tutorial question and additional work

chapter 1

section 1.1-1.3

self test 1.1

self test1.2

read 1.3d-1.3g

(see section 1.3 for explanation)

section 1.5-1.6

Self test 1.7-1.11

Exercises 1.9-1.15, 1.17-1.26, 1.28-1.31 (pp 32-33)

section one general review

Quantum numbers

Introduction

Orbitals are a spacial distribution of electron density.All energy states of electrons within atoms are negative by convention, (as the are considered to be the minimum energy necessary to free that electron from its parent atom)

principle quantum number

n

range

$n \in \mathbb{Z}^+ | n \geq 1$

NOTE: although n is theoretically unbounded values greater than five have not yet been observed in reality.

details

Identifies a specific energy state Orbitals of the same quantum number form an part of the same electron shell

Azimuthal quantum number (orbital angular momentum number)

l

encoding

values of l are given letters for identification

$0 \rightarrow s$

$1 \rightarrow p$

$2 \rightarrow d$

$3 \rightarrow f$

range

$l \in \mathbb{Z} \quad | \quad 0 \leq l \leq n - 1$

details

determines the size and shape of the sub shell/ determines the area around the nucleus which the electron may inhabit.

Magnetic quantum number

m_s

range

$m_l \in \mathbb{Z} \quad | \quad -l \leq m_l \leq l$

details

determines the three dimensional orientation of sub shell.

spacial orientations

P orbitals have three possible orientations

X,Y,Z

D orbitals have five possible orientations

$xy, xz, zy, z^2, x^2 - y^2$
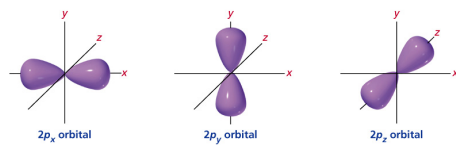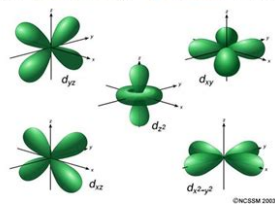
F orbitals have seven possible orientations.

Figure 1: p orbital orientations

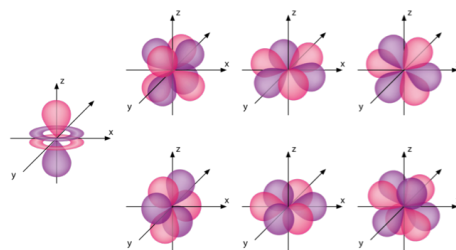Figure 2: d orbital orientations

Figure 3: forbital orientations

magnetic spin number m_s

range

$m_s \in \left(\frac{+1}{2}, \quad \frac{-1}{2} \right)$

details

determines the direction of spin/ gyration of the electron in regard to the magnetic axis of the atom.

representation diagrams

Standard representation

nl^s

Where:

```
n= principle quantum number
l= azimuthal number
x= number of electrons within the l subshell.
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Condensed representation

[noble gases] valence shell in standard representation

Pauli Exclusion Principles.

no too electron within one atom can have the same set of quantum numbers

Aufbau Priciple

electrons must always fill into the lowest energy levels available, this provides the sable ground state for of the atom.

Hundu's

degenerate orbitals must always be filled singly and by electrons with the same spin number before 2 electrons may fill the same orbital, and opposite spin numbers are permissible.
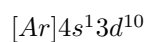
exchange with higher sub-shells

electrons are most lightly to be promoted into higher sub-shells when in doing so they can lead to completely singly filled, or completely double filled orbitals.

examples

Chromium

$[Ar]4s^13d^5$

Copper

$[Ar]4s^13d^{10}$
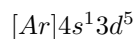
Effective nuclear charge

effective nuclear charge is the charge exerted on a given electron within an atom by the (positively charged) nucleus of that atom

shielding

shielding is the reduction of the full nuclear charge which and in isolation the nucleus would exert on an electron.

$Z_{eff} = Z - \sigma$

where: Z_{eff} = effective nuclear charge Z= nuclear charge σ = shielding effect of other electrons.

this shielding effect is due to the present of other electrons within the atom which repel the electron in question reducing the net attractive force towards the nucleus which it feels.

(this reduction is often expressed as the reduction of $Z \quad to \quad Z_{eff}$)

penetration

the potential for the presence of an electron inside shells of other electrons. (?)

Slater's Rules

Estimated value for sigma

final electron is in a s or p orbital

- n-1 electrons contribute 0.85
- ns and np electrons contribute 0.35 to σ
- n-2 or lower electrons contribute 1.0 to σ

final electron is in a d or f orbital

- nf and nd electrons contribute 0.35 to σ
- electrons in lower shells contribute 1. to σ

Trends

#1

The closer to the nuclear an electron is the smaller the difference between Z and Z_{eff} will be.

#2

In terms of energy levels d>p>s

summary

Increases up and across the periodic table.

Exceptions

Hydrogen

the 2s and 2p orbitals have the same energy level.

potassium and calcium

4s energy level is lower than the 3p (?) (see section 1.3 for explanation)

Periodic table

History

first proposed in 1869 based on increased atomic weight.

families of elements with similar chemical properties (groups) with gaps in these families allowing for prediction.

classifying elements.

Metallic character

metals

Good Conductors High lustre generally solid malleable ductile

metalloids

goo semiconductors some High lustre some low lustre generally solid some malleable some not malleable some ductile some not ductile

Non metals

not malleable low to no lustre not ductile poor conductors brittle gas

mixtures

metals and metals

alloys

non metals and metals

hard
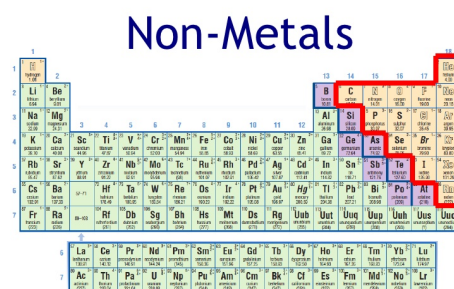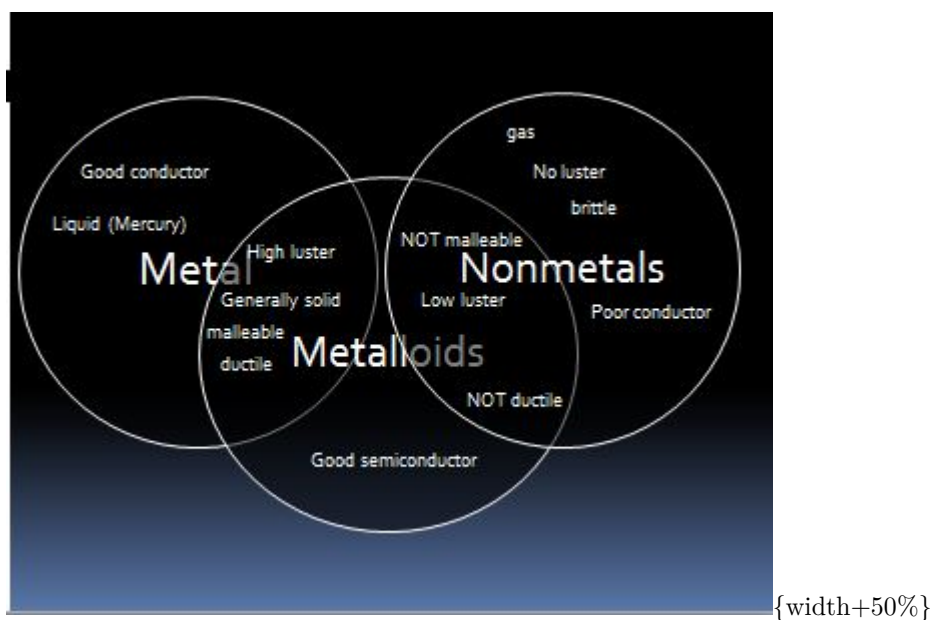
non metals and non metals

volatile

Figure 4: MetallicCharacter

{width+50%}

Atomic properties

Atomic and Ionic radii

radii measures are not very precise

Trends

increases down group and decreases across period.

this trend is offset between strontium and barium because Z_{eff} is increased as there are more protons but few effectively shielding electrons. For orbitals are very bad at shielding (?)

Lanthanoid Contractions

D block elements don't tend to expand or shrink properly

Covalent radius

half of the difference between centres of atoms in covalent bond (there is some overlap)

Ionic Radius

radius of atoms within ionic compounds, an average must be taken over many different ionic compounds as there is no reason to assume it would be half way between the atom centres.

mono atomic cations

monatomic cations are smaller than the parent atoms, as there is less shielding but equal nuclear charge so high effective nuclear charge.

monatomic anions

monoatomic anions are larger than their parent ions because they experience more shielding so lower effective nuclear charge

Metallic

half of the distance between atoms in a solid.

Ionization Energy

Ionisation energy is the energy require to remove an electron from and atom (the standard is measure in gaseous conditions)

Trends

Ionisation energy increases up a group and across a period.

Correlated with atomic radii, but there are often exceptions depending on which sub-shell the electron in question is removed from.

Electron Affinity

Electron enthalpy gain $\Delta_{eg} H^\circ$

$$\Delta_{eg} H^\circ \quad = -E_a - \frac{5}{2RT}$$

E_a is determined by the energy of the lowest unfilled or half filled orbital.

E_a can be high if the electron added can experience a strong effective nuclear charge.

ELectronegativity χ

the power of an element to attract electrons towards itself when it is part of a compound.

Mulliken Electronegativity (χ_M)

Atoms with higher ionisation energies and electron affinities are more likely to gain electrons

Atoms with low ionisation energies and low electron affinities are more likely to lose electrons.

$\chi_M = (I + E_a)$

Pauling Electronegativity

Pauling energetics is related to the energetic of bond formation

If $BE(A - B) > \frac{1}{2}(BE(A - A) + BE(B - B))$ then the covalent bond contains an ionic contribution

Equation (?)

Trends

related to atomic size and electron configuration

increases up group and across period.

###Polarizability the ability of an atom to be distorted by an electric field

polarizable

large highly charged anions are highly polarisable.

Cations that do not have noble gas configuration are easily polarisable.

polarizing or polarizing ability.

small highly charge cations have high polarisability.