ELAINE PEH (COPYRIGHTED) © 70 FT 21,3 M Chapter 1 Atomic Stucture 25 FT



- Relatively straight forward chapter
- 4 key concepts

CHAPTER ANALYSIS



- Always tested
- The foundations for all calculations



• Heavy overall weightage as it is always incorporated into other chapters

KEY CONCEPT

Properties of The Three Sub-Atomic Particles Quantum Mechanical Model of the Atom Writing Electronic Configurations Ionisation Energy

ATOM

- The smallest particle of an element.
- Made up of sub-atomic particles proton, neutron, electron.
- $^{A}_{Z}X$
- X = symbol of the element
- A = atomic mass (nucleon number) = total number of protons and neutrons
- Z = atomic number (proton number)



BEHAVIOUR IN AN ELECTRIC FIELD



• The angle of deflection of particles depends on their mass and charges.

$$\angle$$
 deflection = k $\frac{\text{charge}}{\text{mass}}$
k = proportionality constant



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Protons and neutrons are found in the nucleus of an atom whereas electrons are found in spaces outside the nucleus.

These spaces can be categorised as (1) principal quantum shells (2) subshells (3) orbitals

Based on where they are found, each electron within the same atom have different energy level.

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Each principal quantum number indicates the principal quantum shell. Each principal quantum shell (n = 1, 2, 3, or 4) contains either 1 (s), 2 (s, p), 3 (s, p, d), or 4 (s, p, d, f) subshells. The ssubshell has 1 orbital, p-subshell has 3 orbitals, d-subshell has 5 orbitals. Each orbital holds a maximum of 2 electrons with opposite spins.

Principal	Number	Name of	Number	Maximum
Quantum	of	Subshell	of Orbital	number of
Shell	Subshell			electrons
				(2n ²)
n = 1	1	1s	1	2
n = 2	2	2s, 2p	1+3	8
n = 3	3	3s, 3p, 3d	1+3+5	18
n = 4	4	4s, 4p, 4d,	1+3+5+7	32
		4f		

Electron Located





Quantum Mechanical Model of the Atom

s-SUBSHELL

- Spherical in shape and non-directional
- As *n* increase, the distance of the electrons within the s-subshell also increases; electrons in 1s nearest to the nucleus.
- As *n* increase, the size of the s-subshell increases; size of 1s < size of 2s < size of 1s < size of 3s



p-SUBSHELL

- ٠
- **Dumbbell in shape**, consisting of 3 types of orbitals (p_x, p_y, p_z) As *n* increase, the size of the p-subshell increases; size of 2p < ٠ size of 3p



d-SUBSHELL

- **Dumbbell in shape**, consisting of 5 types of orbitals d_{xy} , d_{yz} , d_{xz} , d_z^2 , $d_x^2 d_y^2$ •
- ٠



RULE 1: AUFBAU / BUILDING-UP PRINCIPLE

1) Orbital with lowest energy level filled first. Note: The writing order is in order of increasing quantum number

2) Filling order = 1s, 2s, 2p, 3s, 3p, **4s**, **3d**, 4p, **5s**, **4d**... Exceptions: $Cr (1s^22s^22p^63s^23p^63d^54s^1)$ and $Cu (1s^22s^22p^63s^23p^63d^{10}4s^1)$ and elements in the same group

Boron has 5 electrons

electronic configuration:

electron-in-box diagram:

1s2 2s2 2p1

15

11 2s



Winder Generation of the second se

RULE 2: HUND'S RULE OF MULTIPLICITY

Orbitals within the same subshells are singly occupied by electrons with the same spin before the electrons are paired







allowed: singly filled with same spins in the same subshell not allowed: pairing without filling all orbitals first

not allowed: different spin

Nitrogen has 7 electrons.

electronic configuration: 1s² 2s² 2p³











2pz

RULE 3: PAULI'S EXCLUSION PRINCIPLE

- 1) An orbital cannot hold more than 2 electrons
- 2) The 2 electrons must be of opposite spins

Note: When 2 electrons are in the orbital, they are referred to as paired electrons. When there is only 1 electron in the orbital, it is referred to as an unpaired electron.

1		1	
1	1		
		L	
1		2	

	-	-	1
1	1		
1			



allowed: opposite spin

Helium has 2 electrons. electronic configuration:

electron-in-box diagram:



1s



not allowed: same spin in the orbital



interview of the second s

ELECTRONIC CONFIGURATION OF IONS

Cations are positively charges ions formed when electrons are lost. Anions are negatively charges ions formed when electrons are gained.

Step 1: Write the electronic configuration of the **atom**

Step 2:

Cation – **Remove** the number of electrons corresponding to the charge of the ion from the outermost shell of the ground state configuration of its atom

Anion – **Add** the number of electrons corresponding to the charge of the ion from the outermost shell of the ground state configuration of its atom

OriginalOr

TYPES OF NOTATION

1. Electrons-in-box Diagram

- Each box represents an orbital
- Boxes are drawn in order of increasing quantum number

2. spdf Notation

$1s^2$

- 1 = the principal quantum number (n = 1, 2, 3, 4)
- s = the subshell (s, p, d, f)
- 2 = number of electrons in the subshell

3. Noble Gas Core Configuration

• Substitute the spdf notation using the noble gas symbol prior to the element on the periodic table

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FIRST IONISATION ENERGY

First IE is the energy required to remove 1 mole of electrons from 1 mole of **gaseous atoms** to form 1 mole of **singly charged** gaseous (cat)ions

- Ca (g) → Ca⁺ (g) + e⁻
- Is always ∆H>0
- Units = kJ mol⁻¹

SECOND IONISATION ENERGY

Second IE is the energy required to remove 1 mole of electrons from 1 mole of singly charged gaseous (cat)ions to form 1 mole of doubly charged gaseous (cat)ions

- $Ca^+(g) \rightarrow Ca^{2+}(g) + e^-$
- Is always ∆H>0

Note: Will touch more on it in Chapter 5: The Period Table & Chapter 7: Chemical Energetics

GENERAL TREND OF IE AMONG ELEMENTS

IE are used to overcome the electrostatic forces of attraction between the valence electrons to be removed in an atom and the nucleus.

- General trend across the period: Increase
- General trend down the group: Decrease

Note: Will touch more on it in Chapter 5: The Periodic Table

Ionisation Energy (IE)

FACTORS AFFECTING THE MAGNITUDE OF IE (for general trend)

FACTOR 1: EFFECTIVE NUCLEAR CHARGE

- Effective Nuclear Charge takes into account both the nuclear charge and the shielding effect and is referred to as the net attractive forces between the nucleus and the valence electrons in an atom.
 - Nuclear Charge is dependent on the number of protons in the nucleus.
 - Shielding Effect is dependent on the number of inner shells present.
- It measures the **actual attraction** on the outer electrons by the nucleus
- Effective Nuclear Charge $\propto \frac{\text{Nuclear Charge}}{\text{Shielding Effect}}$; if both nuclear charge and shielding effect increase, need to compare which increase outweighs the other.

Note: Will touch again in Chapter 5: The Periodic Table

Ionisation Energy (IE)

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FACTORS AFFECTING THE MAGNITUDE OF IE (for exception cases against the general trend)

FACTOR 2: ORBITAL THE ELECTRON IS IN

- The **orbital (or sub-shell)** where the electron to be removed comes from also affects the IE.
- The further the orbital (or sub-shell) is away from the nucleus, the lower the IE is.

Note: The writing of electronic configuration will help in the explanation for this factor

FACTOR 3: INTER-ELECTRONIC REPULSION

- If 2 electrons are present in the **same** orbital, **interelectronic repulsion occurs** as they are of the same charge.
- IE is lowered if the electron to be removed from the orbital is paired with another electron in the same orbital as compared to a singly unpaired electron.

Note: The writing of electronic configuration will help in the explanation for this factor



USING IE TO DETERMINE THE POSITION OF THE ELEMENT

GRAPHICAL REPRESENTATION

- Big Jump = it indicates that the electrons removed come from a different principal quantum shells and hence there is a significant decrease in the shielding effect on the outermost electron due to a decrease in the number of inner shells between the electron to be removed and the nucleus
- Small Jump = it indicates that the electrons removed come from different sub-shells but is still within the same principal quantum shells



Energy

USING IE TO DETERMINE THE POSITION OF THE ELEMENT

MATHEMATICAL REPRESENTATION

- Calculate the difference between ionisation energy to determine where the "big jump" occurs
- Not commonly used to determine the position of the "small jump"

Ionisation Energy (IE)

source

Practice Questions

Question: Suggest the polarity of A and hence calculate the angles of deflection of ${}^{2}H^{+}$ nuclei and ${}^{3}He^{2+}$ nuclei.

Question: Sketch on the diagram below how beams of neutrons, protons, electrons and ${}^{2}H^{+}$ are effected by the electric field.





Answer: A is negatively charged. $\angle^{2}H^{+} = 2$, $\angle^{3}He^{2+} = 2.67$ (3 sf)

Question: Write the electronic configuration of sulfur using (i) Electrons-in-box Diagram (ii) spdf Notation and (iii) Noble Gas Core Configuration

Answer:



Question: Write the electronic configuration of S²⁻.

Answer: 1s² 2s² 2p⁶ 3s² 3p⁶

Question: Draw the electronic configuration of Cl-.



Question: Write the electronic configuration of Ga⁴⁺.

Answer: 1s² 2s² 2p⁶ 3s² 3p⁶ 3d⁹

Question: Draw the electronic configuration of Ca.



Question: Comment and explain the difference in the first ionisation energy of sodium with that of aluminum and potassium.

	Na	Al	К
1 st IE / kJ mol ⁻¹	483	593	429

Answer: The 1st IE of Na is lower than that of AI. Na has lower number of protons hence Na has a lower nuclear charge than AI. Both have approximately the same shielding effect as both have 2 inner electron shells as they belong to Period 3. The increase in nuclear charge thus outweigh the increase in shielding effect as the electron is added to the same valence electron. Therefore, the effective nuclear charge of Na is lower than that of AI hence lesser amount of energy is required to remove the electron in Na than in AI.

The 1st IE of Na is higher than that of K. K has larger number of protons hence K has a higher nuclear charge than Na. However, K has a significantly higher shielding effect than Na due to having 1 more inner electron shell (K is in Period 4 while Na is in Period 3) hence the increase in shielding effect of K outweighs the increase in nuclear charge. Therefore, the effective nuclear charge of K is lower than that of Na hence lesser amount of energy is required to remove the electron in K than in Na.

Question: Explain why the first ionisation of boron is lower than that of beryllium despite boron having a higher effective nuclear than beryllium.

	Ве	В
1 st IE / kJ mol ⁻¹	900	799



The outermost valence electron is removed from the 2s orbital in Be as compared to the removal of the electron in the 2p orbital in B. 2p orbital is further away from the nucleus as compared to 2s orbital. Therefore it is less attracted to the nucleus and hence lesser amount of energy is require to remove the electron from the 2p orbital nucleus as compared to the removal of electron in the 2s orbital. This thus resulted in Be having a higher IE than B.



Question: Explain why the first ionisation of oxygen is lower than that of nitrogen despite oxygen having a higher effective nuclear than beryllium.

	02	N ₂
1 st IE / kJ mol ⁻¹	1310	1400



Electron to be removed in N_2 is unpaired whereas in O_2 , the electron to be removed is paired with another electron in the $2p_x$ orbital. These two electrons in O_2 will experience inter-electronic repulsion hence it is easier to remove one of them than the p electron in N_2 . Hence N_2 has a higher 1st IE than O_2 .



Question: Explain the trend of the graph below for the ionisation energy of sodium

Log IE Successive ionization energy of sodium

Number of electron removed

Answer: There is an increasing in ionisation energy as the number of electrons removed increased. As the number of protons remain the same whereas the number of electrons decreases, shielding effect decreases and hence effective nuclear charge increases. As effective nuclear charge increase, the outermost electron is more strongly attracted to the nucleus hence more energy is required to remove it and hence ionisation increase.

There is a large jump in the ionisation energy between the removal of the 1st and the 2nd electron in Na. For the 1st ionisation energy, the electron removed is from the 3s orbital whereas for the 2nd ionisation energy, the electron removed is from the 2p orbital. This resulted in a significant decrease in the shielding effect as the electron removed from the 3s orbital has 2 inner shells shielding it from the nucleus whereas the electron removed from the 2p orbital only has 1 inner shell shielding it from the nucleus. As nuclear charge remains the same, the large decrease in the shielding effect resulted in a large increase in effective nuclear charge and hence a large jump in ionisation energy.

There is a smaller jump in ionisation energy between the removal of the 7th and the 8th electron in Na. For the 7th ionisation energy, the electron removed is from the 2p orbital whereas for the 8th ionisation energy, the electron removed is from the 2s orbital. As the 2s orbital is nearer to the nucleus as compared to 2p orbital, it is more strongly attracted to the nucleus and hence greater amount of energy is require to remove the electron from the 2s orbital nucleus as compared to the removal of electron in the 2p orbital. This thus resulted in the small jump from the 7th ionisation energy to the 8th ionisation energy.

However as the number of inner shells remain the same, the increase in ionisation energy is smaller as compared to the jump from the 1st ionisation energy to the 2nd ionisation energy where there is a decrease in the number of inner shells.

Question: Explain why the first ionisation of oxygen is lower than that of nitrogen despite oxygen having a higher effective nuclear than beryllium. The following graph on the right shows a sketch of the logarithm of the ionisation energy for the successive removal of all the electrons in an atom. Deduce which group and period the element belongs to in the Periodic Table and hence deduce its identity and write out the electronic configuration.

Answer: Group 7, Period 2, Fluorine, 1s² 2s² 2p⁵

Question: The successive ionisation energies in kJ mol⁻¹ of an element A are as follows: 740, 1500, 7700, 10500, 13600, 18000, 21700 Which group the element A belongs to?

Answer: Group 2



Question: The following graph shows a sketch of the 2nd ionisation energy of eight consecutive elements from A to H in the Periodic Table.

(i) Identify the group element A belongs to

(ii) Explain why the 2nd ionisation energy of B is higher than that of A and C.

Second ionisation energy / kJ mol-1



Answer:

(i) Group 5

(ii) The removal of the 2nd valence electron from B is from a partially filled p orbital as compared to A and B has a greater effective nuclear charge than A, hence resulting in higher amount of energy required.

The 2^{nd} valence electron from C experience inter-electronic repulsion as compared to the 2^{nd} valence electron from B, hence resulting in lower amount of energy required.

Test yourself!

(a) identify and describe protons, neutrons and electrons in terms of their relative charges and relative masses

(b) deduce the behaviour of beams of protons, neutrons and electrons in an electric field

(c) describe the distribution of mass and charges within an atom

(d) deduce the numbers of protons, neutrons and electrons present in both atoms and ions given proton and nucleon numbers (and charge)

(e) understanding nucleon numbers

- i. describe the contribution of protons and neutrons to atomic nuclei in terms of proton number and nucleon number
- ii. distinguish between isotopes on the basis of different numbers of neutrons present

(f) describe the number and relative energies of the s, p and d orbitals for the principal quantum numbers 1, 2 and 3 and also the 4s and 4p orbitals

Test yourself!

(g) describe the shapes of s, p and d orbitals [knowledge of wave functions is **not** required]

(h) state the electronic configuration of atoms and ions given the proton number (and charge)

(i) explain the factors influencing the ionisation energies of elements (link with Chapter 5: The Periodic Table)

(j) deduce the electronic configurations of elements from successive ionisation energy data

(k) interpret successive ionisation energy data of an element in terms of the position of that element within the Periodic Table



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