

Atomic structure HL (answers)

IB CHEMISTRY HL

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

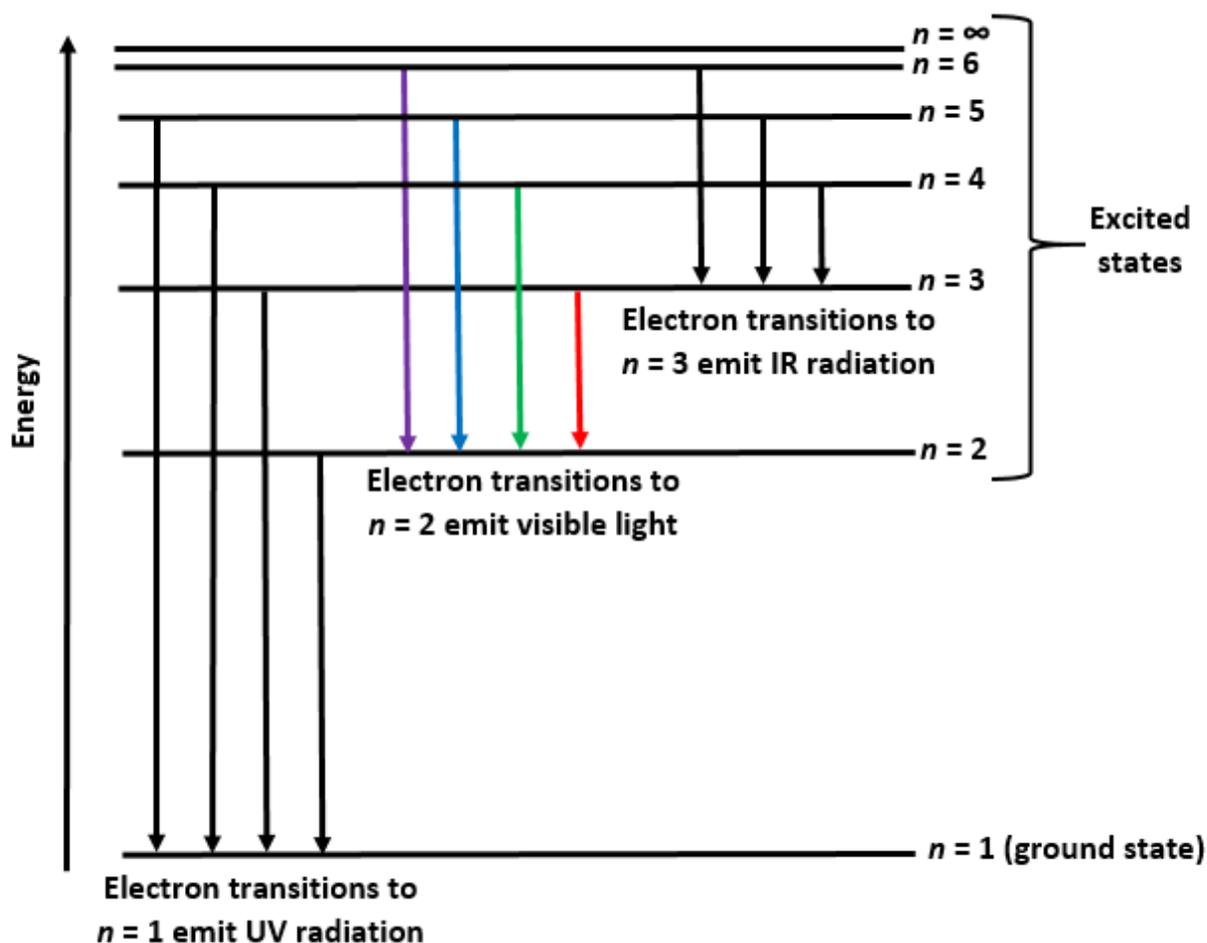
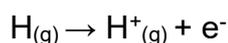
- Solving problems using $E = h\nu$
- Calculation of the value of the first ionization energy from spectral data which gives the wavelength or frequency of the convergence limit. Deduction of the group of an element from its successive ionization energy data.
- Explanation of the trends and discontinuities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

Ionisation energy and convergence limit

- In an atom, the highest possible energy level corresponds to the frequency at which the spectral lines converge ($n = \infty$).
- 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 electron in the hydrogen atom can be promoted from $n = 1$ to the infinity energy level, $n = \infty$.
- At this point, the electron has been removed from the attraction of the nucleus and the atom has been ionized to form a H^+ ion.



Calculations involving $E = hv$

$$E = hv \quad c = \lambda\nu$$

E is energy in Joules (J)

h is Planck's constant (6.63×10^{-34} J·s)

ν is the frequency in s^{-1} (or Hertz, Hz)

c is the speed of light (3.00×10^8 m s^{-1})

λ is the wavelength in m or nm ($1 \text{ m} = 1 \times 10^9$ nm)

Exercises: use the formulas and constants above to answer the following questions.

1. What is the frequency, in s^{-1} , of a photon of light with an energy of 2.24×10^{-19} J?

$$E = hv$$

$$2.24 \times 10^{-19} = 6.63 \times 10^{-34} \nu$$

$$\nu = 2.24 \times 10^{-19} / 6.63 \times 10^{-34}$$

$$\nu = 3.38 \times 10^{14} \text{ s}^{-1} = 8.88 \times 10^{-7} \text{ m} = 888 \text{ nm}$$

2. What is the wavelength, in m, of light with a frequency of $7.11 \times 10^{14} \text{ s}^{-1}$?

$$c = \lambda\nu$$

$$3.00 \times 10^8 = \lambda 7.11 \times 10^{14}$$

$$\lambda = 3.00 \times 10^8 / 7.11 \times 10^{14}$$

$$\lambda = 4.22 \times 10^{-7} \text{ m} = 422 \text{ nm}$$

3. A photon of light has a wavelength of 6.98×10^{-7} m. How much energy does it have in J?

$$c = \lambda\nu$$

$$3.00 \times 10^8 = 6.98 \times 10^{-7} \nu$$

$$\nu = 3.00 \times 10^8 / 6.98 \times 10^{-7}$$

$$\nu = 4.30 \times 10^{14} \text{ s}^{-1}$$

$$E = hv$$

$$E = 6.63 \times 10^{-34} \times 4.30 \times 10^{14}$$

$$E = 2.85 \times 10^{-19} \text{ J}$$

4. How much energy, in J, does a photon of light have if it has a wavelength of 5.26×10^{-7} m?

$$c = \lambda\nu$$

$$3.00 \times 10^8 = 5.26 \times 10^{-7} \nu$$

$$\nu = 3.00 \times 10^8 / 5.26 \times 10^{-7}$$

$$\nu = 5.70 \times 10^{14} \text{ s}^{-1}$$

$$E = hv$$

$$E = 6.63 \times 10^{-34} \times 5.70 \times 10^{14}$$

$$E = 3.78 \times 10^{-19} \text{ J}$$

5. What is the wavelength, in m, of a photon of light if it has an energy of 4.01×10^{-19} J?

$$E = h\nu$$

$$4.01 \times 10^{-19} = 6.63 \times 10^{-34} \nu$$

$$\nu = 4.01 \times 10^{-19} / 6.63 \times 10^{-34}$$

$$\nu = 6.05 \times 10^{14} \text{ s}^{-1}$$

$$c = \lambda\nu$$

$$3.00 \times 10^8 = \lambda 6.05 \times 10^{14} \text{ s}^{-1}$$

$$\lambda = 3.00 \times 10^8 / 6.05 \times 10^{14} \text{ s}^{-1}$$

$$\lambda = 4.96 \times 10^{-7} \text{ m} = 496 \text{ nm}$$

6. What is the wavelength, in m, of a photon of light with an energy of 1.66×10^{-19} J?

$$E = h\nu$$

$$1.66 \times 10^{-19} = 6.63 \times 10^{-34} \nu$$

$$\nu = 1.66 \times 10^{-19} / 6.63 \times 10^{-34}$$

$$\nu = 2.50 \times 10^{14} \text{ s}^{-1}$$

$$c = \lambda\nu$$

$$3.00 \times 10^8 = \lambda 2.50 \times 10^{14}$$

$$\lambda = 3.00 \times 10^8 / 2.50 \times 10^{14}$$

$$\lambda = 1.20 \times 10^{-6} \text{ m} = 1200 \text{ nm}$$

Calculating ionisation energy

Example 1: In the hydrogen emission spectrum, the transition from $n = \infty$ to $n = 1$ produces a line in the UV spectrum with a wavelength of 9.12×10^{-8} m. Calculate the ionisation energy of a hydrogen atom.

- First, convert from wavelength to frequency:

$$c = \lambda \nu$$

$$3.00 \times 10^8 = 9.12 \times 10^{-8} \nu$$

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

- Next, calculate the energy to remove one electron from one hydrogen atom:

$$E = h\nu$$

$$E = 6.63 \times 10^{-34} \times 3.29 \times 10^{15}$$

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

- Finally, calculate the energy to remove one mole of electrons from one mole of hydrogen atom, in kJ mol^{-1}

$$(6.02 \times 10^{23} \times 2.18 \times 10^{-18}) / 1000 = 1310 \text{ kJ mol}^{-1}$$

Example 2: Determine the wavelength of a photon that will cause the first ionisation of helium. The first ionisation energy of helium is 2372 kJ mol^{-1} .

- First, calculate the energy to remove one electron from one helium atom:

$$E = \frac{2372000}{6.02 \times 10^{23}} = 3.94 \times 10^{-18} \text{ J}$$

- Next, calculate the frequency of the photon:

$$E = h\nu$$

$$3.94 \times 10^{-18} = 6.63 \times 10^{-34} \nu$$

$$\nu = 5.94 \times 10^{15} \text{ s}^{-1}$$

- Finally convert from frequency to wavelength:

$$c = \lambda \nu$$

$$3.00 \times 10^8 = 5.94 \times 10^{15} \lambda$$

$$\lambda = \frac{3.00 \times 10^8}{5.94 \times 10^{15}} = 5.05 \times 10^{-8} \text{ m}$$

Exercises:

1. Define the term *convergence limit*.

The convergence limit is the frequency (or wavelength) at which the spectral lines converge – from this the ionisation energy of an atom can be calculated.

2. Which transition corresponds to the ionisation of hydrogen in the ground state?

The transition is from energy level $n = 1$ to $n = \infty$.

3. What has occurred when the electron is in the $n = \infty$ energy level?

When the electron is in the $n = \infty$ energy level, the atom has been ionised. At this point, the electron has been removed from the attraction of the nucleus.

4. The convergence limit for the sodium atom has a wavelength of 2.42×10^{-7} m.
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 = 6.63×10^{-34} J s

$c = 3.00 \times 10^8$ m s⁻¹

You are given the wavelength, so use the equation $c = \lambda\nu$ to find the frequency.

$$c = \lambda\nu$$

$$3.00 \times 10^8 \text{ m s}^{-1} = 2.42 \times 10^{-7} \nu$$

$$\nu = \frac{3.00 \times 10^8}{2.42 \times 10^{-7}} = 1.24 \times 10^{15} \text{ s}^{-1}$$

Next use the equation below to find the energy to remove one electron.

$$E = h\nu$$

$$E = (6.63 \times 10^{-34}) (1.24 \times 10^{15})$$

$$E = 8.22 \times 10^{-19} \text{ J}$$

Multiply by Avogadro's constant to get the energy to remove one mole of electrons (multiply by 6.02×10^{23} and divide by 1000)

$$(6.02 \times 10^{23} \times 8.22 \times 10^{-19}) / 1000 = 495 \text{ kJ mol}^{-1}$$

5. Calculate the frequency of a photon that will cause the first ionisation of copper. The first ionisation energy of copper is 745 kJ mol^{-1} .

First, calculate the energy to remove one electron from one helium atom:

$$E = \frac{745000}{6.02 \times 10^{23}} = 1.24 \times 10^{-18} \text{ J}$$

Next, calculate the frequency of the photon:

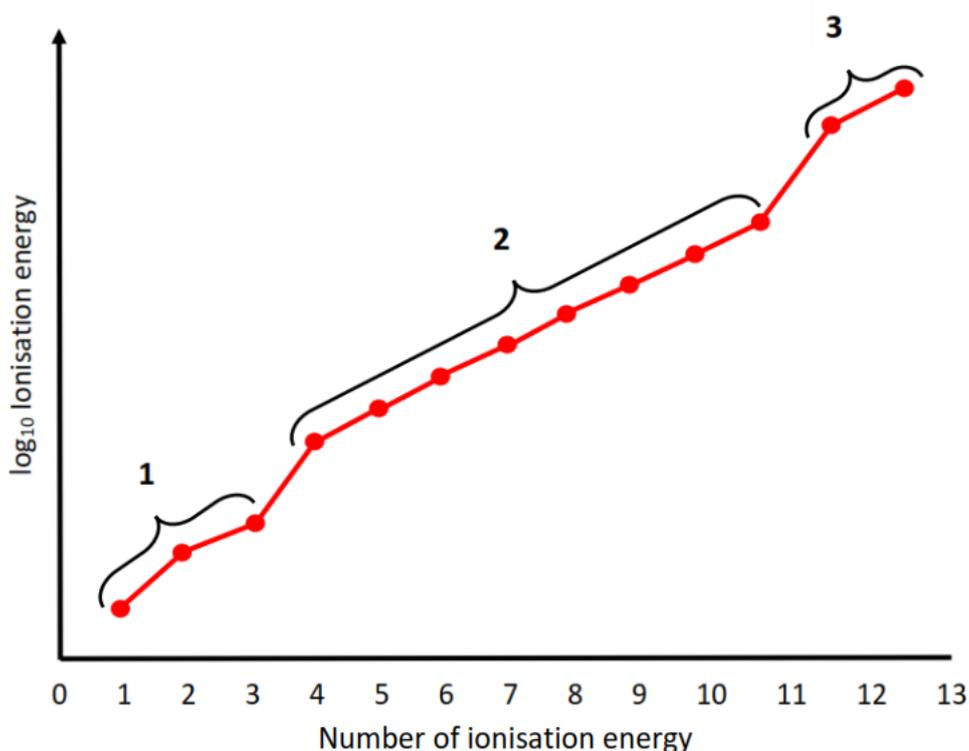
$$E = h\nu$$

$$1.24 \times 10^{-18} = 6.63 \times 10^{-34} \nu$$

$$\nu = 1.87 \times 10^{15} \text{ s}^{-1}$$

Successive ionisation energies

- Successive ionisation energies increase because as more electrons are removed from an atom or ion, the nucleus attracts the remaining electrons more strongly.
- We can determine to which group an element belongs to by looking at a graph of successive ionisation energies.
- The graph below shows the successive ionisation energies of aluminium.

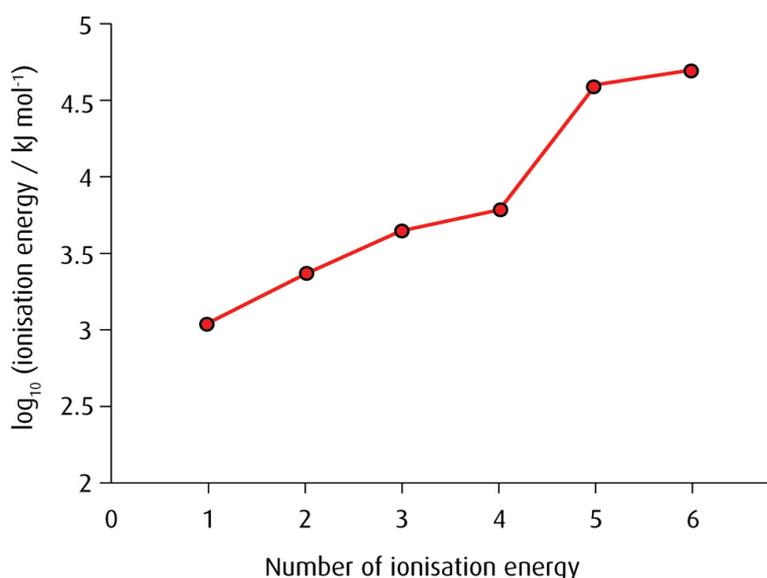


We can divide the graph into three sections:

1. These outer 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 3rd and 4th ionisation energies. This is evidence of the existence of energy levels within the atom and tells us that aluminium is located in group 13 of the periodic table (because it has 3 valence electrons).
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.

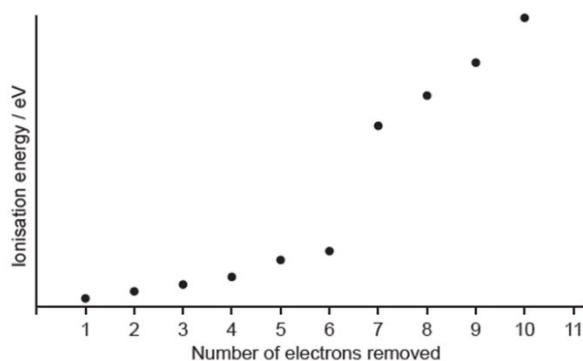
Exercises

1. Explain why the successive ionisation energies of an element show an increase. Successive ionisation energies increase because as more electrons are removed, the nucleus attracts the remaining electrons more strongly (the electrons are being removed from an increasingly positive ion).
2. From the graph of successive ionisation energies below, explain to which group of the periodic table the elements belong.



The element belongs in group 14; there is a large increase in ionisation energy between the 4th and 5th ionisation energies. The 5th electron is being removed from an energy level closer to the nucleus, which experiences electrostatic attraction and requires more energy to remove.

3. The graph below shows the first ten ionisation energies of an element. To which group does the element belong?



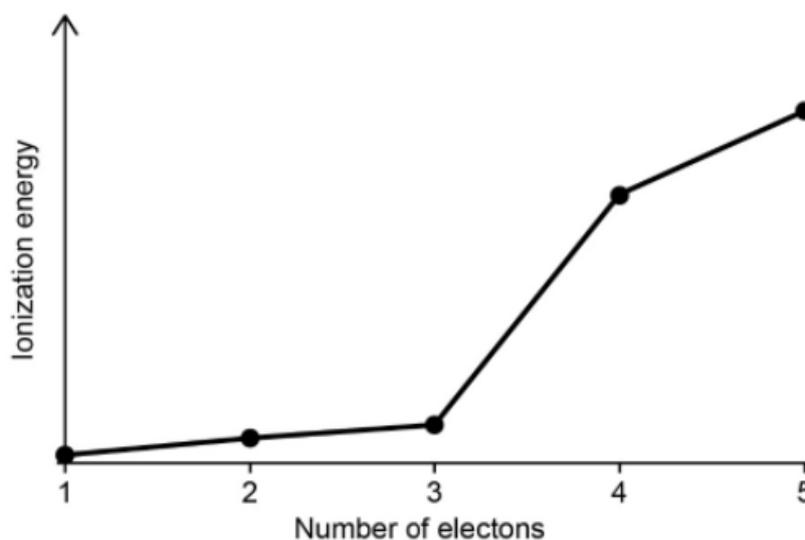
The element is located in group 16 (sulfur) as it has a large increase in ionisation energy after the 6th electron is removed.

4. From the table of data shown below, explain to which group the element belongs.

	1 st	2 nd	3 rd	4 th
Ionisation energy (kJ mol ⁻¹)	420	3600	4400	5900

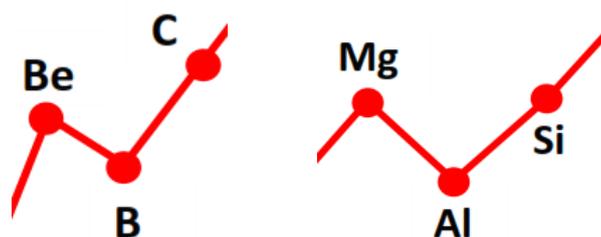
The element belongs to group 1. There is a large increase in ionisation energy between the first and second ionisation energies. The second electron is being removed from an energy level closest to the nucleus, therefore, the energy required to remove the electron shows a large increase.

5. Sketch a graph to show the relative values of the successive ionisation energies of boron.



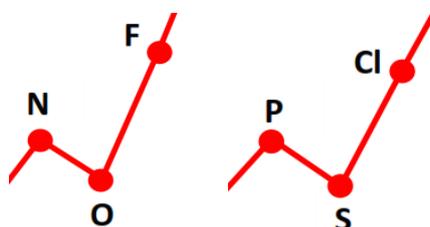
Large increase after 3rd electron is removed (total of 5 electrons removed).

Discontinuities in ionisation energy across a period (Be to B and Mg to Al)



- Be has the electronic configuration $1s^2 2s^2$
- B has the electronic configuration $1s^2 2s^2 2p^1$
- Electrons in p orbitals are of higher energy and further from the nucleus than electrons in s orbitals, therefore they require less energy to remove.
- The same explanation can be applied for the drop in ionisation energy from Mg to Al, except that the electron configurations are $1s^2 2s^2 2p^6 3s^2$ and $1s^2 2s^2 2p^6 3s^2 3p^1$

N to O and P to S



- N has the electronic configuration $1s^2 2s^2 2p^3$
- O has the electronic configuration $1s^2 2s^2 2p^4$
- For oxygen, the electron is removed from a doubly occupied p orbital. An electron in a doubly occupied orbital is repelled by the other electron and requires less energy to remove than an electron in a half-filled orbital.



Exercises:

1. Explain the reason for the decrease in ionisation energy between Mg and Al.

Mg has the electronic configuration $1s^2 2s^2 2p^6 3s^2$, Al has the electronic configuration $1s^2 2s^2 2p^6 3s^2 3p^1$. Electrons in p orbitals are of higher energy and further from the nucleus than electrons in s orbitals, therefore, they require less energy to remove.

2. Explain the reason for the decrease in ionisation energy between P and S.

P has the electronic configuration $1s^2 2s^2 2p^6 3s^2 3p^3$. S has the electronic configuration $1s^2 2s^2 2p^6 3s^2 3p^4$. For sulfur, the electron is removed from a doubly occupied p orbital. An electron in a doubly occupied orbital is repelled by the other electron and requires less energy to remove than an electron in a half-filled orbital.