

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

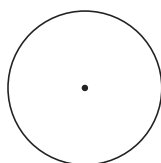
■ Read charge before interpreting a peak

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]

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.

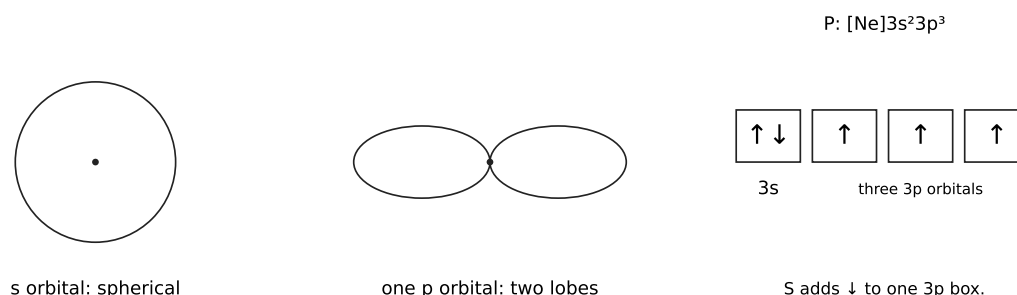
2.3 s: one orbital/two electrons; p: three/six; d: five/ten. Shell $n = 3$ contains 3s, 3p and 3d, with maximum $2 + 6 + 10 = 18$ electrons. A single d orbital holds two, not ten.

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

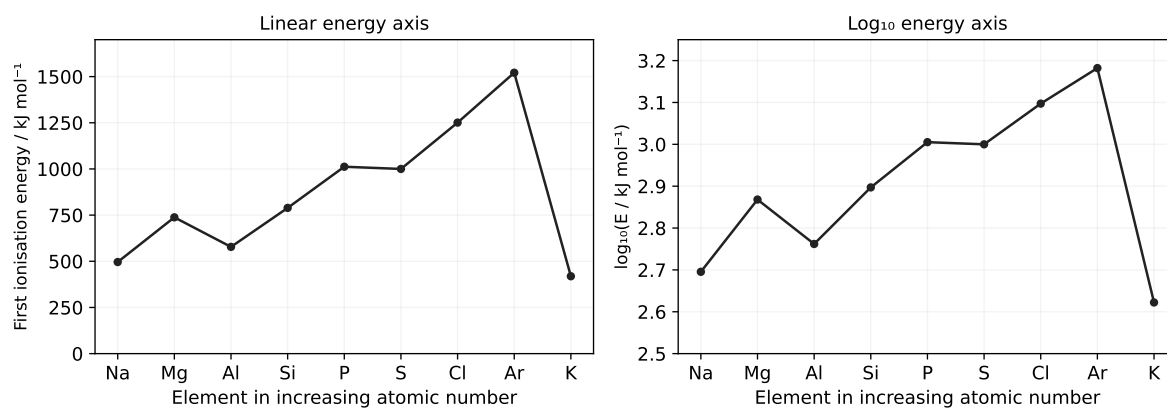


Spherical s region; two-lobed p region about the nucleus; either orbital holds up to two electrons with opposite spins. The electron-box panel is additional occupancy teaching, not a third spatial orbital.

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.