

2.2 Electron configuration

Visible light is part of the electromagnetic spectrum - the spectrum containing all forms of electromagnetic radiation.

All electromagnetic waves travel at the same speed (the speed of light, c) but will have different wavelengths (λ):

$$c = 3.00 \times 10^8 \text{ m s}^{-1}$$



The number of waves that pass a point in 1 second is called the frequency (ν).

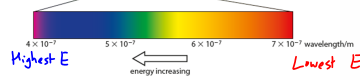
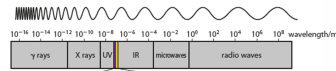
Blue light --- Shorter wavelength --- Higher frequency

Red light --- Longer wavelength --- Lower frequency

We relate ν and λ using the equation:

$$c = \nu \cdot \lambda$$

Hertz
 $\nu \rightarrow \text{Hz}$
 $\lambda \rightarrow \text{m}$



An electromagnetic wave that oscillates more must have a higher energy so we can say:

E is inversely proportional to λ

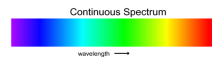
Blue light --- Shorter wavelength --- Higher frequency = Higher energy

Red light --- Longer wavelength --- Lower frequency = Lower energy

$$E \propto \frac{1}{\lambda}$$

SI units : Energy --- J
 Wavelength --- m
 Frequency --- Hz

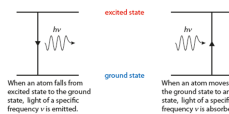
Passing white light through a prism will give a continuous spectrum showing the full range of frequencies.



Exciting a sample and recording the frequencies absorbed or released will produce a line spectrum. In this case an emission spectrum. As used by Bohr.



Line spectra are caused by the absorption or emission of energy by electrons. To jump up to a higher energy level, electrons can absorb light of a specific frequency (corresponding to the energy gap between levels). This creates an atom in an excited state. When it drops back down to the ground state, it releases a packet of energy called a photon.



We can relate the energy of the photon using the Planck constant, h :

$$E_{\text{photon}} = h \cdot \nu \text{ (frequency)} \quad h = 6.63 \times 10^{-34} \text{ J s}$$

This means that energy can only exist in "discrete packets" of energy that we call quanta. So a photon is a quantum of energy.

Rydberg came up with a formula to predict the wavelength of any lines in the hydrogen emission spectrum. It is called the Rydberg equation and uses the Rydberg constant.

$$R_H = 2.18 \times 10^{-18} \text{ J s}$$

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Note - n_2 must be higher than n_1 .

This is used to predict the wavelength of light emitted when an electron drops from one energy level (n_2) to a lower level (n_1).

En el átomo de hidrógeno las líneas de la serie de Paschen se originan en las transiciones electrónicas desde niveles con $n=3$ hasta el nivel $n=2$. Calcule la longitud de onda en nm de la línea de la serie de Paschen correspondiente a la transición desde el nivel $n=7$.

Datos: $R_H = 1.0968 \cdot 10^7 \text{ m}^{-1}$

$$\frac{1}{\lambda} = 1.0968 \times 10^7 \times \left(\frac{1}{3^2} - \frac{1}{7^2} \right) \quad 1 \text{ nm} \rightarrow 10^{-9} \text{ m}$$

$$\frac{1}{\lambda} = 994829.932 \rightarrow \lambda = 1.0052 \times 10^{-6} \text{ m}$$

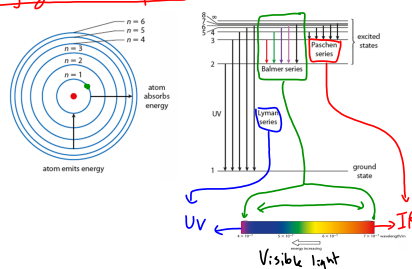
$$1 \text{ nm} \rightarrow 10^{-9} \text{ m}$$

$$\times \rightarrow 1.0052 \times 10^{-6} \text{ m}$$

$$\text{Answer} \quad \lambda = 1.0052 \cdot 10^{-6} \text{ m}$$

$$\lambda = 1005 \text{ nm}$$

Hydrogen emission spectrum



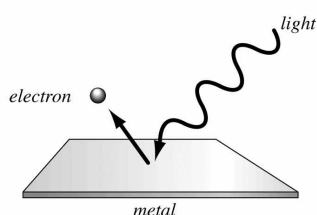
Wave-particle duality

This is a property of light that means it can behave with a particulate-nature and also as a wave:

- We can view light as a stream of photons (packets of energy)
- We can view light as a magnetic wave

Evidence for these 2 characteristics can be found in different phenomena:

Photoelectric effect

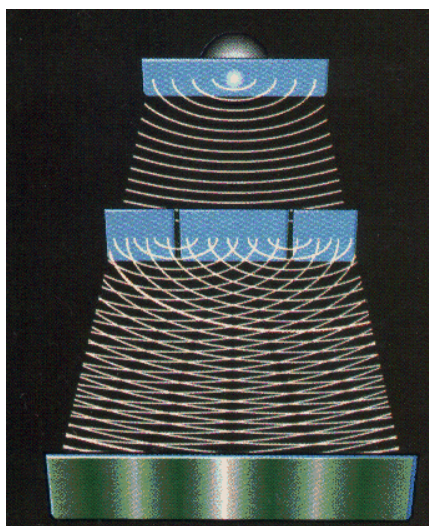
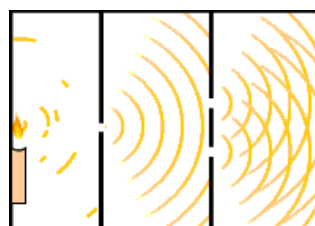


When light is shone at certain materials, a small current is produced as the energy from the photons (packets of energy) is transferred to electrons - freeing them from their positions.

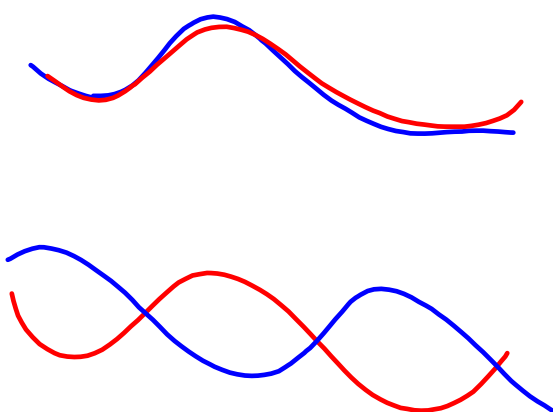
If light is treated as a wave then increasing the brightness of the light should lead to electrons being "knocked out" with more energy. However, this did not happen.

Einstein suggested that if light was treated as a stream of photons then increasing the brightness of the light would only increase then number of electrons being freed not the energy of them. This proved true and he won the Nobel prize!

Double slit experiment



The photosensitive detector shows bands of light reaching it suggesting that the 2 waves interact with their peaks and troughs to produce a detection or cancel it to produce no detection.



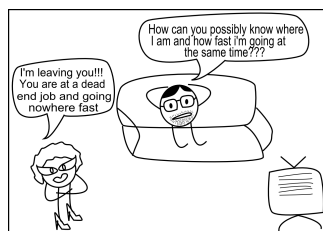
Heisenberg's Uncertainty Principle and the concept of orbitals

A significant problem of Bohr's model was that he assumed the position and movement of an electron could be precisely described.

Heisenberg's Uncertainty Principle states that we can never know precisely the position and momentum of an electron. This is because through the process of trying to locate an electron will disturb its location.

This led to the Schrodinger model of the atom (using the wave-like property of an electron). He stated that electrons must be found in orbitals. An orbital is a region of space where there is a very high chance of finding an electron (90%). This region is calculated using a mathematical function.

The shape of an orbital will depend on the energy of an electron and the higher the energy, the further the orbital can be from the nucleus.



Shell → Energy level (H)

1st energy level

A single s-orbital:

1s

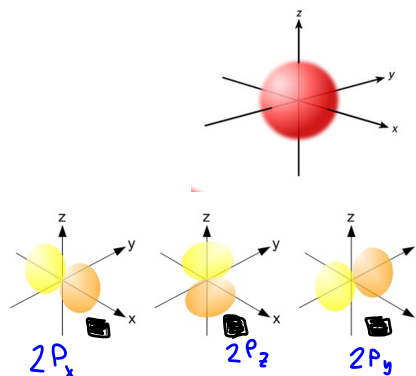


2nd energy level

Split into 2 sub-levels:

2s - larger than the 1s

2p - 3 orbitals
arranged along
different axes.

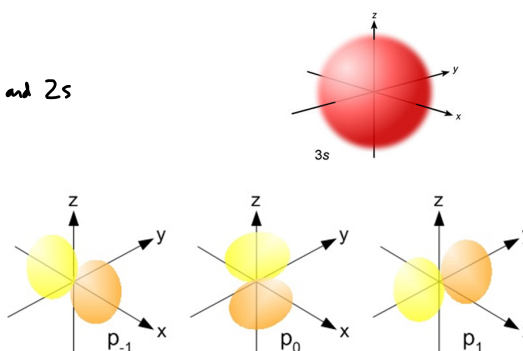


3rd energy level

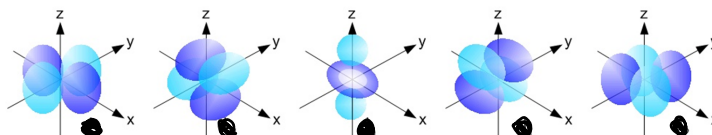
Split into 3 sub-levels:

3s - larger than the 1s and 2s

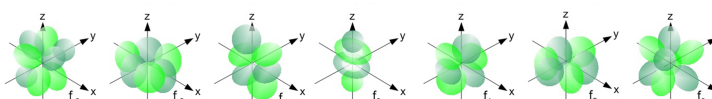
3p - 3 p orbitals
arranged along
different axes.



3d - 5 d orbitals



The 4th energy level also has f orbitals:



Electron configuration → Showing how many electrons an element has and where they are located.

Pauli Exclusion Principle :

- Each orbital can hold a maximum of 2 electrons.
- If there are 2 in an orbital then they must spin in opposite directions.

(This is so that every electron is individually identifiable using its orbital and spin. If 2 electrons were in the same orbital with the same spin then they would be the same electron)

$1s \rightarrow \uparrow\downarrow$ spin

Level	Sub-level	Maximum number of electrons in sub-level	Maximum number of electrons in level
$n = 1$	$1s$	2	2
$n = 2$	$2s, 2p$	2, 6	8
$n = 3$	$3s, 3p, 3d$	2, 6, 10	18
$n = 4$	$4s, 4p, 4d, 4f$	2, 6, 10, 14	32

We can see the following from the table.

The n th energy level of the Bohr atom is divided into n sub-levels. For example, the fourth level ($n = 4$) is made up from four sub-levels. The letters s, p, d, and f are used to identify different sub-levels.

- Each main level can hold a maximum of $2n^2$ electrons. The 3rd energy level, for example, can hold a maximum of 18 electrons ($2 \times 3^2 = 18$).
- s sub-levels can hold a maximum of 2 electrons.
- p sub-levels can hold a maximum of 6 electrons.
- d sub-levels can hold a maximum of 10 electrons.
- f sub-levels can hold a maximum of 14 electrons.

Arranging the different sub-levels in order of energy, you can see that there is overlap between different energy levels.

$Ne \rightarrow 10 e^- : 1s^2 2s^2 2p^6$
 $Ar \rightarrow 18 e^- : 1s^2 2s^2 2p^6 3s^2 3p^6$

Aufbau Principle: orbital diagrams

The electron configuration of the ground state of an atom of an element can be determined using the **Aufbau Principle**, which states that electrons are placed into orbitals of lowest energy first. Boxes can be used to represent the atomic orbitals, with single-headed arrows to represent the spinning electrons. The electron configurations of the first five elements are shown in Figure 2.17. The number of electrons in each sub-level is given as a superscript.

Hund's Rule

Once more than 1 orbital in the same sub-level is available then Hund's rule states that we must half-fill each orbital with electrons of a parallel spin.

What happens when we reach the d-block elements (elements with outer electrons in a d-orbital)?

Element: C, N, O

Orbital diagram for C: $1s^2 2s^2 2p^2$

Electron configuration: $1s^2 2s^2 2p^2$

Worked example

State the full electron configuration of vanadium and deduce the number of unpaired electrons.

Solution

$V = 1s^2 2s^2 2p^6 3s^2 3p^4 4s^2 3d^3$

Unpaired electrons: 3

Abbreviated electron configuration - Write the full configuration for:

- Na: $1s^2 2s^2 2p^6$ (then $3s^1$)
- Ar: $1s^2 2s^2 2p^6 3s^2 3p^6$ (then $4s^1$)

We can use the config. from noble gases and then just add the outer electrons for other elements.

Na → [Ne] $3s^1$
Ti → [Ar] $4s^2 3d^2$

So for the d-block elements we can write their electronic configuration as...

Can you spot the 2 exceptions?

Chromium: [Ar] $4s^1 3d^5$
Copper: [Ar] $4s^1 3d^9$

Periodic table showing electron filling order.

EXERCISES

19 Identify the sub-level which does not exist.
A 5d B 4d C 3d D 2p

20 Which is the correct order of orbital filling according to the Aufbau Principle?
A 4s 4p 4d 4f B 4s 4d 4f 4p C 4s 3d 4p 4d D 4d 4f 4s 4p

21 State the full ground-state electron configuration for the following elements.
(a) V (b) K (c) Sc (d) Sr

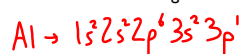
22 Determine the total number of electrons in d orbitals in single isomer atoms.
A 5 B 10 C 15 D 20

23 Identify the excited state (i.e. not a ground state) in the following electron configurations.
A [He] $2s^1 2p^1$ B [He] $2s^1 2p^2$ C [He] $2s^1 2p^3$ D [He] $3s^1 3p^1 3d^1$

24 Deduce the number of unpaired electrons present in the ground state of a titanium atom.
A 1 B 2 C 3 D 4

Electron configuration of ions

The formation of ion simply requires the addition or removal of electrons from a ground state element. E.g. ions of Al:



- Al^+ is $1s^2 2s^2 2p^6 3s^2$
- Al^{2+} is $1s^2 2s^2 2p^6 3s^1$
- Al^{3+} is $1s^2 2s^2 2p^6$, etc.

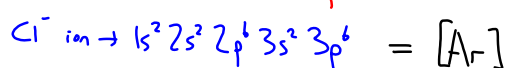
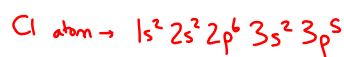
However with the **d-block elements** we must know:

The 4s sub-level is very slightly lower than the 3d sub-level so it is filled (according to the Aufbau principle) beforehand. However, once there are electrons in the 3d sub-level the 4s orbital increases in energy.

This means that if we are writing electron configurations for positive ions such as Fe^{3+} , when we remove electrons to form the ion, they are removed first from the 4s orbital.

For example, Cr is $[\text{Ar}] 3d^5 4s^1$ and Cr^{3+} is $[\text{Ar}] 3d^3$

Write the electron configuration for a Cl^- ion.



K^+ also is an isoelectronic species. ← They are isoelectronic species.

Worked example

State the ground-state electron configuration of the Fe^{3+} ion.

Solution**Exercises**

25 State the full ground-state electron configuration of the following ions.

- (a) O^{2-} (b) Cl^- (c) Ti^{3+} (d) Cu^{2+}

26 State the electron configuration of the following transition metal ions by filling in the boxes below. Use arrows to represent the electron spin.

	Ion	3d	4s
(a)	Ti^{2+}		
(b)	Fe^{2+}		
(c)	Ni^{2+}		
(d)	Zn^{2+}		

27 (a) State the full electron configuration for neon.

(b) State the formulas of two oppositely charged ions which have the same electron configuration as neon.

Exercises

28 Use the Periodic Table to find the full ground-state electron configuration of the following elements.

- (a) Cl (b) Nb (c) Ge (d) Sb

29 Identify the elements which have the following ground-state electron configurations.

- (a) $[\text{Ne}] 3s^2 3p^2$ (b) $[\text{Ar}] 3d^4 4s^2$ (c) $[\text{Kr}] 5s^2$

(d) $1s^2 2s^2 2p^3 3s^2 3p^3 3d^4 4s^2$

30 State the total number of p orbitals containing one or more electrons in tin.

31 How many electrons are there in all the d orbitals in an atom of barium?

32 State the electron configuration of the ion Cd^{2+} .

CHALLENGE YOURSELF

4 Only a few atoms of element 109, meitnerium, have ever been made. Isolation of an observable quantity of the element has never been achieved, and may well never be. This is because meitnerium decays very rapidly.

- (a) Suggest the electron configuration of the ground-state atom of the element.
 (b) There is no g block in the Periodic Table as no elements with outer electrons in g orbitals exist in nature or have been made artificially. Suggest a minimum atomic number for such an element.

5 State the full electron configuration of U^{2+} .

6 Consider how the shape of the Periodic Table is related to the three-dimensional world we live in.

- (a) How many 3p and 3d orbitals would there be if there were only the x and y dimensions?
 (b) How many groups in the p and d block would there be in such a two-dimensional world?