the 3p block.