Atomic Physics Glossary

A

The symbol for mass number - the number of nucleons (protons and neutrons) in an atom's nucleus.

Allotrope

An allotrope is a way of arranging atoms from a single element. For example, graphite, diamond and buckminster fullerine are all allotropes of carbon. The only difference between these forms of the element is the arrangement of carbon atoms. In graphite the atoms are arranged into layers that can slide over each other. Diamond is a rigid structure of tetrahedrons (3 sided pyramids). In buckminster fullerine the carbon atoms are arranged into hollow spheres made up of 60 atoms. Ozone is an allotrope of oxygen - a molecule containing 3 oxygen atoms. (Most atmospheric oxygen is O_2 - a molecule containing two oxygen atoms).

Atom

An atom consists of a nucleus surrounded by electrons. Almost all of the mass of the atom resides in the nucleus. (Protons and neutrons have nearly 2000 times more mass than electrons). The electrons in an atom can exist in only certain specific states. Because of the Pauli Exclusion Principle they are organised into shells and sub-shells. The volume of space an electron in a particular state takes up is called an orbital. The diameter of a nucleus is about 100 000 times smaller than the diameter of the whole atom. (A nucleus is about 10^{-15} m across and an atom is about 10^{-10} m - If a nucleus was the size of a full-stop, a whole atom would be the size of a house).

Atomic number

The number of protons in an atom. Atomic number is sometimes given the symbol 'Z'. The atomic number of an atom determines what type of atom it is, i.e. which element it belongs to.

Atomic physics

The term 'atomic physics' usually refers to the behaviour of electrons in atoms. This distinguishes it from 'nuclear physics' which is deals with the behaviour of nuclei.

Bonds

Bonds are formed when atoms share or exchange electrons in their outer shell. The outer shell of the noble gases is complete and so it is very difficult to add or remove electrons. Because of this, noble gases are unreactive (do not form bonds).

Other elements *do* react to form allotropes or compounds. The most important bonds are the covalent bond and the ionic bond. Atoms will only combine to form compounds if the energy of the compound is less than the energy of the separate atoms. The lower the energy, the more *stable* the atom or compound is. The arrangement of electrons in sodium (Na) is similar to the noble gas neon but sodium also has a single electron in a 3s state (see shells and sub-shells). If sodium loses an electron to become a positive ion then the remaining electrons will be in the same stable arrangement as neon (with full shells).

Bonds tend to result in stable (low energy) arrangements of electrons. If elements from opposite sides of the periodic table react together they exchange electrons and form an ionic bond (e.g. sodium oxide). Elements close to each other on the periodic table most easily achieve a stable arrangement by *sharing* their electrons and so form a covalent bond (e.g. carbon dioxide).

Another way to think of this is that if the difference in the electronegativity of two elements is large then they will form ionic bonds but if it is small they will form covalent bonds.

Covalent bond

A covalent bond is formed when two atoms share their outer electrons. The simplest covalent molecule is the hydrogen molecule, H_2. This is formed when two hydrogen atoms share their electrons between them. Covalent bonds are not as strong as ionic bonds. Some examples of covalent compounds are carbon dioxide (CO_2), sulphur dioxide (SO_2), water (H_2O), Methane (CH_4), hydrogen chloride (HCl). As with all bonds, atoms will only combine if the energy of the compound is less than the energy of the separate atoms.

Electron

A negatively charged fundamental particle. One of the constituents of atoms. It's mass is 9.109 381 88 x 10^{-31} kg (approximately 2000 times less massive than a proton or neutron). Its charge is 1.602176462 x 10^{-19} coulombs. (1998 CODATA recommended values. See *International Aspects of Establishing Recommended Values*, http://physics.nist.gov/cuu/Constants/international.html)

Electronegativity

The electronegativity of an atom is (broadly) a measure of how easy it is to add an electron to its outer shell. Elements on the right hand side of the periodic table are 'electronegative' which means it is easy to turn them into negative ions and it is very hard to turn them into positive ions. Elements on the left hand side are 'electropositive' which means it is easy to turn them into positive ions and it is very hard to turn them into negative ions.

If the difference in the electronegativity of two elements is large then they will form ionic bonds but if it is small they will form covalent bonds .

Many factors affect how electronegative an atom is but there is a general increase *across* the periodic table from left to right. Electronegativity also tends to *decrease* as you go *down* a group.

A useful short hand way to think about it is to say that atoms 'want' to have full shells (i.e. the same arrangement of electrons as the noble gases) and that is why it is easy to add electrons to atoms with nearly full shells. Of course, atoms don't really *want* to have full shells. A partial explanation for the apparent desire goes like this:

1) Electrons are bound in the atom by the positive electric field from the nucleus.

2) Electrons in inner shells screen electrons in outer shells from the field so outer electrons are not held so tightly.

3) The screening effect is much less between electrons in the *same* sub-shell.

4) As the atomic number increases from element to element, the strength of the electric field from the nucleus increases. However, because the screening does not increase in step with the field, electrons in nearly full shells are bound more tightly than electrons in nearly empty shells.

Electrons in outer shells spend more time far way from the nucleus than electrons in inner shells. As you go down a group there are also more electrons in inner shells to screen the nucleus. This is why electron negativity decreases as you go down a group - the pull of the nucleus on an additional electron is not so strong.

Electronvolt, (eV)

A unit of energy used for very small energies. It is equivalent to 1.6 x 10^{-19} joules. This is the energy that an electron acquires when it is accelerated across a voltage of 1 volt. The energies of electrons in atoms are usually in this range so it is a useful unit for atomic physics. In nuclear physics the more usual unit of energy is the mega-electronvolt, MeV i.e. 1 million eV. (See nucleus).

Element

A substance consisting entirely of the same type of atom is called an element. There are about 100 different elements which means there are about 100 different types of atom. An element is defined by the number of protons in an atomic nucleus. If an atom has 1 proton then it is a hydrogen atom; if it has 6 protons then it is a Carbon atom; if it has 92 protons then it is a uranium atom. The number of protons in an element is its atomic number, Z.

The number of neutrons in a nucleus does *not* affect which element an atom belongs to. It determines the isotope of the element. Also, an atom can gain or lose electrons and still be the same element. An atom with more electrons than protons is called a negative ion. One with more protons than electrons is positive ion.

Energy level

Quantum mechanics dictates that the energy of microscopic objects such as electrons in atoms can take on only certain fixed values (no intermediate values). Electrons have energy because of their motion and because of electrostatic interactions with the nucleus and other electrons. The energies that electrons can have within an atom are called 'energy levels'. An electron in a low energy level can absorb a photon and 'jump' into a higher energy level. The energy of the photon must be precisely the difference in energy between the two energy levels. The term 'energy level' is sometimes used synonymously with 'state'.

The energy of molecules and nuclei (and many other microscopic things) is also limited to fixed values or 'energy levels'.

Groups

In the periodic table, elements are arranged into vertical columns called groups. Elements in the same group have similar properties. The groups correspond to the number of electrons present in the outer sub-shell of an atom. In group I elements there is one electron in the outer sub-shell; in group II elements there are two electrons in the outer sub-shell; etc. In group 0 (sometimes called group VIIIa) elements, the outer sub-shell is completely full (see Pauli Exclusion Principle). This is why group 0 elements are very unreactive.

Group 0 elements are called the 'noble gases'; group Ia elements are called the 'alkali metals'; group VIIa elements are called the 'halogens'.

Ion

An ion is a charged atom. A positive ion is charged because it has lost one or more electrons. A negative ion has more electrons than protons. A positive ion and a negative ion will be attracted to each other by electrostatic forces.

Ionic bond

In ionic compounds one atom donates its outer electrons to fill up the spaces in another atom's outer shell. This results in a positively charged ion and a negatively charged ion that are held together by electrostatic forces.

In some elements (those on the left of the periodic table) it is relatively easy to knock outer electrons right out of the atom - that is, to 'ionise' them. We say, the 'ionisation energy' is small. This is because the outer electrons are a long way from the nucleus and shielded from it by the inner electrons. Elements with nearly full outer shells readily accept spare electrons (see electronegativity).

An atom with a high electronegativity (e.g. chlorine) can combine with an atom with a low electronegativity (e.g. sodium) by taking its outer electron. The two ions will be attracted together and will release energy as they move towards each other. Ionic compounds usually form large crystal structures. The ionic compound formed by sodium and chlorine is sodium chloride (also known as salt).

Isotope

Two atoms that have the same atomic number (number of protons) but different numbers of neutrons are different isotopes of the same element. For example carbon has six protons. The nucleus of carbon's most common isotope, C^{12}, also contains six neutrons. However, two other isotopes of carbon can be found occurring naturally. One has 7 neutrons (C^{13}) and one has 8 neutrons (C^{14}). The name of the isotope is given by the mass number (the total number of protons and neutrons) e.g. 'carbon 12' or 'uranium 235'.

Mass number

The number of nucleons (neutrons and protons) present in the nucleus of an atom. For example, the mass number of carbon 12 is 12 and the mass number of carbon 14 is 14 (see isotope). The symbol for mass number is A.

Molecule

A molecule is the smallest particle of any substance - a collection of atoms bound together by covalent bonds. For example carbon dioxide is a gas made up of carbon dioxide molecules. A carbon dioxide molecule is composed of one carbon atom and two oxygen atoms bound together by covalent bonds.

Noble gases

Elements in group 0 (sometimes called group VIIIa) are called noble gases because they are very unreactive. Helium, neon, argon, krypton xenon, and radon do not form bonds because the arrangement of their outer electrons is already stable - their outer shell is complete. Because of this, It always takes more energy to add or remove an electron from the outer shell of a noble gas than you would gain by forming a compound.

When atoms form bonds this usually results in the arrangement of electrons in the atoms being like the arrangement of electrons in noble gases. For instance when sodium reacts with chlorine, sodium loses its spare electron and the arrangement of its remaining electrons is the same as the electrons in neon. The extra electron is taken up by chlorine which completes its outer shell making the arrangement of electrons the same as argon. (See bonds, ionic bonds, covalent bonds, electronegativity).

Neutron

One of the particles found in the nucleus. It has a similar mass to that of a proton but it has no electric charge. Neutrons are bound to each other and to protons by the 'strong nuclear force' (see nucleus).

Nucleon

The collective name for neutrons and protons (the particles in the nucleus).

Nucleus

The central bit of an atom. It contains protons and neutrons. The diameter of a nucleus is about 100 000 times smaller than the diameter of the whole atom. (A nucleus is about 10^{-15} m across and an atom is about 10^{-10} m - If a nucleus was the size of a full-stop, a whole atom would be the size of a house). This means that the nucleus takes up just one thousandth of a trillionth of the *volume* of the atom yet it contains nearly all the mass of the atom. (We know this because of Rutherford's scattering experiments). Protons are positively charged and neutrons have no charge. From the point of view of atomic physics we can think of the nucleus simply as the source of the electric field that holds electrons in atoms. However, the nucleus is very interesting in its own right. The protons and neutrons are held together by a force called the 'strong nuclear force'. This is much stronger than electromagnetism (which is why the protons can stick together) but it only operates over a very short distance. This distance is smaller than most nuclei. Nucleons (protons or neutrons) cling to their nearest neighbours and this is how the whole nucleus stays together.

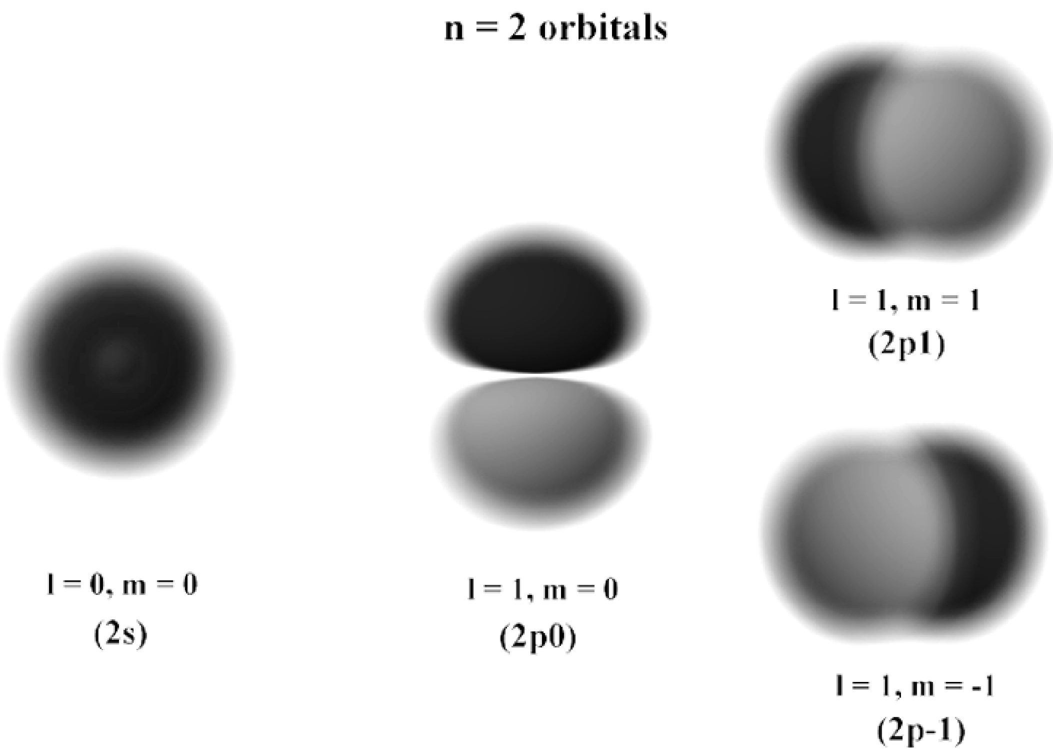
The nucleus can vibrate and has energy levels much like electrons in atoms. Nuclear energy levels are much much greater than electron energy levels. (Typically measured in millions of electron volts rather than electron volts). When the nucleus undergoes a transition from a high energy level to a low energy level the electromagnetic radiation that it emits is in the gamma-ray part of the spectrum rather than the visible part of the spectrum. By looking at the spectrum of gamma rays emitted by a nucleus we can learn about the energy levels in the nucleus. (Compare this with visible light spectroscopy which tells us about the energy levels of electrons in atoms).

Some nuclei are unstable and can break up. We say, these nuclei are 'radioactive'. One way this happens is that a neutron turns into a proton and emits an electron. This is called beta radiation. Another way it happens is that the nucleus spits out an alpha particle (two protons and two neutrons). This is called alpha radiation. Yet another way it can happen is a (very large) nucleus can break up into smaller nuclei. This is called fission.

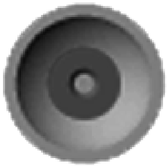
Orbitals

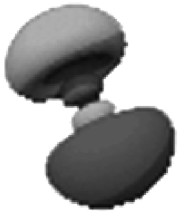
An orbital is the volume of space in an atom occupied by an electron in a particular **state**. It is not strictly correct to think of electrons orbiting nuclei like little planets orbiting a sun (though this is a useful picture to keep hold of). Quantum mechanics makes our picture of electrons (and therefore our picture of atoms) much more complicated. The word 'orbital' is chosen to convey a more hazy and complex idea than the 'orbit' of a planet.

An orbital describes the probability of finding an electron in a particular place. (Some people like to think of the electron as a cloud of negative charge. It's fine if you find this helpful but I personally don't like this picture of electrons). The shape of the orbital depends on the electron's **state** i.e. on the value of n, ℓ and m_ℓ (see quantum numbers). The number of protons in the atom and interactions with other electrons in the atom can also affect the size and shape of orbitals. For high quantum numbers, the shape of the orbital can be very complex.



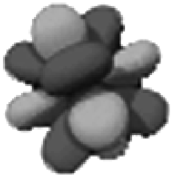
The shape of the orbitals for the possible states in the n = 2 shell. The three p-orbitals (l = 1 orbitals) are the same shape (and energy) but oriented at right angles to each other.


n=3, l=0, m=0


n=3, l=1, m=0

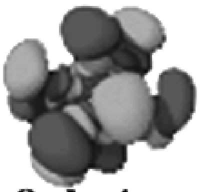

n=3, l=2, m=0

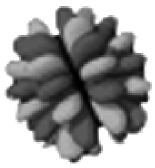

n=5, l=2, m=0


n=5, l=4, m=2


n=6, l=1, m=0


n=9, l=0, m=0


n=8, l=4, m=3


n=10, l=10, m=4

Some other examples of orbitals. These pictures represent surfaces of constant probability (i.e. the probability of finding an electron is the same at any point on the surface). This is why they are not fuzzy like the pictures of orbitals above. Plotting them this way makes the shape clearer.

Pauli Exclusion Principle

No two electrons in an atom can be in the same **state** i.e. no two electrons can have the same set of quantum numbers. This gives rise to shells and sub-shells and so to the chemical properties of the elements and the structure of the periodic table.

The reason the principle is true for electrons is a little technical. It arises from the symmetry of electron waves (see quantum mechanics) and from the fact that electrons are indistinguishable.

Periodic Table

An arrangement of the 100 or so chemical elements in order of their atomic number. Elements are arranged in a way that demonstrates the periodic patterns in their properties. Elements with similar properties occur at regular intervals and fall into groups of related elements. The elements between group IIa and group IIIa are called the transition elements.

The outer electrons in group Ia and group IIa elements are in an ‘s-state’ ($\ell = 0$). The outer electrons in the other main groups are in a ‘p-state’ ($\ell = 1$). The outer electrons in the transition elements are in ‘d-state’ ($\ell = 2$).

Photon

A photon is a particle of light (or other electromagnetic radiation). Because of quantum mechanics we are forced to think of light in two incompatible ways: both as a wave and a particle. The energy of a photon is given by the equation:

$E=hf$ or, alternatively $E=hc/\lambda$ where E is energy, f is the frequency of the light, λ (lambda) is the wavelength of the light, c is the speed of light and h is Planck’s constant.

Planck’s constant

In quantum mechanics many quantities such as energy and angular momentum can only be increased in jumps. Planck’s constant determines the size of the jumps. Its value is 6.629196×10^{-34} joule seconds. (A very small quantity - which is why we don’t notice quantum mechanics at normal scales). Planck’s constant is a universal constant of nature. Like the charge on an electron, Newton’s gravitational constant and other constants of nature, nobody knows why it has the value it has - it just does.

Proton

A positively charged particle and constituent of the nucleus of atoms. Protons feel the ‘strong force’ (see nucleus) as well as the electromagnetic force which is why they can be bound together in nuclei. Its mass is $1.672\,621\,58 \times 10^{-27}$ kg. That is, 1836 times the mass of the electron on and 0.9986 times that of the neutron. (1998 CODATA recommended values. See *International Aspects of Establishing Recommended Values*, http://physics.nist.gov/cuu/Constants/international.html)

Quantum mechanics

Quantum mechanics is a way of describing the behaviour of matter at small scales (atoms, molecules and smaller particles). At these scales the behaviour of matter seems strange. Most importantly, quantities like the energy and angular momentum of an electron can only take on specific values. Also the energy in electromagnetic radiation is delivered in ‘chunks’. This makes light seem to behave like little particles. Particles of electromagnetic radiation are called ‘photons’. Things that we normally take to be particles like electrons and protons can be shown under some circumstances to behave like waves. This confused nature of matter and light is called ‘wave-particle duality’.

Quantum numbers

In quantum mechanics it is often found that the properties of a physical system, such as its angular momentum and energy, can only take on discrete values. Where this occurs the property is said to be ‘quantised’ and its various possible values are labelled by a set of numbers called quantum numbers. Regions in an atom where an electron may move (electron orbitals) are characterised by the quantum numbers n, ℓ and m_ℓ. Each electron can be in one of two spin states. (Roughly, we can think of the electron spinning on its axis like a little spinning top but, because of quantum mechanics, it is actually little more complicated than that). The spin of the electron is given by the quantum number m_s. The value of m_s is either labelled ‘up’ and ‘down’ or given the value + ½ or - ½. No two electrons in an atom can have the same set of quantum numbers n, ℓ, m_ℓ and m_s. (Pauli Exclusion Principle). The set of quantum numbers possessed by an electron determines its **state**.

The possible values of ℓ can vary between 0 and n-1. For example if n is 1 then the only possible value of ℓ is 0; if n is 4 then ℓ can be 0, 1, 2, or 3. The possible values of m_ℓ can vary between $-\ell$ and $+\ell$. For example, if ℓ is 2 then m_ℓ can be -2, -1, 0, 1 or 2. (see table in Shells and Sub-Shells)

Shells and Sub-Shells

Electrons in atoms tend to occupy state with the low energy. However, because of the Pauli Exclusion Principle the low energy states can get full. Low energy states have low values of n and ℓ. Each value of n defines a 'shell'. There are two possible states when n = 1 so two electrons can fit into the n = 1 shell. There are eight possible states with n = 2 so eight electrons can fit into the n = 2 shell. Eighteen electrons can fit into the n = 3 shell and thirty two can fit into the n = 4 shell.

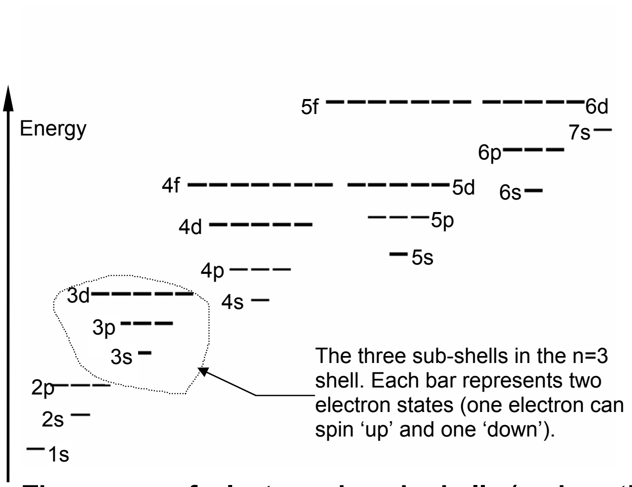
n	l	m_l	m_s
2	0	0	up
2	0	0	down
2	1	0	up
2	1	0	down
2	1	1	up
2	1	1	down
2	1	-1	up
2	1	-1	down

the eight possible states in the n = 2 shell

Shells are divided into sub-shells according to the value of the quantum number ℓ. There are two sub-shells in the n = 2 shell corresponding to $\ell = 0$ and $\ell = 1$. Sometimes the sub-shells are given letters instead of numbers. This comes from the early history of spectroscopy - before anybody had thought of quantum numbers. The letters correspond to the appearance of the lines in a spectrum .

ℓ	spectroscopic notation	historical reason for name (description of line)
0	s	sharp
1	p	principal
2	d	diffuse
3	f	fine
4	g	
5	h	
6	etc.	

notation for sub-shells



The energy of electrons in sub-shells (and so, the order in which sub-shells are filled). Note that the 4s sub-shell is less energetic than the 3d sub-shell . This means that the 4s sub-shell will be filled before the n = 3 shell is completely full.

n (shell)	ℓ	possible values of m_ℓ	sub-shell name	no. of states in sub-shell	no. of states in shell
1	0	0	1s	2	**2**
2	0	0	2s	2	
2	1	-1,0, 1	2p	6	**8**
3	0	0	3s	2	
3	1	-1,0, 1	3p	6	
3	2	-2,-1,0, 1, 2	3d	10	**18**
4	0	0	4s	2	
4	1	-1,0, 1	4p	6	
4	2	-2,-1,0, 1, 2	4d	10	
4	3	-3,-2,-1,0, 1, 2, 3	4f	14	**32**

The number of states in each shell depends on the possible values of l and ml for a given value of n. (See quantum numbers).

see table of n = 2 states and diagram of n = 2 orbitals above.

Shells and sub-shells are not physical shells (like sea-shells) around an atom. You should think of them as a sort of catalogue. They are a way of organising the changing behaviour of electrons as energy levels get filled up in atoms.

From the point of view of chemistry the most important shell in an atom is the outer sub-shell. The chemical behaviour of an element depends on how full or empty the outer sub-shell is.

When the s and p sub-shells of a given shell are both complete, we say the shell is complete. The d and f sub-shells are treated slightly differently in as much as they do not have to be full for the shell itself to be classified as complete.

Transition Elements

Elements in the groups between group IIa and group IIIa in the periodic table. (i.e., in period 4: scandium, titanium, vanadium, chromium, ..., copper, zinc). These differ from elements in the main groups in that one of their inner shells is only partially complete. That means that bonding goes on with electrons in this inner shell as well as the outer shell.

Z

The symbol for atomic number - the number of protons in an atom's nucleus (the quantity that identifies which element an atom belongs to).