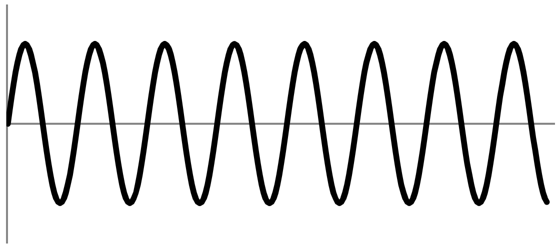
QUANTUM CHEMISTRY

Model 1: Light and Waves

The picture below shows a light wave. The wavelength is the distance between peaks (or the distance between troughs). The amplitude is the height of the wave.

We cannot see these waves. Instead, our eyes detect the ***intensity*** of the light which is given by the ***square*** of the wave.

Squaring means multiplying the wave at each point by itself, remembering that positive × positive and negative × negative are both positive.



Critical thinking questions

1. Label the diagram showing how the wavelength (λ) and the amplitude (A) of the wave can be measured.

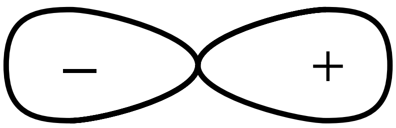
2. Put an asterisk ('*") to mark the positions where the wave is zero. These are 'nodes'.

3. Peaks are where the wave is positive. Troughs are where the wave is negative. Labels these with "+" and "–" signs respectively. *Lightly* shade the "–" areas.

4. On top of the picture, draw a sketch of the ***intensity*** of the light.

Model 2: Electron Waves

The picture below is a lobe representation of a 2-dimensional wave for an electron. The line encapsulates 90% of the electron density. We cannot see or measure the wave. Instead, the electron density can be measured and this is given by the ***square*** of the wave.



Critical thinking questions

5. Mark the position of the node and *lightly* shade the "–" area.

6. Draw a sketch of the ***electron density*** for this electron.

Model 3: Atomic Orbitals and Quantum Numbers

The wave functions for electrons in atoms are given the special name 'atomic orbitals'.

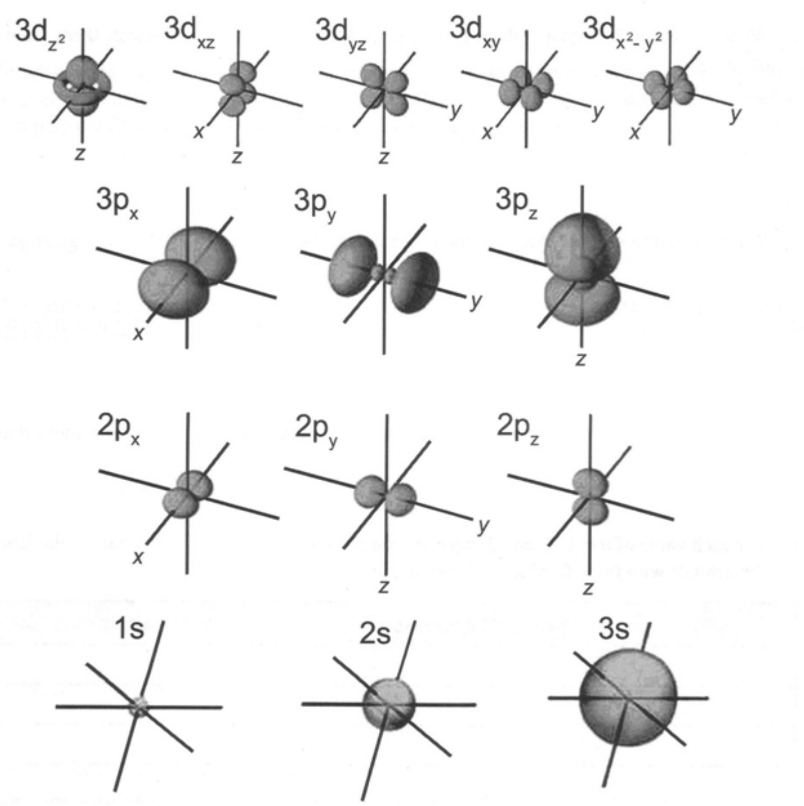
As explored in worksheet 1, the energy levels of hydrogen-like (one-electron) atoms are determined by a single quantum number, *n*. For other atoms, more quantities are involved in determining the shape and orientation of the atomic orbitals, these are the *angular momentum quantum number, l,* and *magnetic quantum number,* m_l.

Name	Characterizes	symbol	Allowed values
Principal	Size Energy	*n*	***n* = 1, 2, 3, … (to infinity)**
Angular Momentum	Shape Energy in multi-electron atoms *l* planar nodes	*l*	***l* = 0, 1, 2,… *n*-1**
Magnetic	Orientation	m_l	**m_l = -*l*, 1-l,…0… *l*-1, +*l***

Orbitals are labelled with their *n* value and a letter to represent the *l* value: *l* = 0, 1, 2 and 3 correspond to *s*, *p*, *d* and *f* respectively.

For example, for *n* = 2:

- *l* has values from 0 to *n* – 1. When *n* = 2, *n* – 1 = 1 and so *l* = 0 and 1 only.
- m_l can have values from –*l* to +*l*.
  - When *l* = 0, m_l = 0 only. There is only one orbital with *n* = 2 and *l* = 0. It is labelled 2*s*.
  - When *l* = 1, m_l = -1, 0 and +1 only. There are three orbitals with *n* = 2 and *l* = 1. They are called the 2*p* orbitals.
- To distinguish the individual orbitals, a subscript is added with gives an indication of the orientation of the orbitals in space. The three 2*p* orbitals are called $2p_x$, $2p_y$ and $2p_z$ as they point along the *x*, *y* and *z* axes respectively.



Critical thinking questions

1. What are the characteristic shapes of *s*, *p*, and *d* orbitals?

2. Which quantum number identifies the shape of an orbital?

3. For each value of n = 1, 2, and 3, what are the possible values for l, and what labels correspond to these orbitals?.

n	**Possible *l* values**	**Orbital labels**
1		
2		
3		

4. For each value of l = 0, 1, 2, what are the possible values for m_l, and what are the labels for the orbitals with this set of m_l values?

l	**Possible m_l values**	**Number of orbitals in the set**
1		
2		
3		

5. Which orbitals have a plane where the probability of finding the electron is zero (a *nodal plane*)?

6. What is the relationship between the value of the angular momentum quantum number and the number of such *nodal planes*?

Model 4: Electronic Configurations in Atoms

Critical thinking questions

7. Look up definitions for the following and write down your own definition in one or two sentences.

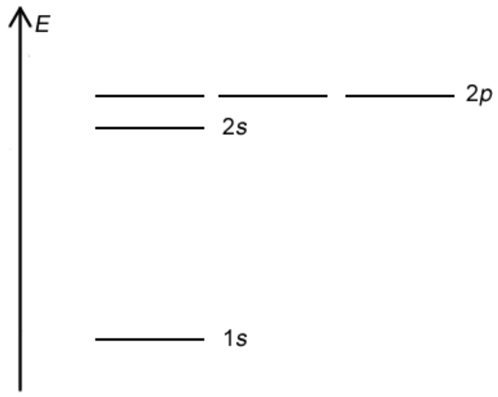
   (a) *The Aufbau Principle*

   (b) *Pauli Exclusion Principle*

   (c) *Hund's Rule*

Possible sources: http://en.wikipedia.org/wiki/Aufbau_principle, http://en.wikipedia.org/wiki/Hund's_rule and http://en.wikipedia.org/wiki/Pauli_exclusion_principle

8. Fill in the ground state electronic configuration for a carbon atom on the diagram below.



(a) Why is the electron configuration of carbon *not* $1s^2\ 2s^3\ 2p^1$?

(b) Why is the configuration *not* $1s^2\ 2s^2\ 2p_x^2$?