Atomic structure Part two (answers)

IB CHEMISTRY SL

25	16		6	2	25
Mn	S	J	C	He	Mn
Manganese	Sulfur		Carbon	Helium	Manganese
54.938045	32.065		12.0107	4.002602	54.938045

2.2 Electron configurations

Understandings:

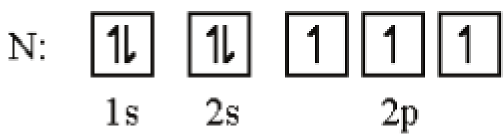
- Emission spectra are produced when photons are emitted from atoms as excited electrons return to a lower energy level.
- The line emission spectrum of hydrogen provides evidence for the existence of electrons in discrete energy levels, which converge at higher energies.
- The main energy level or shell is given an integer number, n, and can hold a maximum number of electrons, $2n^2$.
- A more detailed model of the atom describes the division of the main energy level into s, p, d and f sub-levels of successively higher energies.
- Sub-levels contain a fixed number of orbitals, regions of space where there is a high probability of finding an electron.
- Each orbital has a defined energy state for a given electronic configuration and chemical environment and can hold two electrons of opposite spin

Applications and skills:

- Description of the relationship between colour, wavelength, frequency and energy across the electromagnetic spectrum.
- Distinction between a continuous spectrum and a line spectrum.
- Description of the emission spectrum of the hydrogen atom, including the relationships between the lines and energy transitions to the first, second and third energy levels.
- Recognition of the shape of an s atomic orbital and the p_x, p_y and p_z atomic orbitals.
- Application of the Aufbau principle, Hund's rule and the Pauli exclusion principle to write electron configurations for atoms and ions up to Z = 36.

Guidance:

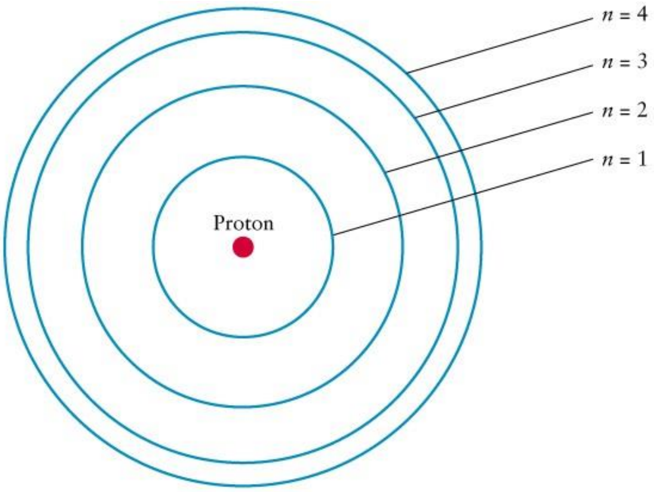
- Details of the electromagnetic spectrum are given in the data booklet in section 3.
- The names of the different series in the hydrogen line emission spectrum are not required.
- Full electron configurations (eg $1s^22s^22p^63s^23p^4$) and condensed electron configurations (eg [Ne] $3s^23p^4$) should be covered.
- Orbital diagrams should be used to represent the character and relative energy of orbitals. Orbital diagrams refer to arrow-in-box diagrams, such as the one given below.



- The electron configurations of Cr and Cu as exceptions should be covered.

Electron configurations

- The Bohr model of the atom has the electrons located in energy levels, which are assigned the letter *n*.



- *n*=1 is closest to the nucleus and has lowest energy. As the value of *n* increases, the energy also increases.
- The main energy levels are divided into sub-levels.
- Each main energy level can hold $2n^2$ electrons.

<table>
<tr><th>Energy level</th><th>sub-level</th><th>maximum number of electrons in sub-level</th><th>maximum number of electrons in level</th></tr>
<tr><td>n = 1</td><td>1s</td><td>2</td><td>2</td></tr>
<tr><td rowspan="2">n = 2</td><td>2s</td><td>2</td><td rowspan="2">8</td></tr>
<tr><td>2p</td><td>6</td></tr>
<tr><td rowspan="3">n = 3</td><td>3s</td><td>2</td><td rowspan="3">18</td></tr>
<tr><td>3p</td><td>6</td></tr>
<tr><td>3d</td><td>10</td></tr>
<tr><td rowspan="4">n = 4</td><td>4s</td><td>2</td><td rowspan="4">32</td></tr>
<tr><td>4p</td><td>6</td></tr>
<tr><td>4d</td><td>10</td></tr>
<tr><td>4f</td><td>14</td></tr>
</table>

Summary:

- The s sub-level can hold a maximum of 2 electrons.
- The p sub-level can hold a maximum of 6 electrons.
- The d sub-level can hold a maximum of 10 electrons.
- The f sub-level can hold a maximum of 14 electrons.

Heisenberg's Uncertainty principle

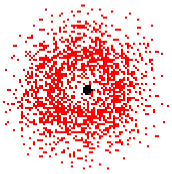
- One limitation of the Bohr model of the atom is that it assumes that an electron's trajectory can be precisely known.
- The Uncertainty principle basically states that the velocity and position of an electron cannot be simultaneously measured with high precision (simply you cannot know where an electron is and how fast it is moving at the same time).

Atomic orbitals

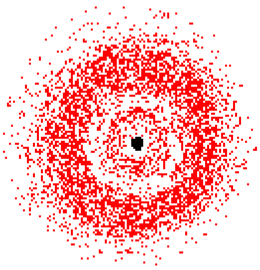
- Atomic orbitals describe the probability of finding an electron in an area of space.
- They represent the region around the nucleus where there is a 95% chance of finding an electron.

s atomic orbitals

- s orbitals are spherical in shape.



a 1s orbital

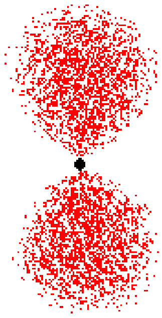


a 2s orbital

- The orbital on the right is a 2s orbital. This is similar to a 1s orbital except that the region where there is the greatest chance of finding an electron is further from the nucleus.

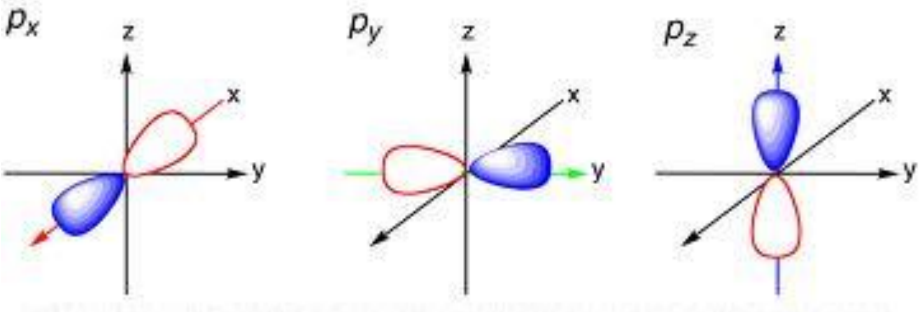
p atomic orbitals

- A p orbital is like 2 identical balloons tied together at the centre (dumbbell shaped).



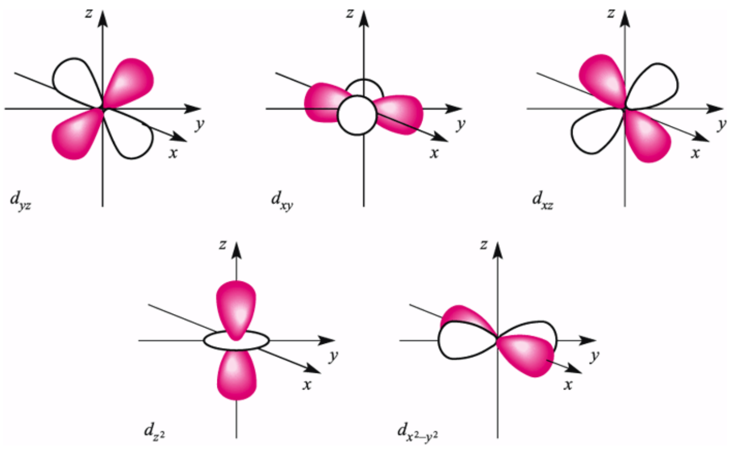
a p orbital

- The p sub-level contains 3 p orbitals of equal energy (degenerate orbitals).
- They are arranged at right angles to each other with the nucleus at the centre.



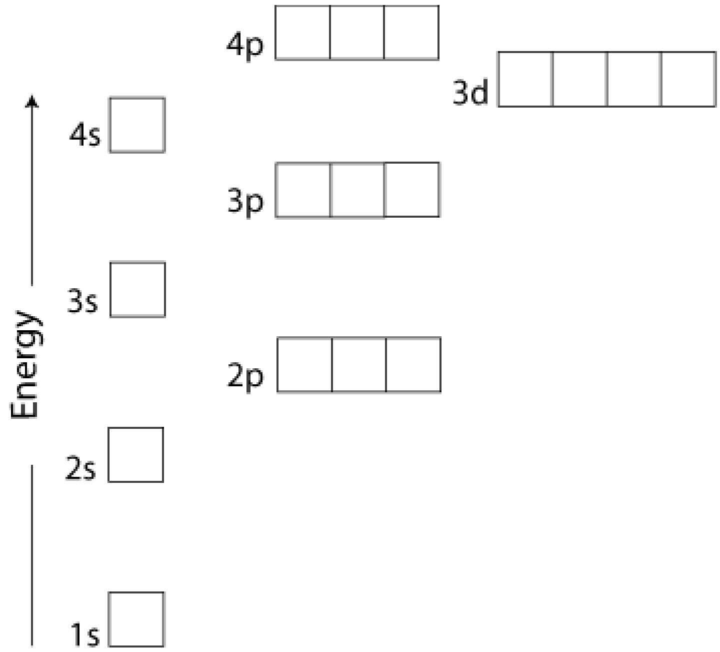
d and f atomic orbitals (shape of f orbitals not shown)

- The d sub-level is made from five d atomic orbitals. Their shapes are shown below (you are not required to know the shapes of d and f orbitals).

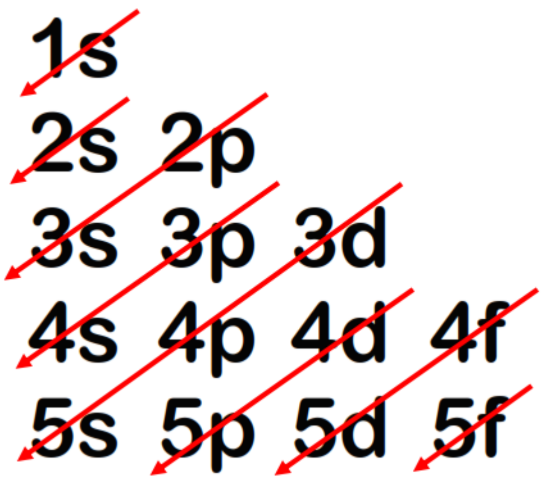


The Aufbau Principle

- The Aufbau Principle states that electrons are placed into orbitals of lowest energy first.
- The following diagram show the sub-levels in order of increasing energy.
- Note the overlap between the 4s and 3d sub-levels.



- The filling of the sub-levels follows the pattern below:



Electron spin and the Pauli Exclusion Principle

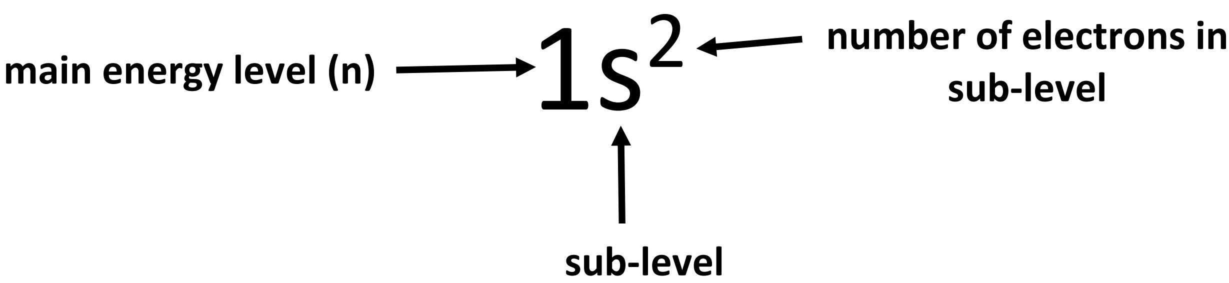
- The Pauli Exclusion Principle states that no two electrons in the same orbital can have the same quantum number.
- This means that no more than two electrons can occupy an orbital and they must spin in opposite directions.
- Electrons and their spins are represented by single-headed arrows (↿ or ⇂).

Hund's rule

- Hund's rule states that if more than one degenerate orbital in a sub-level is available, electrons occupy separate orbitals with opposite spins (simply put, always fill orbitals of equal energy singly with one electron first and then add the second electron once each orbital has one electron in it).

Writing electron configurations

- Electron configurations show how electrons are arranged in sub-levels.
- The first number shows the main energy level (or principle quantum number).
- The letter shows the sub-level (s, p, d or f).
- The number in superscript shows the number of electrons in the sub-level.



Example: Write the full electron configuration of the magnesium atom (Z=12)

$1s^2\ 2s^2\ 2p^6\ 3s^2$

Abbreviated electron configurations

Example – the full and abbreviated electron configuration of rubidium (Rb) are shown below

- Rb $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^1$
- Rb [Ar] $5s^1$

Write the abbreviated electron configuration for Al:

- Al $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$
  [Ne] $3s^2\ 3p^1$

Concept check:

Write **full** electronic configurations for the following atoms:

1) He $1s^1$

2) Li $1s^2\ 2s^1$

3) B $1s^2\ 2s^2\ 2p^1$

4) C $1s^2\ 2s^2\ 2p^2$

5) O $1s^2\ 2s^2\ 2p^4$

6) Ne $1s^2\ 2s^2\ 2p^6$

7) Na $1s^2\ 2s^2\ 2p^6\ 3s^1$

8) Al $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$

9) P $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$

10) Cl $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$

11) Ar $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$

12) Ca $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2$

13) Ti $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^2$

14) Mn $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^5$

15) Ni $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^8$

16) Zn $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}$

17) Ge $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^2$

18) Se $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^4$

19) Br $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^5$

20) Kr $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6$

Write **abbreviated** electron configurations for the following atoms:

11) Li [He] $2s^1$

12) Mg [Ne] $3s^2$

13) S [Ne] $3s^2\ 3p^4$

14) Ca [Ar] $4s^2$

15) Ga [Ar] $4s^2\ 3d^{10}\ 4p^1$

Electron configurations of ions

- Note that First row d-block elements (Sc – Zn) lose their 4s electrons first when they form ions.

Write the electron configuration for the Ni^{2+} ion:

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^8$

Write the electronic configuration for the Mn^{2+} ion:

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^5$

Exercise: write abbreviated electron configurations for the following ions:

1) Na^+

2) S^{2-}

3) Ca^{2+}

4) Cr^{3+}

5) Cu^+

Na^+ [He] $2s^2\ 2p^6$

S^{2-} [Ne] $3s^2\ 3p^6$

Ca^{2+} [Ar] $4s^2$

Cr^{3+} [Ar] $3d^3$

Cu^+ [Ar] $3d^{10}$

Exceptions to the Aufbau principle – copper (Cu) and chromium (Cr)

Copper Z=29

- The full electron configuration for the Cu atom is:
  $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1\ 3d^{10}$

Chromium Z= 24

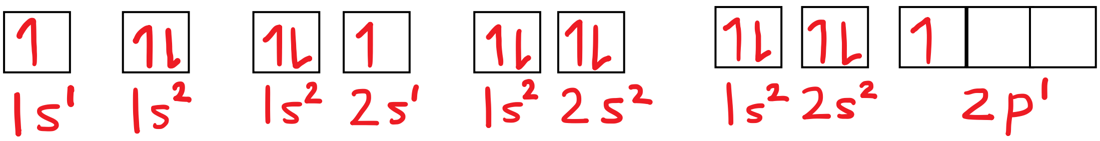
- The abbreviated electron configuration for the Cr atom is:
  $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1\ 3d^5$

Orbital diagrams – electrons in boxes

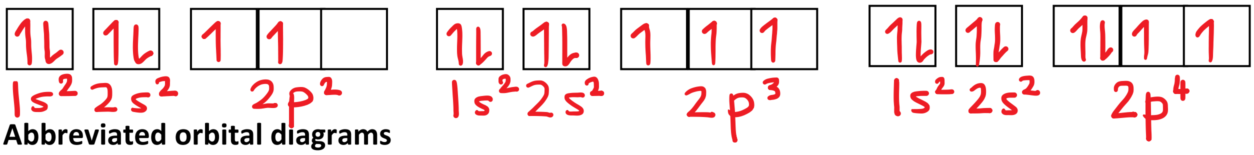
- Boxes can be used to represent the atomic orbitals with single headed arrows used to represent the spinning electrons.
- Recall that electrons fill orbitals according to Hund's rule and the Pauli exclusion principle; an orbital can hold a maximum of two electrons which must have opposite spins, ↿ or ⇂, and electrons fill degenerate orbitals singly before being doubly occupied.

Exercise: Draw electrons in boxes (orbital diagrams) for the first 7 elements below:

H He Li Be Boron

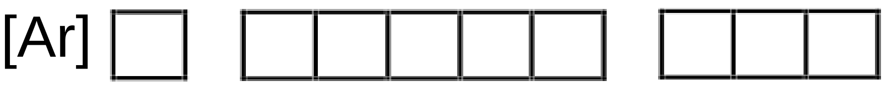


Carbon Nitrogen Oxygen



Abbreviated orbital diagrams

- These use the configuration of a noble gas (just as for electron configurations)



Exercise:

Draw abbreviated orbital diagrams for the following:

1) Ca

2) V

3) Mn

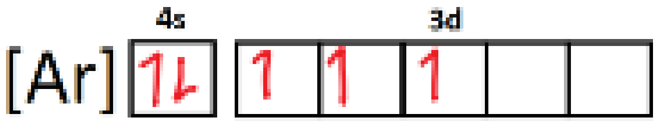
4) Cr^{3+}

5) Cu^{2+}

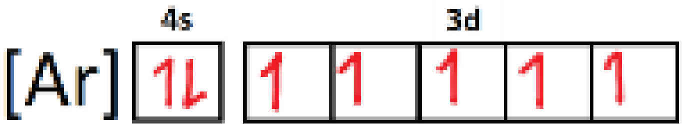
Answers:

1) $[Ar]4s^2$

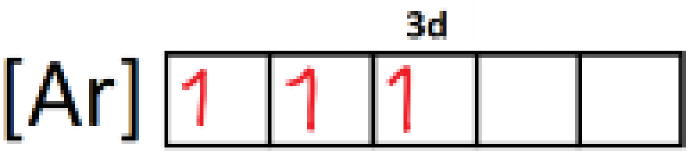
2) $[Ar]4s^2 3d^3$



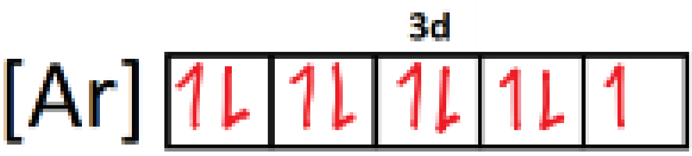
3) $[Ar]4s^2 3d^5$



4) $[Ar]3d^3$

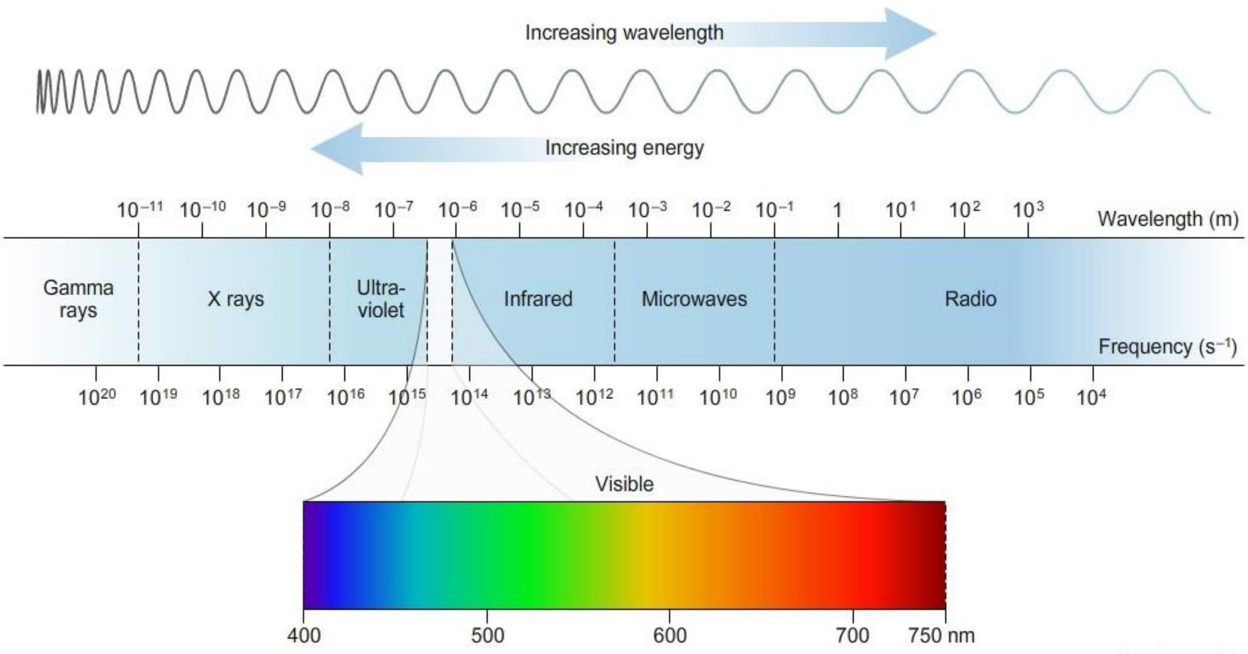


5) $[Ar]3d^9$

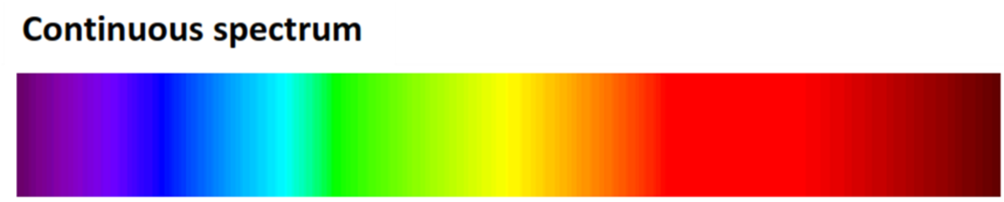


The electromagnetic spectrum

- The electromagnetic spectrum is the range of wavelengths, or frequencies, of electromagnetic radiation.
- It extends from radio rays (low energy, long wavelength, low frequency) to gamma rays (high energy, short wavelength, high frequency).

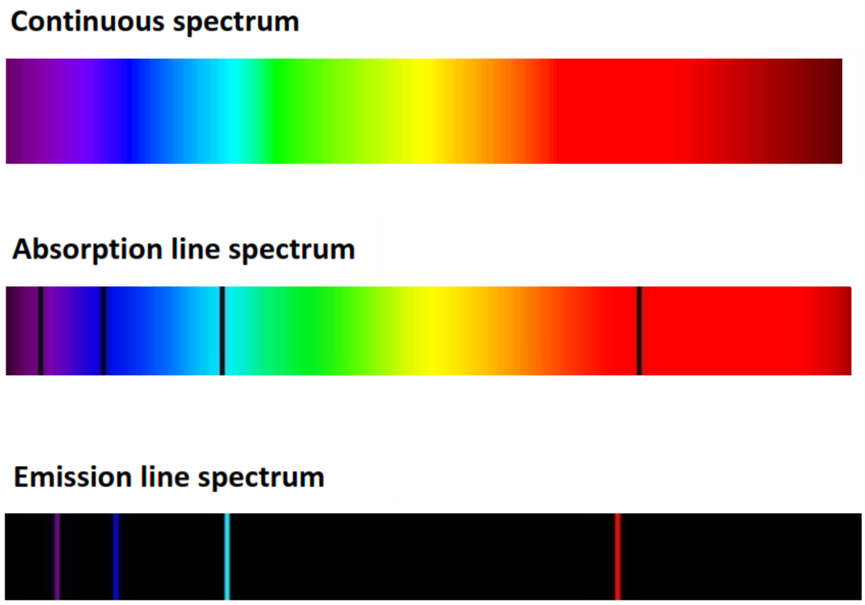


- Higher energy corresponds to higher frequency and shorter wavelength.
- Lower energy corresponds to lower frequency and longer wavelength.
- A continuous spectrum (shown below) shows all the wavelengths, or frequencies, of visible light.

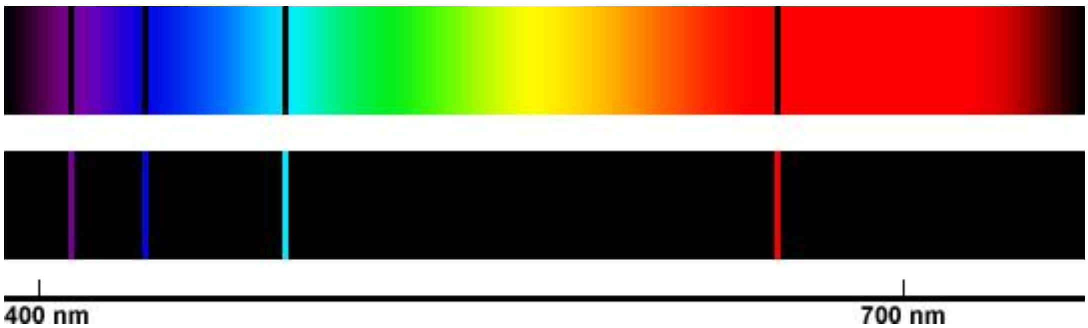


Line spectra

- The two kinds of line spectra are absorption line spectra and emission line spectra.
- Different elements have different line spectra, and they can be used to identify unknown elements.
- They are shown below compared to a continuous spectrum.



Concept check:



1) Label the spectra above as absorption or emission line spectra.

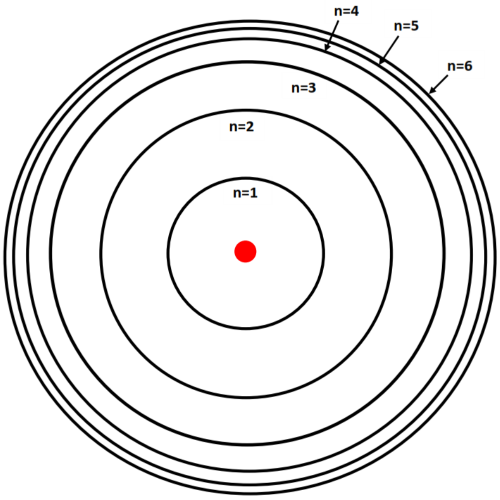
Top spectrum is absorption, bottom one is emission.

2) Describe the difference between the two line spectra.

Emission spectra have coloured lines on a black background, absorption spectra have black lines on a coloured background.

How are line spectra produced?

- The Bohr model of the atom has the protons and neutrons located in the nucleus and the electrons in energy levels around the nucleus.
- An electron can only have a certain amount of energy; its energy is quantised.



- Energy levels closest to the nucleus have lower energy and those further from the nucleus have higher energy.
- Electrons can transition between energy levels by either absorbing or emitting energy.
- An electron absorbs energy when it transitions to a higher energy level.
- An electron emits energy when it transitions to a lower energy level.
- The energy is in the form of photons of light (small packets of energy) and is related to the position of the light in the electromagnetic spectrum by the equation below (note that the use of this equation will not be assessed).

$$\mathbf{E = hf}$$

h = Plank's constant 6.63×10^{-34} J s^{-1}

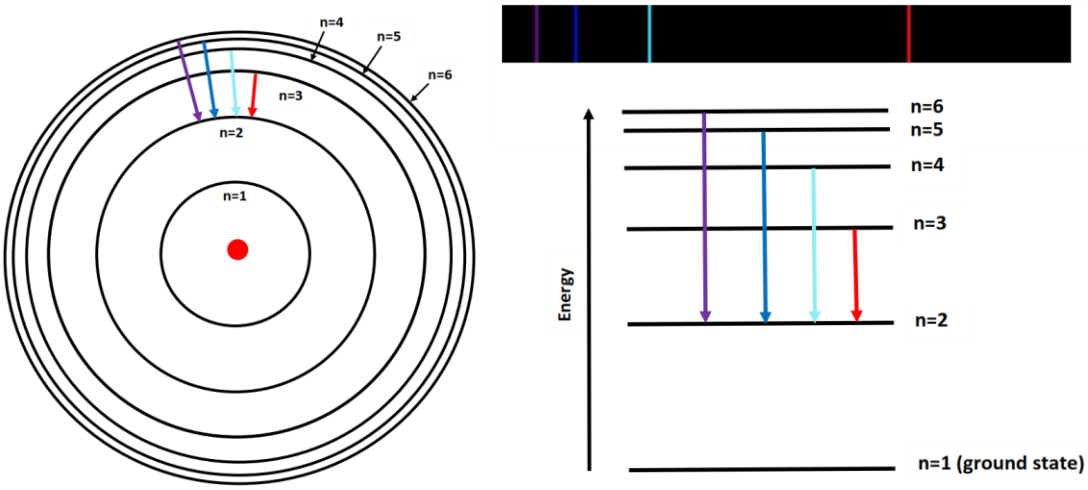
f = frequency

Summary:

- Electrons are located in energy levels within the atom.
- Electrons can only exist at certain energy levels.
- Electrons can transition to higher energy levels by absorbing energy.
- Electrons can transition to lower energy levels by emitting energy.

How is an emission line spectrum produced?

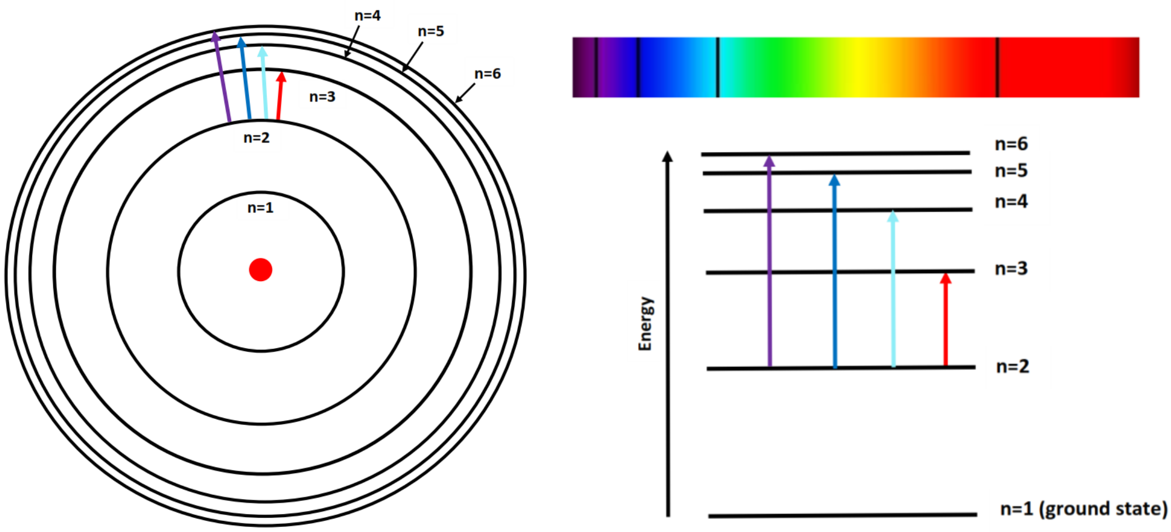
- The emission line spectrum of hydrogen is shown below.
- It has four colours on a black background that converge at higher energy (to the left).



- The emission line spectrum above is produced when an electron emits energy and transitions to a lower energy level (to n=2).
- The energy emitted by the electron corresponds to the wavelength, or frequency, of visible light.
- For example, when an electron transition from n=3 to n=2, the energy that is emitted corresponds to the wavelength, or frequency, of red light. This explains why a red line appears in the emission line spectrum above.

How is an absorption line spectrum produced?

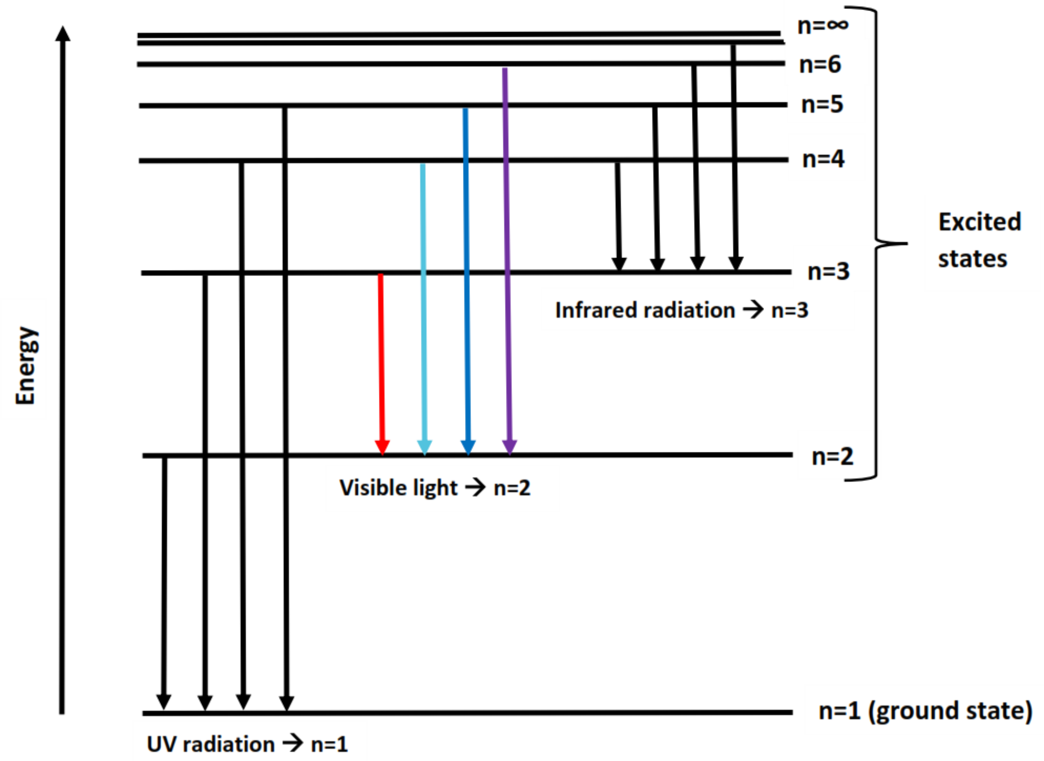
- The absorption line spectrum of hydrogen is shown below.
- It has 4 black lines on a coloured background. The black lines are in the same positions as the coloured lines on the emission line spectrum shown above.



- The absorption line spectrum above is produced when an electron absorbs energy and transitions to a higher energy level (from n=2).
- The energy absorbed by the electron corresponds to the to the wavelength, or frequency, of visible light.
- For example, when an electron transition from n=2 to n=3, the energy that is absorbed corresponds to the wavelength, or frequency, of red light. This explains why the colour red is missing in the absorption line spectrum above.

The hydrogen emission spectrum

- The hydrogen emission spectrum is shown below.



- Electron transitions to the first energy level (n=1) release the highest amount of energy and are in the UV region of the electromagnetic spectrum.
- Electron transitions to the n=2 energy level emit energy that corresponds to the frequency, or wavelength of visible light.
- Electron transitions to the n=3 energy level emit energy in the infra-red region of the electromagnetic spectrum.
- The longer the arrow, the greater the amount of energy emitted (or absorbed).
- Higher energy corresponds to higher frequency and shorter wavelength.
- Lower energy corresponds to lower frequency and longer wavelength.