

tutorial question and additional work

chapter 1

section 1.1-1.3

self test 1.1

self test 1.2

read 1.3d-1.3g

(see section 1.3 for explanation)

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 they 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.

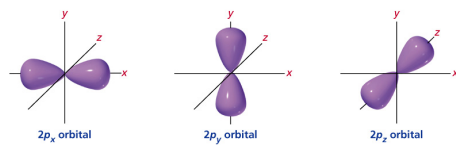
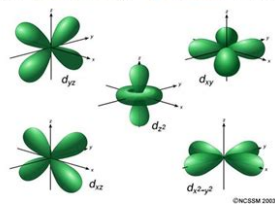


Figure 1: p orbital orientations

“d” shape (cloverleaf) – 5 orbital orientations (m)



“f” shape (indeterminate) – 7 orbital orientations (m)

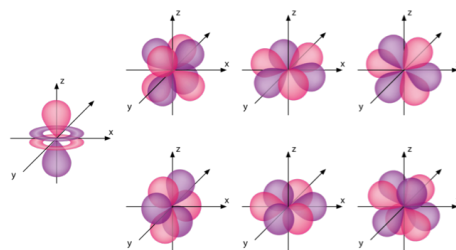


Figure 3: f orbital orientations

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.

Condensed representation

[noble gases] valence shell in standard representation

Pauli Exclusion Principles.

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

Aufbau Principle

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

Hund'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 likely 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 $[Ar]4s^13d^5$

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 presence 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 to 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)