

# Atomic structure

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IB CHEMISTRY HL

Michael Sugiyama Jones  
[WWW.MSJCHEM.COM](http://WWW.MSJCHEM.COM)

**Understandings:**

- In an emission spectrum, the limit of convergence at higher frequency corresponds to the first ionization energy.
- Trends in first ionization energy across periods account for the existence of main energy levels and sub-levels in atoms.
- Successive ionization energy data for an element give information that shows relations to electron configurations.

**Applications and skills:**

- Solving problems using  $E = h\nu$
- Calculation of the value of the first ionization energy from spectral data which gives the wavelength or frequency of the convergence limit. Deduction of the group of an element from its successive ionization energy data.
- Explanation of the trends and discontinuities in first ionization energy across a period.

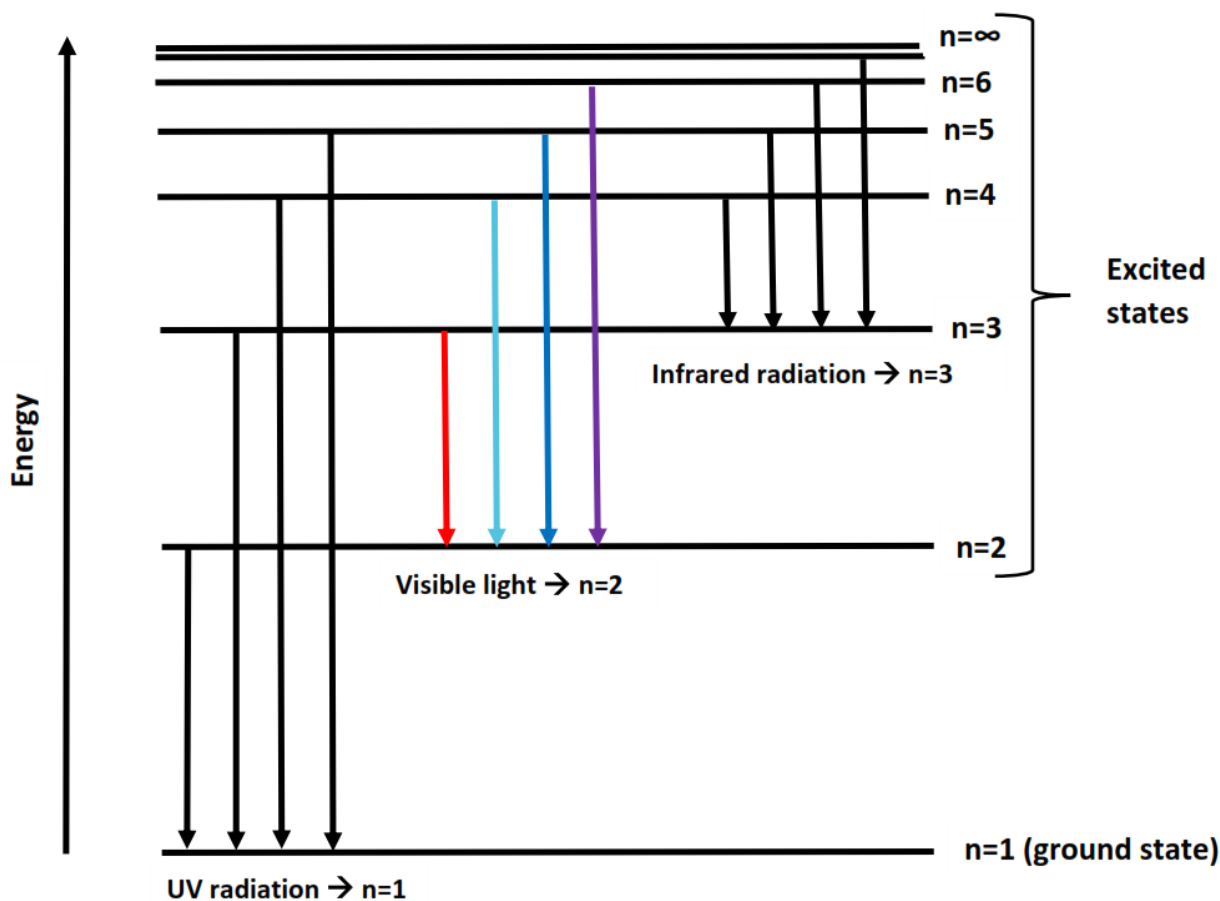
**Guidance:**

- The value of Planck's constant ( $h$ ) and  $E = h\nu$  are given in the data booklet in sections 1 and 2.
- Use of the Rydberg formula is not expected in calculations of ionization energy.

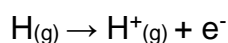
## Electrons in the atom

### Convergence limit

- In an atom, the highest possible energy level corresponds to the frequency at which the spectral lines converge.
- By determining the frequency at which the spectral lines converge (known as the convergence limit) the ionisation energy can be calculated.



- If enough energy is supplied, the one electron in the hydrogen atom can be promoted to the infinity level.
- At this point, the electron has been removed from the attraction of the nucleus and the atom has been ionized to form the  $H^+$  ion.



- The amount of energy required to ionize the hydrogen atom corresponds to the energy the electron would emit if it fell back down to the  $n=1$  energy level from  $n=\infty$

**Example:**

In the hydrogen emission spectrum, the transition from  $n=\infty$  to  $n=1$  produces a line in the UV spectrum with a wavelength of 91.2 nm (convergence limit).

$$c = \lambda\nu$$

$$3.00 \times 10^8 \text{ ms}^{-1} = (9.12 \times 10^{-8} \text{ m})\nu$$

$$\nu = \frac{3.00 \times 10^8}{9.12 \times 10^{-8}} = 3.29 \times 10^{15} \text{ s}^{-1}$$

$$E = h\nu$$

$$E = (6.63 \times 10^{-34} \text{ Js})(3.29 \times 10^{15} \text{ s}^{-1})$$

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

$$(6.02 \times 10^{23})(2.18 \times 10^{-18} \text{ J}) = 1310 \text{ kJmol}^{-1}$$

**Exercises:**

- 1) Define the term *convergence limit*.
- 2) From what transition between energy levels can the convergence limit be found for the hydrogen atom?
- 3) What has occurred when the electron is said to be in the  $n=\infty$  energy level?
- 4) The convergence limit for the sodium atom has a wavelength of 242nm. Calculate the first ionization energy of sodium from this data.

The two equations you need are  $c = \lambda\nu$  and  $E=h\nu$

Planck's constant =  $6.63 \times 10^{-34} \text{ Js}$

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

## Calculating ionisation energy

Follow this link:

<http://physics.nist.gov/PhysRefData/Handbook/periodictable.htm>

Part 1 – Calculating ionisation energy from the convergence limit.

- 1) Click on hydrogen from the periodic table.
- 2) At the top of the screen, click on energy levels.

**Hydrogen (H)**

Main Page	Other Elements				Neutral Atom				
	Finding List	Element Name	Atomic Number	Periodic Table	Atomic Data	Strong Lines	Persistent Lines	Energy Levels	Ref.
Switch to ASCII Version									

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- 3) Scroll to the bottom of the table:

H	Limit	109678.7717	MK00a
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Convergence limit

- 4) The circled value is the wavenumber for the convergence limit of the hydrogen atom. The wavenumber can be converted to wavelength by taking the reciprocal (1/wavenumber).

- 5) Now that you have calculated the wavelength of the convergence limit, the ionisation energy can be calculated.

(i) Convert from wavelength to frequency

(ii) Use the equation below to find the energy to remove one electron.

(ii) Multiply by Avogadro's constant to get the energy to remove one mole of electrons.

## Part 2

- Choose 2 other elements from the periodic table and calculate the ionisation energy using the method above.
- For elements other than hydrogen, be sure to click on the neutral atom tab (see example for carbon below):
- Compare your answer to the value in the data booklet in table 8.

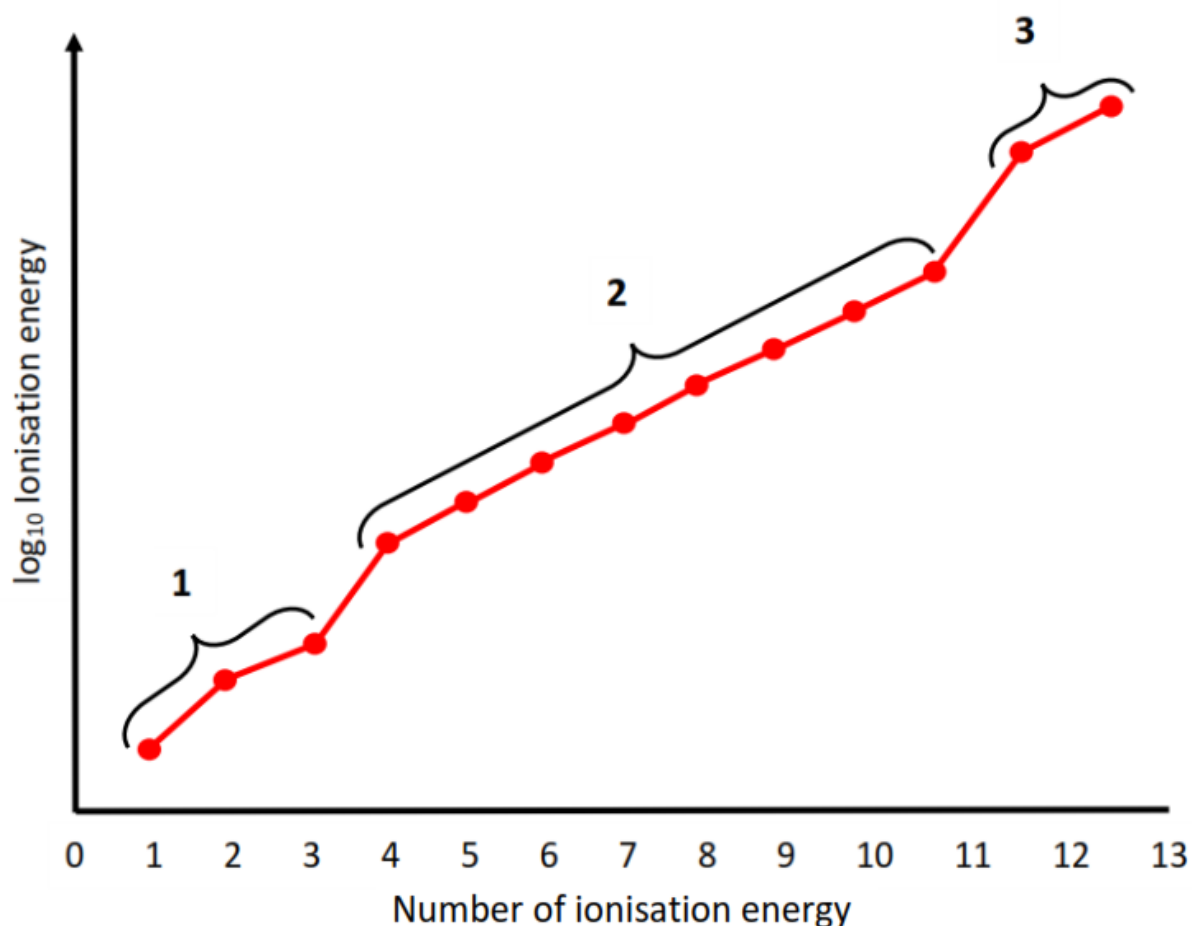
**Carbon (C)**

<b>Main Page</b> Switch to ASCII Version	<b>Finding List</b>	<b>Other Elements</b>			<b>Atomic Data</b>	<b>Strong Lines</b>	<b>Neutral Atom</b>		<b>Singly Ionized</b>		<b>Ref.</b>
		<b>Element Name</b>	<b>Atomic Number</b>	<b>Periodic Table</b>			<b>Persistent Lines</b>	<b>Energy Levels</b>	<b>Persistent Lines</b>	<b>Energy Levels</b>	

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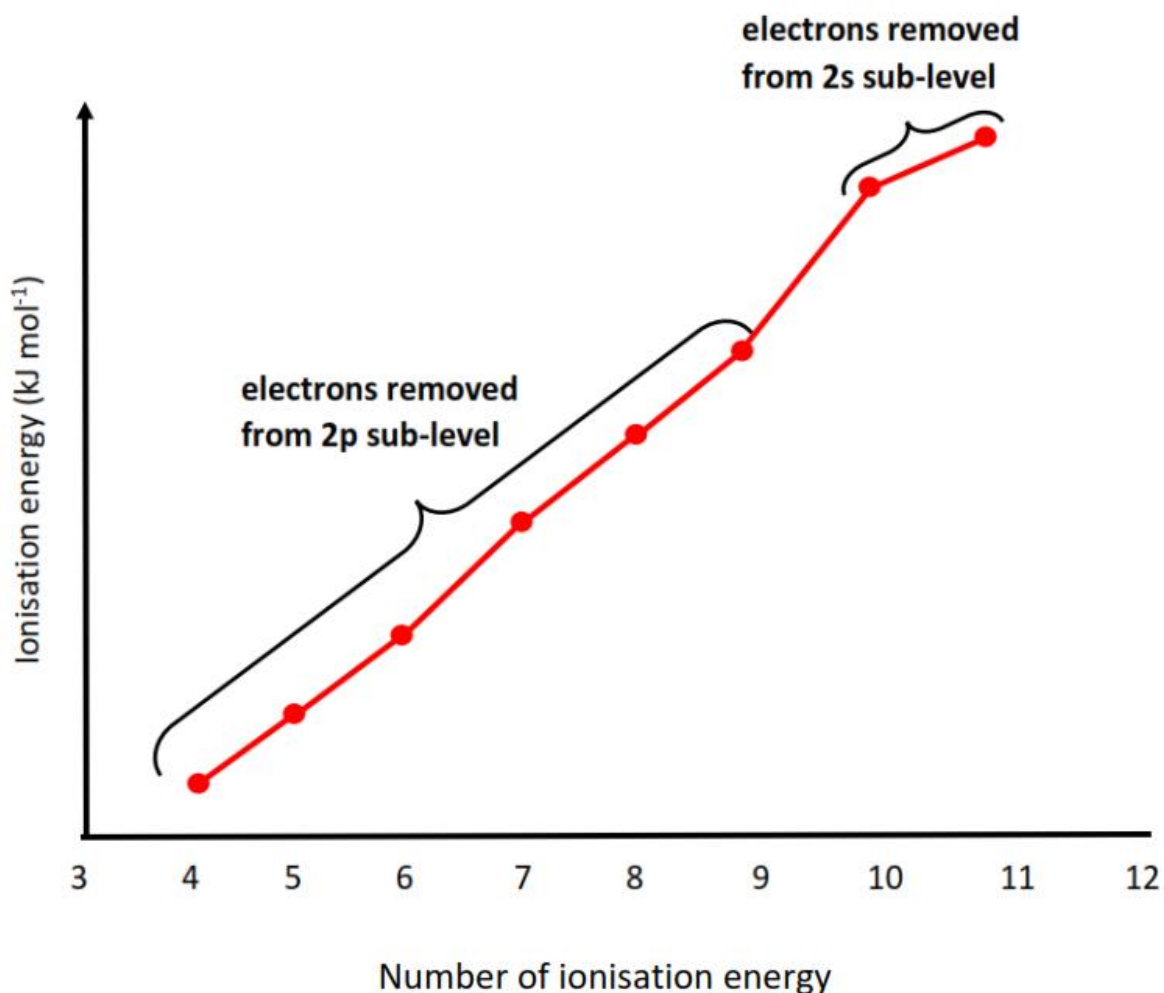
## Evidence from ionisation energies

Successive ionisation energies of aluminium



1. These electrons are removed from the energy level furthest from the nucleus ( $n=3$ ), therefore they require the less energy to remove (weaker electrostatic attraction from the nucleus and shielding by inner electrons).
2. These electrons are removed from the second main energy level ( $n=2$ ). Notice the jump between the 3<sup>rd</sup> and 4<sup>th</sup> ionization energy. This is evidence of the existence of energy levels within the atom.
3. These electrons are being removed from the energy level closest to the nucleus ( $n=1$ ). These electrons require the most energy to remove because of the strong electrostatic attraction from the nucleus, and the lack of shielding from the positive nucleus.

## 4<sup>th</sup> to 11<sup>th</sup> ionisation energies of aluminium

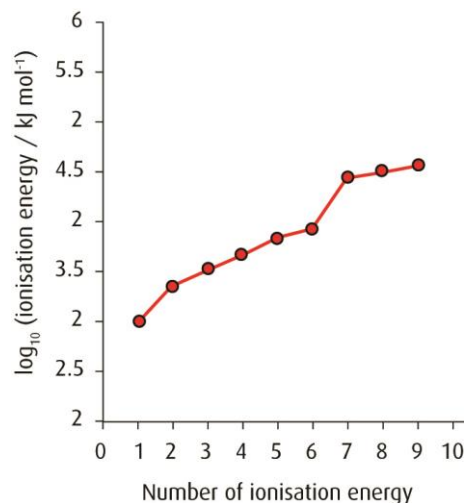
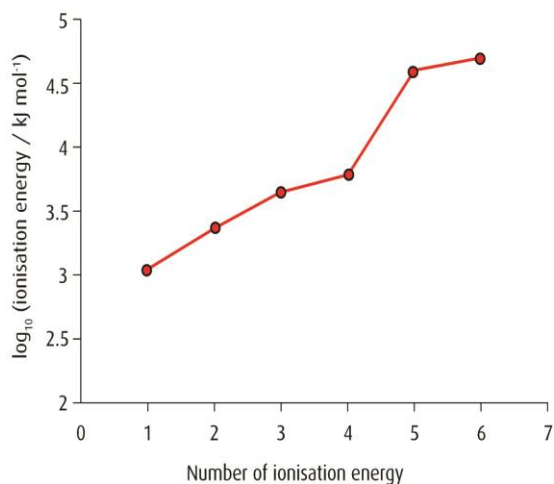


- The jump in ionisation energy between the 9<sup>th</sup> and 10<sup>th</sup> ionisation energy occurs because the 10<sup>th</sup> electron is being removed from the 2s orbital which is closer to the nucleus and experiences a stronger electrostatic attraction from the nucleus.
- The bigger jump in ionisation energy between the 6<sup>th</sup> and 7<sup>th</sup> compared to the 5<sup>th</sup> and 6<sup>th</sup> occurs because the 6<sup>th</sup> electron is removed from a doubly occupied p orbital.
- This requires less energy to remove due to the repulsion between electrons.



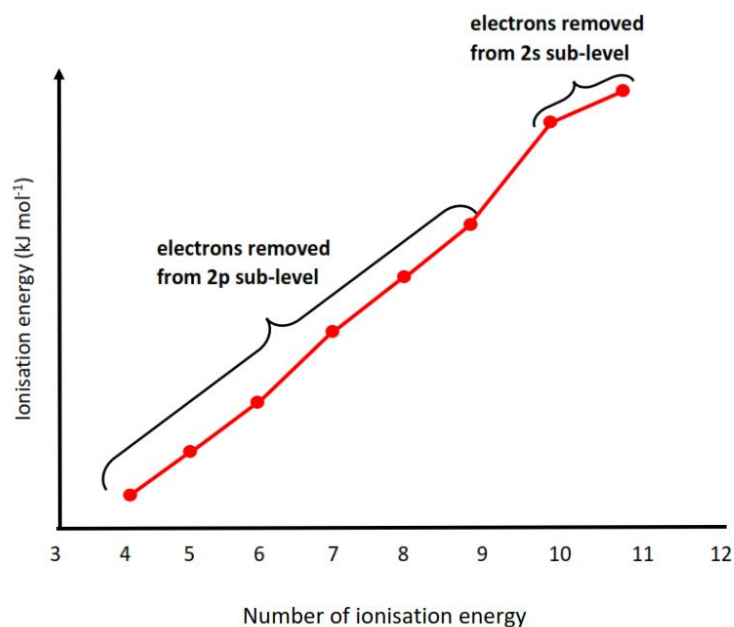
## Exercises:

- 1) From the graphs of successive ionisation energies below, explain which group of the periodic table the elements belong to.



- 2) Study the graph of 4<sup>th</sup> to 11<sup>th</sup> ionisation energies for aluminium.

a) Explain why there is a large increase in ionisation energy between the 9<sup>th</sup> and 10<sup>th</sup> ionisation energies.



b) Explain why the increase between the 6<sup>th</sup> and 7<sup>th</sup> ionisation energies is greater than the increase between the 5<sup>th</sup> and 6<sup>th</sup> ionisation energies.