Mr G's Little Book on

Quantum

Numbers

Summary

In any atom of a specific atomic number - the number of protons in the nucleus - there is a unique pattern of orbiting electrons. Each electron has a specific "address" in the electron cloud defined by 4 quantum numbers.

Quantum Numbers

The **first quantum numbers** is **n** a positive integer giving the overall relative energy of each orbital.

Electrons with the same n value are said to be in the same electron shell.

n = 1 is called the K shell

n = 2 is called the L shell

n = 3 is called the M shell

n = 4 is called the O shell etc.

The **second quantum number** is ℓ the azimuthal quantum number roughly the shape of the orbital.

ℓ can take the values 0 to n–1.

for n = 1 ℓ = 0 called the s subshell

for n = 2 ℓ = 0 called the s subshell

and ℓ = 1 called the p subshell

for n = 3 ℓ = 0 called the s subshell

and ℓ = 1 called the p subshell

and ℓ = 2 called the d subshell

for n = 4 ℓ = 0 called the s subshell

and ℓ = 1 called the p subshell

and ℓ = 2 called the d subshell

and ℓ = 3 called the f subshell

While commonly thought **s** stands for spherical and **p** polar these letters derive from the original spectrograph investigations and stand for **s**harp, **p**rincipal, **d**iffuse and **f**undamental. These terms have little relevance now. Subsequent subshells are just labelled g for ℓ = 5 and h for ℓ = 6 though these do not occur naturally in nature.. Never let it be assumed these sub-orbitals can actually be seen. However by solving certain equations a probability density can be ascribed to each which may be interpreted as shape.

The **third quantum number** is m and roughly equates to the angular momentum vector – that is the orientation the sub-shell and can take The values can take $-\ell$ to $+\ell$.

For ℓ = 0 m = 0

and the s orbital is a sphere

For ℓ = 1 m = –1, 0 or +1

and the three p orbitals are all figure of eight paths, one along along each axis.

For $\ell = 2$ m = –2, –1, 0, +1 or +2

Four of the five **d** orbitals are clover leaf in shape and the fifth a figure of eight with a halo round the middle.

This pattern continues although the shape of each **f** suborbital becomes more complex.

The **fourth quantum number** is **s,** the angular momentum of the electron and colloquially called "spin" though it should never be supposed that anything is actually spinning.

Spin down is defined as –½ and spin up as +½.

Electrons having the same first 3 quantum numbers will then usually pair up for the fourth though exceptions are detailed later.

Shell "Capacity"

No two electrons can have the same 4 quantum numbers so there is a theoretical maximum to the number of electrons in each shell.

K shell is 1s and because there is only one m value maximum is

$(1) \times 2 = 2$

L shell is 2s and 2p and because there are 3 **m** values maximum is

$(1+3) \times 2 = 8$

M shell is 3s, 3p and 3d and because there are 5 **m** values maximum is

$(1+3+5) \times 2 = 18$

N shell is 4s, 4p, 4d and 4f and because there are 7 **m** values maximum is

$(1+3+5+7) \times 2 = 32$

N shell is 5s, 5p, 5d, 5f and a theoretical 5g. Because there are 7 **m** values the theoretical maximum is

$(1+3+5+7+9) \times 2 = 50$

Although sub-orbital 5g does not occur shells O, P and Q do occur to accommodate lower energy sub orbitals.

Maximum Practical Shell Size

The outer configuration of electrons largely determines the chemical properties of the element. The periodic table consists of columns and rows. Columns are labelled as Groups 1 to 18 and contain similar outer electron configurations but in increasingly higher energy shells.

The rows are labelled Period-1 through to Period-7 each ending with an inert gas having the most stable outer configuration of s^2 p^6 - that is 8 electrons called an octet

It is worth analysing the actual electron distribution for the inert gases.

Helium Total 2

K shell 2

Neon Total 10

K shell 2 L shell 8

Argon Total 18

K shell 2 L shell 8 M shell 8

Krypton Total 36

K shell 2 L shell 8 M shell 18

N shell 8

Xenon Total 54

K shell 2 L shell 8 M shell 18

N shell 18 O shell 8

Radon Total 86

K shell 2 L shell 8 M shell 18

N shell 32 O shell 18 P shell 8

Oganessium Total 118

K shell 2 L shell 8 M shell 18

N shell 32 O shell 32 P shell 18

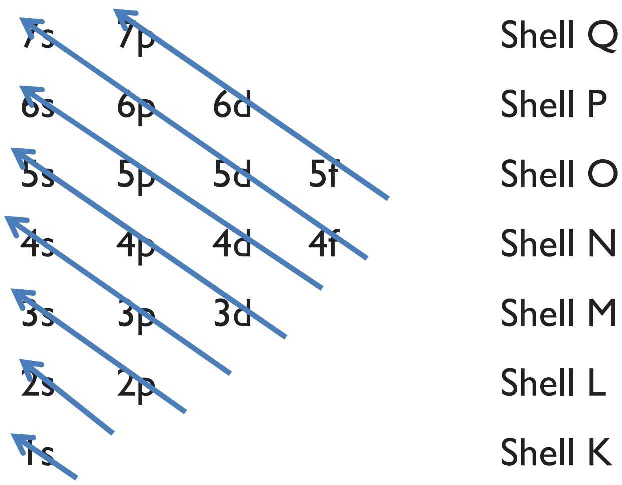
Q shell 8

So the maximum number electrons in any shell is 32

Aufbau Rules

In the ground state of an atom, electrons fill atomic orbitals of the lowest available energy level before occupying higher energy levels.

The increasing energy levels generally follow a specific pattern



giving the sequence as

1s>2s>2p>3s>3p>4s>3d>4p>5s etc.

Exceptions to Aufbau Rules

Electrons join sub orbitals from lowest to highest energy levels but where two suborbitals have very similar energy level electrons will join each in turn before pairing up.

Thus at higher energy levels there is an increasing overlap between sublevels leading to “exceptions” to the expected pattern. The author analysed these in 1990. The full chart is available as an attachment to this booklet but the exceptions are summarised here.

Chromium is	[Ar] $4s^1$ $3d^5$
and not	[Ar] $4s^2$ $3d^4$
Copper is	[Ar] $4s^1$ $3d^{10}$
and not	[Ar] $4s^2$ $3d^9$
Niobium is	[Kr] $5s^1$ $4d^4$
and not	[Kr] $5s^2$ $4d^3$
Molybdenum is	[Kr] $5s^1$ $4d^5$
and not	[Kr] $5s^2$ $4d^4$
Ruthenium is	[Kr] $5s^1$ $4d^7$
and not	[Kr] $5s^2$ $4d^6$
Rhodium is	[Kr] $5s^1$ $4d^8$
and not	[Kr] $5s^2$ $4d^7$
Palladium is	[Kr] $5s^0$ $4d^{10}$
and not	[Kr] $5s^2$ $4d^8$
Silver is	[Kr] $5s^1$ $4d^{10}$
and not	[Kr] $5s^2$ $4d^9$
Gadolinium is	[Xe] $6s^2$ $4f^7$ $5d^1$
and not	[Xe] $6s^2$ $4f^8$ $5d^0$
Platinum is	[Xe] $6s^0$ $4f^4$ $5d^{10}$
and not	[Xe] $6s^2$ $4f^8$ $5d^8$
Gold is	[Xe] $6s^1$ $4f^{14}$ $5d^{10}$
and not	[Xe] $6s^2$ $4f^8$ $5d^9$
Actinium is	[Xe] $7s^2$ $5f^0$ $6d^1$
and not	[Xe] $7s^2$ $5f^1$ $6d^0$
Thorium is	[Xe] $7s^1$ $5f^0$ $6d^2$
and not	[Xe] $7s^2$ $5f^2$ $6d^0$
Protectinium is	[Xe] $7s^2$ $5f^2$ $6d^1$
and not	[Xe] $7s^2$ $5f^3$ $6d^0$
Uranium is	[Xe] $7s^2$ $5f^3$ $6d^1$
and not	[Xe] $7s^2$ $5f^4$ $6d^0$
Neprunium is	[Xe] $7s^2$ $5f^4$ $6d^1$
and not	[Xe] $7s^2$ $5f^5$ $6d^0$
Curium is	[Xe] $7s^2$ $5f^7$ $6d^1$
and not	[Xe] $7s^2$ $5f^8$ $6d^0$

Most of these elements you’ve never heard of but one might reflect that three elements, Silver, Gold and Platinum, only exist because having set up all the laws of the Universe someone decide that they then needed to be adjusted.

- On My TI Calculator what's the difference between Sx and σx?

  It's not what I thought for the first 40 years of the scientific calculator

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  An investigation into the pitfalls of medical screening

- Hypercomplex Numbers

  Instead of making $i^2 = -1$ *as in complex numbers what if we just make* $i^2 = 1$

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