QUANTUM THEORY - Beginnings

Derived from the study of light! (Kirchhoff)

1. Blackbody Radiation – the colour of light given off by an object solely due to its temperature.

(Figure 2 Colour distribution of an object as it gets hotter)

Why does the intensity increase but not increase to infinity?
Why does the shape of the graph gradually shift to the UV side?
Why does the shape drop off at the UV region?

Classical theory – as the frequency increases the wavelengths get smaller and the energy gets higher.

Why doesn't the graph continue to increase to infinity?

Max Planck was able to mathematically describe (beyond my ability) the relationship of the light and intensity graph of blackbody radiation by making a radical hypothesis – the energy of the light frequencies are all multiples of some smallest packet of energy – energy is not continuous – it is QUANTIZED.

(Planck originally dismissed this idea but it worked, Einstein was also involved and supported this idea)

2. Photoelectric Effect – light of certain frequencies shone onto some metals cause the metals to give off electrons. (calculators)

Light lower frequencies (colours) did not produce a current even at huge intensities. Light at higher freqencies could produce electricity even at low intensities.

Light (specifically colours) must be made up of specific energy packets called photons with their own energy level. This is an example of QUANTIZED energy.

Both blackbody radiation and the photoelectric effect proved that classical physics does not work at the atomic level (common sense no longer applies so don't even try to use logic).

Bohr Atomic Theory

Rutherford – the electron was circling the nucleus – BUT – a moving charge radiates energy (radio towers, antennas etc.)

Bohr – if energy is quantized for electrons that can explain why Rutherford's atoms did not implode – proof – Emission Spectra

(demo-what do you see)

Colours represent very discrete energy being emitted from an excited electron dropping down to the ground state

For an electron to jump a level it must absorb the exact amount of energy between the levels – no partial jumps allowed!! Also the electron jumps from one level to the next without ever being in between.

Bohr's model explained the hydrogen spectra and also predicted the spectral lines in the IR an UV regions

Unfortunately the theory did not agree with the empirical evidence for line spectra of elements that have greater than 1 electron (it is a starting point though)

QUANTUM NUMBERS (pg 181)

Based on Atomic Spectra Analysis!

Bohr – Described electrons jumping up and down from specific energy levels. This is the principal quantum number. Relates to the period number.

Arnold Sommerfeld – Secondary quantum number. Each spectral line is actually several lines close together

Pieter Zeeman – Spectral analysis of gases in a magnetic field created more spectral lines – Magnetic quantum number – orbits can also be at various angles

Wolfgang Pauli – electrons can have 2 different spins. Similar but different magnetic fields (magnets) – Spin quantum number

All values are quantized – whole number values

Each value has a rule – page 184 *copy rules*

n	1 to infinity
ℓ	0 to n-1
m_ℓ	$-\ell$ to $+\ell$
m_s	+1/2 and -1/2

At this point the electron still has an orbit with a size, shape, orientation and energy value

Review:
What clues in the 3 separate experiments provided support for the idea of quantum theory?

Why do we need to include four quantum numbers?

What does each quantum number describe?

How many electrons can exist in the 4^{th} energy level?

Atomic Structure and the Periodic Table

- Bohr Rutherford theory described elements 1-20. Quantum can include all atoms of the periodic table
- Each electron can be described by the four quantum numbers.
- We will be concerned mainly with the first 2 quantum numbers (n and ℓ) but we need to make some changes

Principal quantum number = shell
Secondary quantum number = subshell
Third quantum number = number of orbitals
Fourth quantum number = 2 electrons per orbital

- Electrons in the same sublevel all have the same energy
- Secondary quantum number changes to letters

ℓ-Number	Letter	Orbitals (m_ℓ)
0	s	1
1	p	3
2	d	5
3	f	7
4	g	9

Ex. quantum numbers ➔ Atomic Orbital
n = 2, l = 1 2p

- For any main energy level / shell the subshell energy always follows this pattern s < p < d < f
- As the atoms become larger the subshells of different energy levels begin to overlap

Energy Level Diagram and Electron Configurations

1. Figure 2 page 187 – that is what they should look like

2. Rules page 188
   a. Pauli Exclusion Principle
   b. Aufbau Principle
   c. Hund's Rule

3. Figure 5 page 185 – order of energy levels

Examples… Try Some…

4. Electron Configurations pg 192-193

Examples… Try Some…

Explaining the Periodic Table, Ion Charges, Magnetism, and Exceptions to the Rules

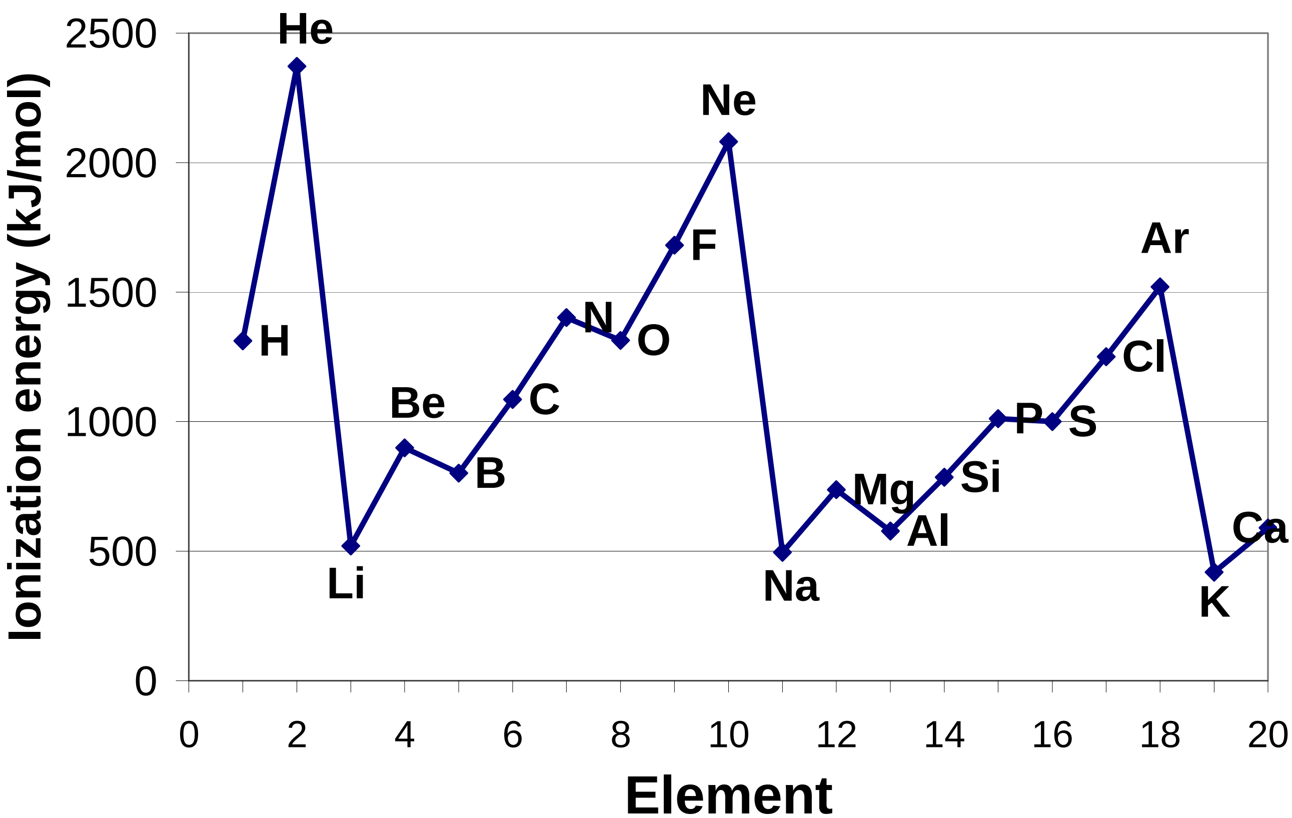
1. regions of the periodic table

2. losing and gaining electrons

3. unpaired electrons … magnets

4. Full d subshell or half d subshell is more stable than full s subshell

5. Ionization Energy Trends



Wave Mechanics and Orbitals

Quantum theory and electron configurations help explain atomic structure and periodic trends but it can also give some idea of what the electron is doing inside the atom.

Louis DeBroglie (1923)

- (Already understood – photon is a quantum of energy, light has wave and particle duality – we think light as a wave.)

- He suggested that all particles should also have wave like properties. Large masses would have an insignificant wave like property but particles as small as electrons could have a particle and wave duality

- Based on Max Planck's and Albert Einstein's work and experiments, such as the double slit experiment. (a beam of electrons that pass through a double slit cause interference patterns similar to light)

Schrodinger
- Described the wave function of electron
- Electrons can only have quantized energies
- Whole numbers of wave lengths would fit in an orbit
- Provided the mathematical framework that included the first three quantum numbers to describe the

electron's orbital and that each orbital could hold a maximum of 2 electrons
  - n = relative distance from the nucleus
  - ℓ = shape of the orbital
  - m_ℓ = orientation of the orbital

Heisenberg Uncertainty Principle
- Act of looking interferes with measurement
- Impossible to know that position and speed of a particle

Electron Probability Density
- Electron clouds - derived from wave equation
- Reinforced the idea of an orbital with a probability of electron location instead of orbit that assumed a definite path and location
- Each orbital had a specific shape (s = shere; p= dumbbell; d = pairs of dumbbells; f = weirder shapes)

Limitation of Quantum Mechanics
- Limits to what we can observe
- Rules are not the same at subatomic levels
- Superconductors-still don't know how they work just that they do

HW. R&MN 3.3-3.5 3.3 Q 1,5,6,7 3.4 Q 2,6,10,13a-c 3.5 Q 2-5

Quantum Theory Challenge