

## 3.1 Physical Chemistry

includes:

- atomic structure
- amount of substance
- structure and bonding
- energetics
- kinetics
- equilibria
- redox
- (the following are A2 only)
- thermodynamics
- rate equations
- Kp
- electrode potentials
- acids and bases

### 3.1.1 Atomic Structure

Section: Completed?

fundamental particles yes

mass number, isotopes no

electron configuration yes

#### Fundamental Particles

plum pudding model a sphere of positive charge with balls of negative charge embedded within: essentially looks like a plum pudding

electron shell model small, dense positive charged nucleus with protons and neutrons; electrons orbit in shells

Rutherford's gold foil experiment (Geiger-Marsdon experiment)

shot alpha particles through thin gold foil

- vast majority pass through

- few deflected by large angles

- ~1/10000 deflected back to side it came from

Rutherford's conclusions

- nucleus is small, positive, dense, massive (heavy)

- most of the atom is empty space

relative mass proton/neutron = 1; electron = 1/1840

relative charge proton = +1; neutron = 0; electron = -1

### Electron Configuration (1.1)

four atomic orbitals s, p, d, f

s orbitals are spherical

p orbitals are dumbbell shaped

(go practice some of these questions on paper)

spin electrons in same orbital have opposite spin

first ionisation energy *energy required to remove 1mol of electrons from 1mol of gaseous atoms*

always refer to "1 mole"

lower ionisation energy = easier to form ion

general equation (ionisation energy)  $X_{(g)} \rightarrow X^+_{(g)} + e^-$

state symbols are important!!

#### factors affecting ionisation energy:

> nuclear charge more protons = more positively charged = stronger  $e^-$  attraction = higher ionisation energy

> distance from nucleus  $e^-$  closer to nucleus = stronger attraction = higher ionisation energy

> shielding higher num orbitals between nucleus and outer  $e^-$  = weaker attraction = lower ionisation energy

#### trends in ionisation energy

down a group: decreases

> each element down a group has an extra  $e^-$  shell

## Electron Configuration (1.1) (cont)

- extra inner shells shield outer  $e^-$  from attraction to nucleus

- extra shells also mean outer  $e^-$  are further from nucleus

across a period generally increases

> proton num increasing

- which means there's a stronger nuclear attraction

> little extra shielding or nuclear distance

- as all elements across period have same number of shells

(across a period cont) focusing on period three elements

dip between group 2 and 3 ie between Mg and Al

Mg is  $1s^2 2s^2 2p^6 3s^2$

Al is  $1s^2 2s^2 2p^6 3s^2 3p^1$

Al outer  $e^-$  is in 3p orbital

- 3p has a slightly higher energy level so is slightly further from nucleus

- shielded by 3s orbital

so ionisation energy drops slightly

provides evidence for electron subshell theory

dip between group 5 and 6 ie P and S

P is  $1s^2 2s^2 2p^6 3s^2 3p^3$

S is  $1s^2 2s^2 2p^6 3s^2 3p^4$

## Electron Configuration (1.1) (cont)

$e^-$  from S is being removed from orbital with two  $e^-$

repulsion between  $e^-$  in same orbital means  $e^-$  are easier to remove

(P has single occupied orbital so no added repulsion)

## equations and associated calculations

### Mass num, Isotopes (1.1)

mass num (A) = num protons + num neutrons

atomic num (Z) = num protons

isotope atom with same number of protons but a different number of neutrons

### mass spectrometry

#### stage 1: ionisation

the sample can be ionised by either *electrospray* or *electron impact*

*electrospray* Sample (X) is dissolved in violent solvent; injected through a hypodermic needle to produce a fine mist; tip of needle is attached to positive terminal of high voltage power supply; ionised by gaining a proton; solvent evaporates;  $XH^+$  ions attracted to negative plate - accelerated

*electron impact* sample (X) is vaporised; high energy electron fired from electron gun - knocks off one outer shell electron from each particle;  $1^+$  ions attracted to negative plate - accelerated

#### stage 2: acceleration



## Mass num, Isotopes (1.1) (cont)

positive ions accelerated using electric field so all ions have the same kinetic energy ( $E_k$ )

$$E_k = \frac{1}{2}mv^2 \quad (E_k = \frac{1}{2} * \text{mass} * \text{velocity}^2)$$

lighter ion = higher velocity

stage 3: flight tube (drift region)

lighter ions move faster than heavier ones ( $E_k$  is the same)

lighter ions reach the detector first

$$s = vt \quad (\text{distance} = \text{velocity} * \text{time})$$

stage 4: detection

positive ion hits negatively charged plate

ion gains an electron

why use mass spec?

## moles, Avagadro const

Avogadro constant      number of particles in a mole

## empirical and molecular formula

empirical formula      simplest whole number ratio of atoms of each element in a compound

molecular formula      actual number of atoms of each element in a compound

## 3.1.2 Amount of Substance

Section:      Completed?

Mr, Ar      yes

moles, Avogadro const      no

ideal gas equation      no

empirical and molecular formula      no

equations and associated calculations      no

## Ar, Mr (1.2)

relative atomic mass (Ar)      mean mass of an atom of an element divided by  $\frac{1}{12}$  mean mass of atom of  $C^{12}$  isotope

relative molecular mass (Mr)      mean mass of molecule of a compound divided by  $\frac{1}{12}$  of mean mass of an atom of  $C^{12}$

known as relative formula mass for ionic compounds

## ideal gas equation

equation:       $pV = nRT$

## 3.1.3 bonding

Section:      Completed?

ionic      no

covalent, dative covalent      no

metallic      no

physical properties      no

shapes of molecules and ions      no

bond polarity      no

forces between molecules (imf)      no

