

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

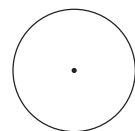
■ Read charge before interpreting a peak

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.

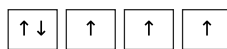
First ionisation is $\text{X}(\text{g}) \rightarrow \text{X}^+(\text{g}) + \text{e}^-$; third ionisation is $\text{X}^{2+}(\text{g}) \rightarrow \text{X}^{3+}(\text{g}) + \text{e}^-$. Both require energy. A graph of log ionisation energy shows multiplicative changes: a one-unit increase in $\log_{10}$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



s orbital: spherical



one p orbital: two lobes



3s three 3p orbitals

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

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]

Solutions

Original marking guidance; accept equivalent notation.

2.1 16 protons and 18 neutrons, 16 electrons in the neutral atom, 18 electrons in the 2- ion. The nucleus is unchanged by electron gain.

2.2 The instrument separates m/z , not mass alone. A single mass-40 isotope could form both 1+ and 2+ ions. Determine the ion charges independently, or obtain a charge-resolved spectrum before assigning two isotope masses. The peak pair alone cannot distinguish these possibilities.

2.3 s: one orbital/two electrons; p: three/six; d: five/ten. Shell $n = 3$ contains 3s, 3p and 3d, with maximum $2 + 6 + 10 = 18$ electrons. A single d orbital holds two, not ten.

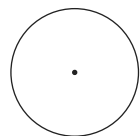
3.1 K: $[\text{Ar}]4s^1$; Br: $[\text{Ar}]3d^{10}4s^24p^5$; Cu^+ : $[\text{Ar}]3d^{10}$. Neutral copper is $[\text{Ar}]3d^{10}4s^1$; its 4s electron is removed first when the positive ion forms.

3.2 Difference in logarithms $= 4.2 - 3.0 = 1.2$, so energy ratio $= 10^{1.2} = 15.8$. A large jump after removal of two electrons supports two outer electrons, assuming the stated jump separates outer and inner shells. $\text{X}^{2+}(\text{g}) \rightarrow \text{X}^{3+}(\text{g}) + \text{e}^-$; the energy change is positive/endothermic.

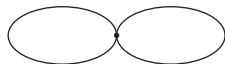
3.3 The 3p electron is higher in energy and more easily removed than a 3s electron; this outweighs the increase in nuclear charge across Mg to Al. For P to S, removal remains from 3p; sulfur has the first paired 3p electrons, whose repulsion makes one easier to remove despite the greater nuclear charge. An extra inner shell is not added in either comparison.

3.4

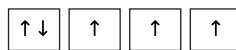
P: $[\text{Ne}]3s^23p^3$



s orbital: spherical



one p orbital: two lobes



3s

three 3p orbitals

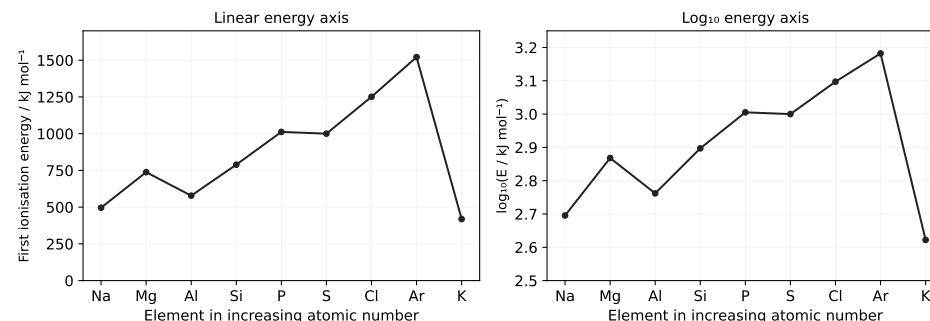
S adds ↓ to one 3p box.

Spherical s region; two-lobed p region about the nucleus; either orbital holds up to two electrons with opposite spins. The electron-box panel is additional occupancy teaching, not a third spatial orbital.

3.5 Both have one outer electron and tend to form 1+ ions, giving similar chemical behaviour. Potassium's outer electron is further from the nucleus with greater shielding by occupied inner shells; these outweigh its higher nuclear charge, so it is more easily removed.

3.6 Relative molecular mass $= 29 \times 2 = 58$. $\text{C}_3\text{H}_6\text{O}$ has mass $3 \times 12 + 6 + 16 = 58$; the other candidates are 46 and 74. Structural isomers such as propanal and propanone share $\text{C}_3\text{H}_6\text{O}$ and the same molecular mass, so further structural evidence is needed.

3.7



Award labelled axes/consistent scales, correct linear points, and correct logarithmic points. K begins a new occupied outer shell, increasing distance and shielding relative to Ar; the large decrease after a noble-gas maximum is part of the repeating periodic pattern. A logarithmic axis preserves order but compresses large values.