Atomic structure (answers)

IB CHEMISTRY HL

Michael Sugiyama Jones
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 $E = \mathrm{h}\upsilon$
- 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.

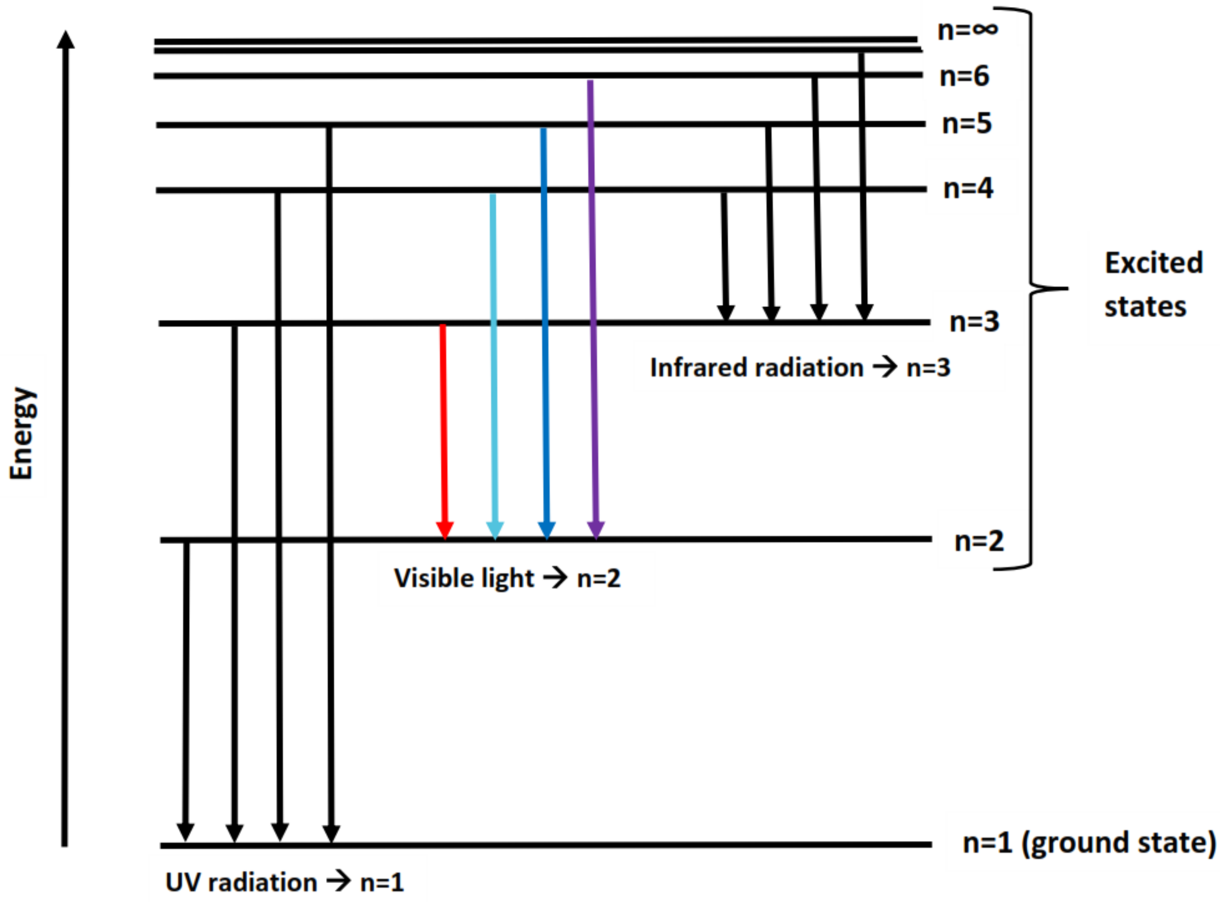
Guidance:

- The value of Planck's constant (h) and $E= hv$ 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.

$$H_{(g)} \rightarrow H^{+}_{(g)} + e^{-}$$

- 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=∞

Example:

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

$$c = \lambda\nu$$

$$3.00 \text{ x } 10^{8} \text{ ms}^{-1} = (9.12\times10^{-8})\nu$$

$$\nu = \frac{3.00\times10^{8}}{9.12\times10^{-8}} = 3.29 \text{ x } 10^{15} \text{ s}^{-1}$$

$$E=h\nu$$

$$E = (6.63 \text{ x } 10^{-34})(3.29 \text{ x } 10^{15})$$

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

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

Exercises:

1) Define the term *convergence limit*.

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

2) From what transition between energy levels can the convergence limit be found for the hydrogen atom?

The convergence limit for the hydrogen atom can be found from the transition from energy level n=∞ to n=1.

3) What has occurred when the electron is said to be in the n=∞ energy level?

When the electron is said to be in the n=∞ energy level, the atom has been ionised.

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=hv

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

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

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

$$c = \lambda\nu$$

$$3.00 \text{ x } 10^{8} \text{ ms}^{-1} = \left(\frac{242}{1000000000}\right)\nu$$

$$\nu = \frac{3.00\times10^{8}}{2.42\times10^{-7}} = 1.24 \text{ x } 10^{15} \text{ s}^{-1}$$

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}

$$(6.02 \times 10^{23})(8.22 \times 10^{-19}) = 495 \text{ kJmol}^{-1}$$

Calculating ionisation energy

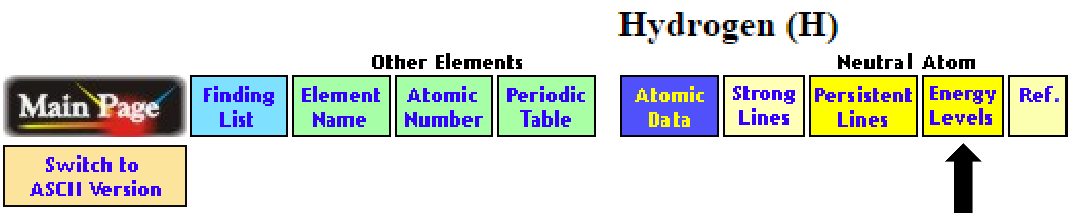
Follow this link:

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

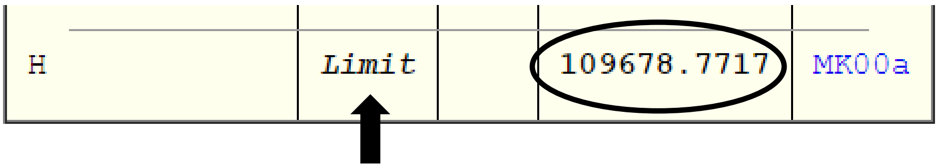
Part 1 – Calculating ionisation energy from the convergence limit.

1) Click on hydrogen from the periodic table.

2) At the top of the screen, click on energy levels.



3) Scroll to the bottom of the table:



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.

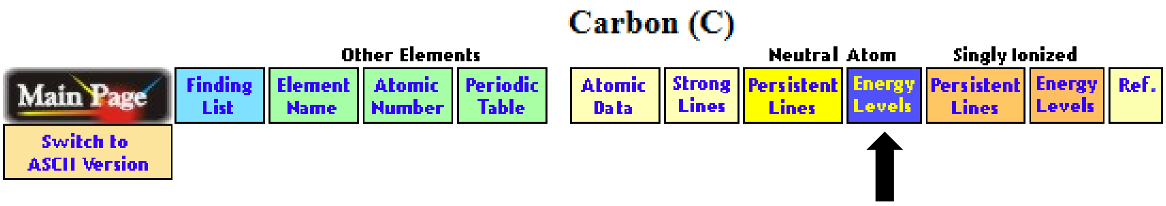
(i) Convert from wavelength to frequency

(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.

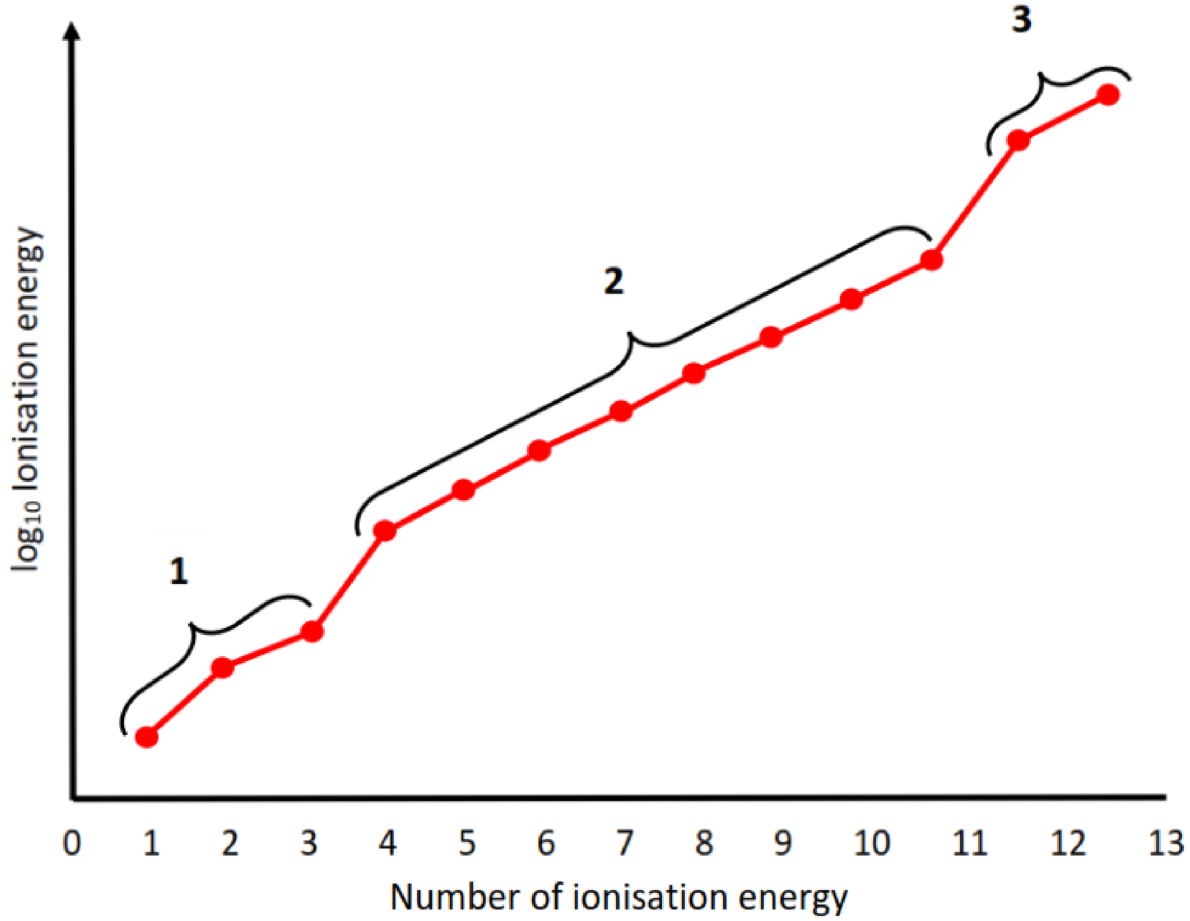
Part 2

- 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 you answer to the value in the data booklet in table 8.



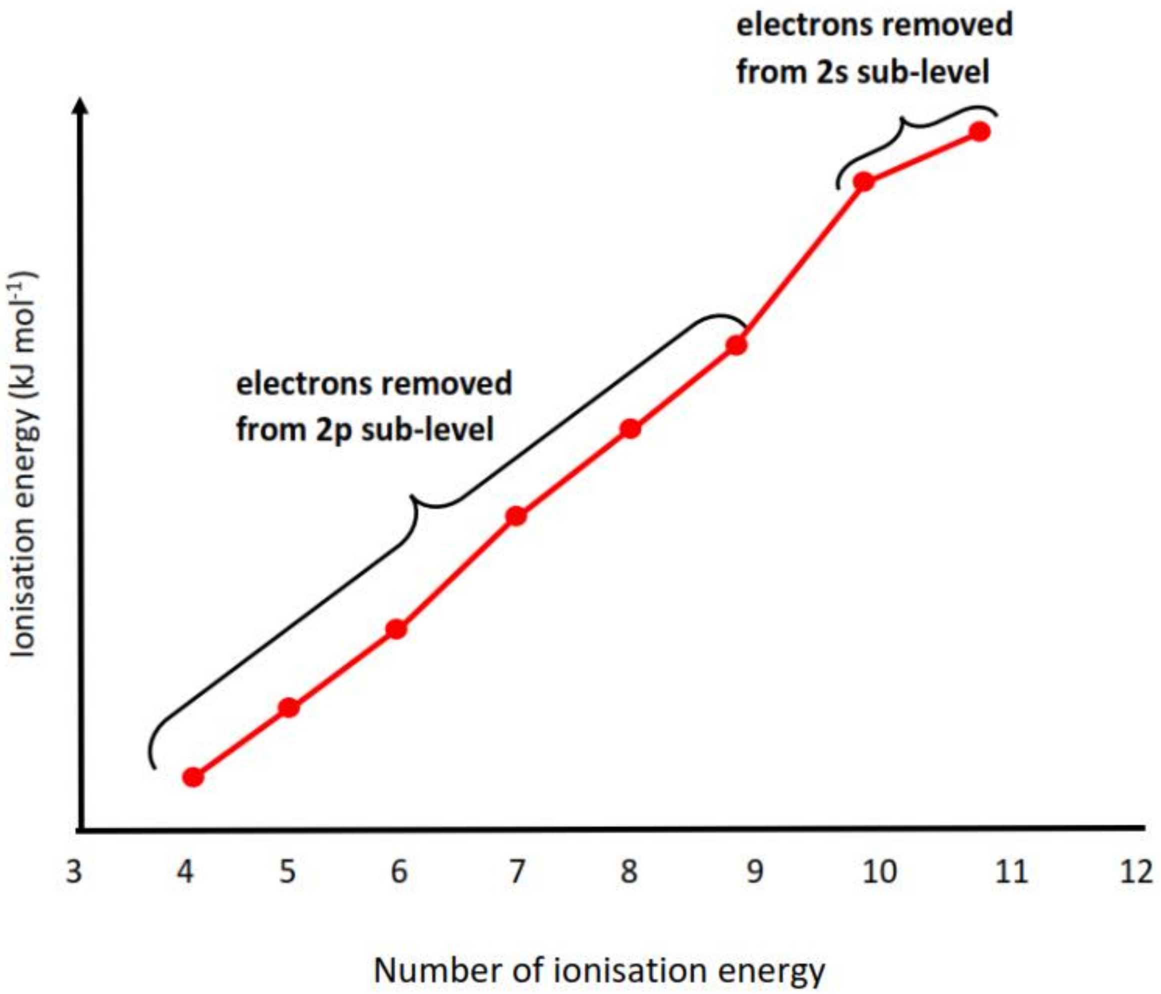
Evidence from ionisation energies

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 3rd and 4th 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.

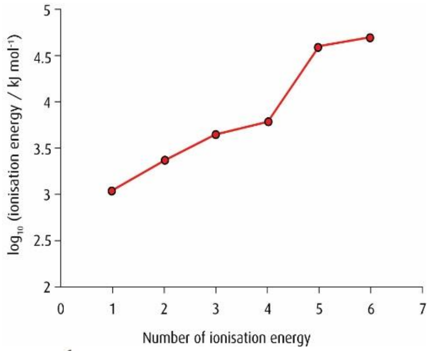
4th to 11th ionisation energies of aluminium



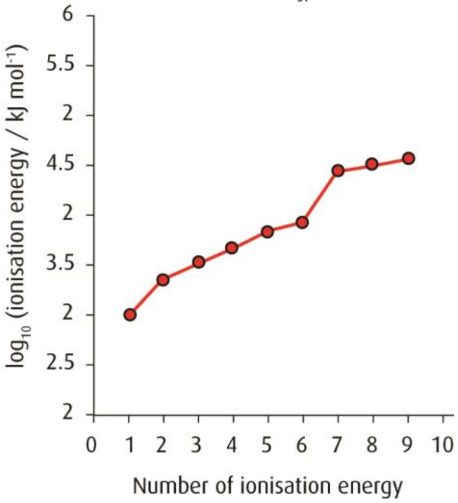
- The jump in ionisation energy between the 9th and 10th ionisation energy occurs because the 10th electron is being removed from the 2s orbital which is closer to the nucleus and experiences a stronger electrostatic attraction from the nucleus.
- The bigger jump in ionisation energy between the 6th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

Exercises:

1)



The element belongs in group 4 – there is a big jump 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 has a stronger electrostatic attraction and therefore requires more energy to remove.



The element belongs in group 6 – there is a big jump in ionisation energy between the 6th and 7th ionisation energies. The 7th electron is being removed from an energy level closer to the nucleus, which has a stronger electrostatic attraction and therefore requires more energy to remove.

2)

a) The jump in ionisation energy between the 9th and 10th occurs because the 10th electron is being removed from the 2s orbital which is closer to the nucleus and experiences a stronger electrostatic attraction.

b) The bigger jump in ionisation energy between the 6th and 7th compared to the 5th and 6th is because the 6th electron is removed from a doubly occupied p orbital. This requires less energy to remove due to the repulsion between electrons.