Quantum Chemistry

So far:

- Atom (basic unit)
- Dalton's Model of the atom (different types of atoms)
- Thomson Model (add electrons)
- Rutherford (add the nucleus)

Bohr:

- added fixed energy orbits for electrons at fixed distance from the nucleus
- the reason for fixed orbits is due to resonant de Broglie wave patterns which introduces in integer value to the description of the hydrogen atom (i.e. n = 1,2,3,4,5 etc) where n is the number of deBroglie wave lengths
- this is a quantum mechanical property

Quantum Mechanical Model:

- uses the same value of n as did Bohr, but with **MUCH** more sophisticated mathematics
- it also introduces three more quantum numbers (in addition to n)
- best description we have at present of the atom and how electrons behave in the atom – lays the theoretical basis for the shape of the periodic table
- in this model electrons are described using wave functions (i.e. the electron is a wave not a particle)

QUANTUM NUMBERS: there are four quantum numbers that are used to describe all behaviours of electrons confined to an atom.

1. Principle Quantum Number

- has the symbol n (this is the n in the equations we have used)
- represent the number of de Broglie wavelength for the orbiting electron
- allowed values are: $\{n \in I \mid 0 < n\}$

2. Angular Momentum Quantum Number

- has the symbol ℓ
- represents the angular momentum of the orbiting electrons
- allowed values are: $\{ \ell \in I \mid 0 \leq \ell < n\}$
- eg if $n = 1$ $\ell = 0$

  if $n = 2$ $\ell = 0,1$

  if $n = 3$ $\ell = 0,1,2$
- other names for l are as follows:

ℓ value	0	1	2	3
other name	s	p	d	f

- **Magnetic Quantum Number:**

- has the symbol m_ℓ

- represents the magnetic field that is generated by the motion of the orbiting electron (electromagnetic principle)

- allowed values: $\{ m_\ell \in I \mid -\ell \leq m_\ell \leq \ell \}$

eg if $n = 1$ $\ell = 0$ $m_\ell = 0$

if $n = 2$ $\ell = 0$ $m_\ell = 0$
$\ell = 1$ $m_\ell = -1, 0, 1$

if $n = 3$ $\ell = 0$ $m_\ell = 0$
$\ell = 1$ $m_\ell = -1, 0, 1$
$\ell = 2$ $m_\ell = -2, -1, 0, 1, 2$

if $n = 4$ $\ell = 0$ $m_\ell = 0$
$\ell = 1$ $m_\ell = -1, 0, 1$
$\ell = 2$ $m_\ell = -2, -1, 0, 1, 2$
$\ell = 3$ $m_\ell = -3, -2, -1, 0, 1, 2, 3$

4. **Spin Quantum Number:**

- symbol is m_S

- the only independent quantum number – inherent to the electron

- represents the spin possessed by the electron (like the spin of the earth as it orbits)

- allowed values: $\{m_S \in R \mid m_S = \pm \frac{1}{2}\}$

Additional Points:

Aufbau Principle: when adding electrons to a bare nucleus to build a neutral atom, electrons will fill the lowest atomic energy levels first (build outwards)

Pauli Exclusion Principle: no two electrons in a multi-electron atom can have all four quantum numbers the same (this would place the electrons in exactly the same place), at least one quantum number must be different

Hund's Rule: electrons of equal energy (same n value) will fill orbitals one electron at a time first)

Other Terms Concepts or Models You Should Know:

- Heisenberg uncertainty principle
- photoelectric effect
- quantum hypothesis
- line spectra
- absorption spectra
- emission spectra
- Thomson
- Rutherford
- Bohr