

1.2.1 Mass spectra, orbitals and ionisation evidence

Name: _____ Class: _____ Date: _____

Total: 37 marks

KEY WORDS mass-to-charge ratio • orbital • ionisation energy

Objective

Connect mass-to-charge, orbital occupancy and periodic data to justified atomic-structure conclusions. Distinguish evidence from assumptions.

1 Key knowledge and worked examples

■ Read charge before interpreting a peak

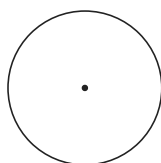
A mass-40 ion with charge 2+ appears at $m/z = 20$. A molecular ion of charge 1+ has an m/z equal to its relative molecular mass. A mass spectrometer ionises gaseous particles, accelerates ions, separates them by m/z and detects their abundance; the detector does not count neutrons directly.

■ Occupy orbitals before pairing

An s subshell has one orbital; p has three; d has five. Each orbital holds up to two electrons with opposite spins. Phosphorus is $[\text{Ne}]3s^23p^3$ with one electron in each 3p orbital. Sulfur is $[\text{Ne}]3s^23p^4$ with a pair in one 3p orbital, giving greater repulsion for that paired electron.

First ionisation is $\text{X}(\text{g}) \rightarrow \text{X}^+(\text{g}) + \text{e}^-$; third ionisation is $\text{X}^{2+}(\text{g}) \rightarrow \text{X}^{3+}(\text{g}) + \text{e}^-$. Both require energy. A graph of log ionisation energy shows multiplicative changes: a one-unit increase in $\log_{10}$ means ten times the energy.

P: $[\text{Ne}]3s^23p^3$



s orbital: spherical



one p orbital: two lobes



3s

three 3p orbitals

S adds ↓ to one 3p box.

2 Practice

2.1 An atom has $Z = 16$ and $A = 34$. State its proton, neutron and electron counts, then give the electron count of its $2-$ ion. [3]

2.2 A sample gives two ion peaks: $m/z = 20$ and 40 . Explain why these peaks alone do not prove that the sample contains two isotopes. Give one alternative interpretation and one further observation needed. [3]

2.3 Give the numbers of orbitals and maximum electrons in an s, a p and a d subshell. State the maximum total electrons in quantum shell $n = 3$. [4]

3 Exam-style questions

3.1 Write electron configurations for K, Br and Cu^+ , using the atomic numbers 19, 35 and 29. Explain why forming Cu^+ does not leave a 4s electron. [4]

3.2 An element has successive ionisation energies whose $\log_{10}$ values rise from 3.0 to 4.2 between the second and third removals. Calculate the energy ratio and infer the outer-electron count. Write the third-ionisation equation and state its energy sign. [5]

3.3 Two successive elements in Period 3 have outer configurations $3s^2$ and $3s^23p^1$. Explain the decrease in first ionisation energy. Contrast this with the decrease from $3p^3$ to $3p^4$. [4]

3.4 Draw the shapes of an s and a p orbital, indicating the nucleus. State the maximum number of electrons in either orbital. [3]

3.5 Sodium and potassium have outer configurations $3s^1$ and $4s^1$. Explain their similar reaction patterns and why potassium has lower first ionisation energy despite its larger nuclear charge. [3]

3.6 A molecular ion of charge $2+$ gives $m/z = 29$. Which formula fits its mass: C_3H_6O , C_2H_6O or $C_4H_{10}O$? Use $C = 12$, $H = 1$, $O = 16$. Explain why this evidence does not identify one unique structure. [3]

3.7 The first ionisation energies in kJ mol^{-1} are Na 496, Mg 738, Al 578, Si 789, P 1012, S 1000, Cl 1251, Ar 1521 and K 419. Plot the values against increasing atomic number using both a linear energy axis and a $\log_{10}$ energy axis. Explain how the Ar-to-K change supports periodicity. [5]
