2.1 Atomic Structure

AQA 7405 · Calculator allowed · about 195 minutes · Write-in edition

Total Marks

Name: _____ Date: ____ / ____ / _____

Answer ALL questions. Show all your working.

1 This question is about the sub-atomic particles found in atoms and ions, and the concept of isotopes.

(a) Complete the table below to show the relative mass and relative charge of a proton, a neutron and an electron. **(3)**

Particle	Relative mass	Relative charge
Proton	1	+1
Neutron	...	...
Electron	...	...

(b) Define the term isotopes. **(1)**

(c) Chlorine exists naturally as two isotopes, 35Cl and 37Cl. Chlorine has atomic number 17. State the number of protons, neutrons and electrons in one atom of 37Cl. **(3)**

(d) 35Cl and 37Cl are chemically identical to one another but can have slightly different physical properties, such as density. Explain why. **(2)**

(Total for Question 1 is 9 marks)

2 This question tests key definitions and facts about atomic structure. For each part, identify the correct option.

(a) Potassium-39 has atomic number 19. Which row correctly gives the number of protons and neutrons in one atom of potassium-39? **(1)**

- ☐ A) 19 protons, 19 neutrons
- ☐ B) 19 protons, 20 neutrons
- ☐ C) 20 protons, 19 neutrons
- ☐ D) 39 protons, 19 neutrons

(b) Which statement correctly defines the relative atomic mass of an element? **(1)**

- ☐ A) The mass of one atom of the element compared with the mass of one atom of hydrogen-1.
- ☐ B) The average mass of all the isotopes of the element compared with the mass of one atom of carbon-12.
- ☐ C) The weighted mean mass of the isotopes of an element compared with 1/12 the mass of one atom of carbon-12.
- ☐ D) The mass number of the most abundant isotope of the element.

(c) How many orbitals are there in total within a p sub-shell? **(1)**

- ☐ A) 1
- ☐ B) 2
- ☐ C) 3
- ☐ D) 5

(d) Which ionisation method is typically used in a modern time-of-flight mass spectrometer to ionise large or delicate molecules without breaking them apart? **(1)**

- ☐ A) Electron impact ionisation
- ☐ B) Electrospray ionisation
- ☐ C) Thermal ionisation
- ☐ D) Flame ionisation

(Total for Question 2 is 4 marks)

3 This question is about the numbers of sub-atomic particles present in ions.

(a) An ion has the formula $^{24}Mg^{2+}$ (magnesium has atomic number 12). State the number of protons, neutrons and electrons present in this ion. **(3)**

(b) An ion has the formula $^{79}Br^{-}$ (bromine has atomic number 35). State the number of protons, neutrons and electrons present in this ion. **(3)**

(c) Explain, in terms of sub-atomic particles, why atoms are electrically neutral overall, but ions such as Mg^{2+} and Br^{-} are not. **(2)**

(Total for Question 3 is 8 marks)

4 This question is about atomic orbitals and sub-shells.

(a) State the maximum number of electrons that can occupy: (i) a single atomic orbital, (ii) an s sub-shell, (iii) a p sub-shell. **(3)**

(b) State the number of orbitals within a p sub-shell and describe their shape and relative orientation to one another. **(2)**

(c) Nitrogen has the electron configuration 1s2 2s2 2p3. Complete a diagram of boxes to show how the three 2p electrons are arranged within the three 2p orbitals, and use Hund's rule to explain the arrangement you have shown. **(3)**

2p: [ ] [ ] [ ]

(Total for Question 4 is 8 marks)

5 This question is about writing electron configurations, including for a transition metal and its ion.

(a) Write the full electron configuration of a chlorine atom (atomic number 17). **(1)**

(b) Write the full electron configuration of the Ca^{2+} ion (calcium has atomic number 20). **(1)**

(c) Write the full electron configuration of (i) an iron atom, Fe (atomic number 26), and (ii) the Fe^{3+} ion. **(2)**

(d) Explain why electrons are removed from the 4s sub-shell before the 3d sub-shell when a d-block atom such as iron forms a positive ion, even though the 4s sub-shell fills before the 3d sub-shell when building up the atom's electron configuration. **(2)**

(e) Complete a diagram of boxes to show the arrangement of electrons within the five 3d orbitals of the Fe^{3+} ion, and hence state the number of unpaired electrons in Fe^{3+}. **(2)**

3d: [ ] [ ] [ ] [ ] [ ]

(Total for Question 5 is 8 marks)

6 A time-of-flight (TOF) mass spectrometer is used to analyse a sample of magnesium. Singly charged Mg+ ions (relative mass 24, charge = 1.60×10^{-19} C) are accelerated through a potential difference of 15.0 kV before travelling along a flight tube of length 2.00 m to the detector.

You may use: energy gained during acceleration, Ek = q x V, where q is the ion's charge and V is the accelerating voltage; kinetic energy, $Ek = 1/2 \times m \times v^2$; time of flight, t = distance / v; 1 unified atomic mass unit = 1.66×10^{-27} kg.

(a) State, in order, the four main stages a sample passes through in a TOF mass spectrometer, and describe what happens to the sample during the ionisation stage. **(2)**

(b) Explain why the entire flight tube of the mass spectrometer must be maintained under a high vacuum. **(2)**

(c) Calculate the velocity of the Mg+ ions as they leave the acceleration stage and enter the flight tube. Give your answer to 3 significant figures. **(4)**

(d) Hence calculate the time taken for the Mg+ ions to travel along the 2.00 m flight tube. Give your answer to 3 significant figures. **(2)**

(Total for Question 6 is 10 marks)

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7 Successive ionisation energy data for a single element, and the pattern of first ionisation energies across a period, both provide evidence for the arrangement of electrons into shells and sub-shells. Discuss how this evidence supports the shell and sub-shell model of electron arrangement in atoms. You should refer to both successive ionisation energies within one element and the trend in first ionisation energy across a period.

(Total for Question 7 is 6 marks)

8 The mass spectrum of 2-chloropropane (C_3H_7Cl) shows two molecular ion peaks, at m/z = 78 and m/z = 80, in an approximate intensity ratio of 3:1.

(a) Explain the origin of the molecular ion peak at m/z = 80. **(2)**

(b) State what the approximate 3:1 ratio of peak intensities tells you about the relative natural abundance of the isotopes 35Cl and 37Cl. **(2)**

(c) Using Ar(C) = 12.0, Ar(H) = 1.0 and Ar(Cl) = 35.5, calculate the relative molecular mass, Mr, of 2-chloropropane, and explain why this value is not equal to either of the mass spectrum peaks at m/z = 78 or m/z = 80. **(3)**

(Total for Question 8 is 7 marks)

9 The first ionisation energy of hydrogen can be found from the minimum frequency of electromagnetic radiation needed to remove the single electron from a hydrogen atom in its ground state.

You may use: $E = h f$, where $h = 6.63 \times 10^{-34}$ J s and f is frequency in Hz; Avogadro constant, $NA = 6.02 \times 10^{23}$ mol^{-1}.

(a) The minimum frequency of radiation needed to ionise a single hydrogen atom is 3.29×10^{15} Hz. Calculate the energy, in J, needed to ionise one hydrogen atom. **(2)**

(b) Calculate the first ionisation energy of hydrogen in kJ/mol, using your answer to (a) and the Avogadro constant. Give your answer to 3 significant figures. **(3)**

(c) Suggest, in terms of quantum theory, why only photons with a frequency equal to or greater than this minimum value can ionise a hydrogen atom, while a very intense beam of lower-frequency photons cannot. **(2)**

(Total for Question 9 is 7 marks)

10 The table shows the first ionisation energies of the elements in Period 3, from sodium to argon.

Element	Na	Mg	Al	Si	P	S	Cl	Ar
First IE (kJ/mol)	496	738	578	786	1012	1000	1251	1521

(a) Describe and explain the general trend in first ionisation energy across Period 3, from sodium to argon. **(3)**

(b) Explain why the first ionisation energy of aluminium (578 kJ/mol) is lower than that of magnesium (738 kJ/mol), even though aluminium has a greater nuclear charge. **(3)**

(c) Explain why the first ionisation energy of sulfur (1000 kJ/mol) is lower than that of phosphorus (1012 kJ/mol), even though sulfur has a greater nuclear charge. **(3)**

(Total for Question 10 is 9 marks)

11 Element Y is in Period 2 of the Periodic Table. The table shows its first five successive ionisation energies.

Ionisation	IE1	IE2	IE3	IE4	IE5
Energy (kJ/mol)	801	2427	3660	25026	32827

(a) Explain why successive ionisation energies always increase for a given element. **(2)**

(b) Calculate the ratio of IE4 to IE3, and use it to show that there is a much larger increase between the removal of the 3rd and 4th electrons than between other consecutive electrons removed. **(2)**

(c) Use this information to deduce the group of the Periodic Table to which element Y belongs, explaining your reasoning. **(2)**

(d) Given that element Y is in Period 2, state its full electron configuration. **(1)**

(Total for Question 11 is 7 marks)

12 A student used a mass spectrometer's chart recorder to measure the relative abundance of magnesium's three isotopes from the height of each peak, which is proportional to abundance. Each peak height was measured with an uncertainty of ± 0.5 mm. The measured peak heights were: 24Mg = 78.9 mm, 25Mg = 10.0 mm, 26Mg = 11.1 mm.

(a) Calculate the percentage abundance of 24Mg, given that the three peak heights sum to 100.0 mm in total. **(2)**

(b) Calculate the percentage uncertainty in the measured peak height of 24Mg (78.9 ± 0.5 mm), to 2 significant figures. **(2)**

(c) Using your percentage uncertainty from part (b), calculate the absolute uncertainty (in percentage points) in the calculated percentage abundance of 24Mg found in part (a). **(2)**

(d) Given this level of uncertainty, state and justify how many significant figures the final calculated relative atomic mass of magnesium should be quoted to. **(2)**

(Total for Question 12 is 8 marks)

13 This final synoptic question draws together mass spectrometry, electron configuration and ionisation energy to identify an unknown Period 4 element, Z.

(a) A sample of element Z, when analysed by mass spectrometry, gives four isotopic peaks with the following relative abundances: 54Z 5.8%, 56Z 91.7%, 57Z 2.2%, 58Z 0.3%. Calculate the relative atomic mass of Z, to 3 significant figures. **(3)**

(b) Given that Z is a Period 4 transition metal with atomic number 26, write its full electron configuration as a neutral atom. **(2)**

(c) The first six successive ionisation energies of Z (in kJ/mol) are: 762, 1562, 2957, 5290, 7240, 9600. Explain why there is no very large jump between the 2nd and 3rd ionisation energies of Z, unlike the pattern typically seen for a Group 2 element such as magnesium. **(3)**

(d) Calculate the percentage increase from the 1st to the 2nd ionisation energy of Z, and comment on whether this is consistent with Z having 2 electrons in its 4s sub-shell. **(1)**

(Total for Question 13 is 9 marks)

14 The successive ionisation energies of an element, Y, are given below (in kJ/mol): 1st = 738, 2nd = 1451, 3rd = 7733, 4th = 10540, 5th = 13630, 6th = 18020.

(a) Deduce the group of the Periodic Table that element Y belongs to, explaining your reasoning using the data. **(3)**

(b) Calculate the percentage increase in ionisation energy between the 2nd and 3rd ionisation energies. **(2)**

(c) Write the full electron configuration of element Y, given that Y is in Period 3 of the Periodic Table. **(1)**

(d) Explain why the 4th, 5th and 6th ionisation energies increase steadily (rather than showing another very large jump), even though electrons are still being removed from the same inner shell as the 3rd electron. **(2)**

(Total for Question 14 is 8 marks)

15 Evaluate the trend in first ionisation energy down Group 2 of the Periodic Table (beryllium to barium), explaining the balance of factors that determines this trend.

(Total for Question 15 is 6 marks)

16 First ionisation energies across Period 2 (lithium to neon) show a general increasing trend, but with two exceptions: a small drop from beryllium to boron, and a small drop from nitrogen to oxygen.

(a) Explain the general increase in first ionisation energy across Period 2, from lithium to neon. **(2)**

(b) Beryllium's outer electron configuration is 2s2, and boron's is 2s2 2p1. Explain why boron's first ionisation energy is lower than beryllium's, despite boron having a greater nuclear charge. **(3)**

(c) Nitrogen's outer electron configuration is 2p3 (one electron in each of the three 2p orbitals, all unpaired), and oxygen's is 2p4 (one orbital now contains a pair of electrons). Explain why oxygen's first ionisation energy is lower than nitrogen's. **(3)**

(Total for Question 16 is 8 marks)

17 The line emission spectrum of atomic hydrogen contains a series of converging lines in the ultraviolet region (the Lyman series), corresponding to electron transitions from higher energy levels down to the n = 1 energy level. The convergence limit of this series corresponds to an electron falling from n = infinity (a free electron) to n = 1, and its frequency can be used to calculate the ionisation energy of hydrogen.

(a) Explain why the lines in the Lyman series converge (get closer together) at higher frequency, rather than being evenly spaced. **(2)**

(b) The convergence limit of the Lyman series occurs at a frequency of 3.28×10^{15} Hz. Using E = hf, where Planck's constant h = 6.63×10^{-34} J s, calculate the energy in joules required to ionise a single hydrogen atom. **(2)**

(c) Using your answer to part (b) and the Avogadro constant (NA = 6.02×10^{23} per mole), calculate the first ionisation energy of hydrogen in kJ/mol, to 3 significant figures. **(3)**

(d) Suggest why this method (using the convergence limit of the Lyman series) gives a highly accurate value for the ionisation energy, compared with methods based on chemical reactivity trends alone. **(1)**

(Total for Question 17 is 8 marks)

18 Copper (atomic number 29) is a d-block element whose electron configuration is exceptional, in a similar way to chromium.

(a) Write the full ground-state electron configuration of a copper atom, noting that the expected 3d9 4s2 arrangement is not adopted. **(2)**

(b) Explain why the 3d10 4s1 configuration is more stable for copper than the 3d9 4s2 configuration predicted by the simple filling order. **(2)**

(c) Write the electron configurations of the Cu^{+} ion and the Cu^{2+} ion. **(2)**

(d) Explain why the second electron removed (to form Cu^{2+} from Cu^{+}) comes from the 3d sub-shell rather than the 4s sub-shell. **(1)**

(Total for Question 18 is 7 marks)

Mark scheme · 2.1 Atomic Structure

Question 1

(a) neutron: relative mass 1 AND relative charge 0 **B1**

(a) electron: relative mass 1/1840 (accept approx 0.00055 or 5.5 x 10^{-4} or 'negligible') **B1**

(a) electron: relative charge -1 **B1**

(a) Answer: Neutron: mass 1, charge 0. Electron: mass 1/1840 (approx 0.00055), charge -1.

(b) atoms of the same element (same number of protons/same atomic number) with different numbers of neutrons (different mass numbers) oe **B1**

(b) Answer: Atoms of the same element with the same number of protons but different numbers of neutrons.

(c) protons = 17 **B1**

(c) neutrons = 20 **B1**

(c) electrons = 17 **B1**

(c) Answer: Protons = 17, neutrons = 20, electrons = 17.

(d) chemical properties depend on the number and arrangement of electrons, which is identical for both isotopes (same atomic number) oe **B1**

(d) physical properties (e.g. density) depend on the mass of the atom, which differs because the isotopes have different numbers of neutrons (different mass numbers) oe **B1**

(d) Answer: Isotopes have identical electron arrangements so identical chemical properties, but different numbers of neutrons give different masses, so physical properties differ slightly.

Question 2

(a) B **B1**

(a) Answer: B

(b) C **B1**

(b) Answer: C

(c) C **B1**

(c) Answer: C

(d) B **B1**

(d) Answer: B

Question 3

(a) protons = 12 **B1**

(a) neutrons = 12 **B1**

(a) electrons = 10 **B1**

(a) Answer: Protons = 12, neutrons = 12, electrons = 10.

(b) protons = 35 **B1**

(b) neutrons = 44 **B1**

(b) electrons = 36 **B1**

(b) Answer: Protons = 35, neutrons = 44, electrons = 36.

(c) atoms have equal numbers of protons and electrons, so the positive and negative charges cancel, giving no overall (net) charge oe **B1**

(c) ions have unequal numbers of protons and electrons (electrons have been lost or gained), giving an overall positive or negative charge oe **B1**

(c) Answer: Atoms have equal numbers of protons and electrons so their charges cancel; ions have unequal numbers of protons and electrons, giving a net charge.

Question 4

(a) (i) 2 **B1**

(a) (ii) 2 **B1**

(a) (iii) 6 **B1**

(a) Answer: Orbital: 2. s sub-shell: 2. p sub-shell: 6.

(b) 3 orbitals (px, py, pz) **B1**

(b) each is dumbbell (figure-of-eight) shaped, and the three orbitals are oriented at right angles (90 degrees) to each other along the x, y and z axes oe **B1**

(b) Answer: 3 orbitals, each dumbbell-shaped, arranged at 90 degrees to one another along the x, y and z axes.

(c) three separate 2p boxes each shown with a single (unpaired) arrow, all pointing the same direction (no pairing shown) **M1**

(c) states Hund's rule: electrons occupy separate orbitals of equal energy (degenerate orbitals) singly, with parallel spins, before any pairing occurs oe **B1**

(c) this arrangement minimises the repulsion between electrons, giving a more stable (lower energy) configuration oe **B1**

(c) Answer: 2p: one electron in each of the three 2p orbitals, all spins parallel (up, up, up).

Question 5

(a) 1s2 2s2 2p6 3s2 3p5 **B1**

(a) Answer: 1s2 2s2 2p6 3s2 3p5

(b) 1s2 2s2 2p6 3s2 3p6 **B1**

(b) Answer: 1s2 2s2 2p6 3s2 3p6

(c) (i) Fe: 1s2 2s2 2p6 3s2 3p6 3d6 4s2 **B1**

(c) (ii) Fe^{3+}: 1s2 2s2 2p6 3s2 3p6 3d5 **B1**

(c) Answer: Fe: 1s2 2s2 2p6 3s2 3p6 3d6 4s2. Fe^{3+}: 1s2 2s2 2p6 3s2 3p6 3d5.

(d) once the 3d sub-shell begins to fill, the 3d electrons drop to a lower energy than the 4s electrons (3d becomes lower in energy than 4s in the resulting atom/ion) oe **B1**

(d) electrons are always removed from the highest energy (outermost) sub-shell first, which is now 4s, not 3d oe **B1**

(d) Answer: Once 3d starts filling it drops below 4s in energy, so 4s (now the higher-energy, outermost sub-shell) loses its electrons first.

(e) five separate 3d boxes each shown with a single (unpaired) arrow, all parallel spins (half-filled sub-shell, per Hund's rule) **M1**

(e) 5 unpaired electrons **A1**

(e) Answer: 5 unpaired electrons (one in each of the five 3d orbitals).

Question 6

(a) correct order of the four stages: ionisation, acceleration, ion drift (flight tube), detection **B1**

(a) describes ionisation, e.g. the sample is vaporised and ionised, for example by electrospray ionisation, in which molecules gain a proton (H^+) to form positive ions such as [M+H]+ oe **B1**

(a) Answer: Ionisation, acceleration, ion drift, detection. In ionisation the sample is vaporised and converted into positive ions, e.g. by electrospray ionisation.

(b) prevents the (positive) ions colliding with air/gas molecules oe **B1**

(b) such collisions would deflect/scatter the ions or cause them to lose energy, giving inaccurate flight times and an unreliable spectrum oe **B1**

(b) Answer: A vacuum prevents ions colliding with air molecules, which would otherwise deflect them and give inaccurate flight times.

(c) $Ek = qV = 1.60 \times 10^{-19} \times 1.50 \times 10^{4} = 2.40 \times 10^{-15}$ J **M1**

(c) mass of ion in kg = $24 \times 1.66 \times 10^{-27} = 3.98 \times 10^{-26}$ kg **M1**

(c) rearranges $Ek = 1/2\ m\ v^2$ to $v = \sqrt{2\ Ek / m}$ and substitutes values **M1**

(c) v = awrt 3.47×10^{5} m/s **A1**

(c) Answer: v = 3.47×10^{5} m/s

(d) t = d / v = 2.00 / (their answer to (c)) (ft/ecf from (c)) **M1**

(d) t = awrt 5.76×10^{-6} s **A1**

(d) Answer: t = 5.76×10^{-6} s

Question 7

Level 3 A detailed, coherent and logically structured discussion that correctly uses both successive ionisation energy data (large jumps between shells) and the periodic trend in first ionisation energy (including sub-shell anomalies) to support the existence of shells and sub-shells. Accurate scientific terminology is used throughout. **5-6**

Level 2 Some relevant scientific points relating to either shells or sub-shells are made, with some structure and reference to ionisation energy evidence, but the discussion is not fully developed, may focus mainly on one type of evidence, or contains minor inaccuracies. **3-4**

Level 1 Basic, isolated relevant statements are made with little structure or use of data. Limited or inaccurate use of scientific terminology. **1-2**

Level 0 No relevant content, or the answer does not relate to the question. **0**

Indicative content:

- Within one element, successive ionisation energies increase steadily because each remaining electron experiences a greater effective nuclear attraction as electrons are removed (less repulsion, same nuclear charge).
- A very large jump between two successive ionisation energies occurs when the next electron removed comes from a shell closer to the nucleus (an inner shell), which is less shielded and more strongly attracted.
- The position of this large jump indicates the number of electrons in the outer shell, and therefore the group of the element; this provides direct evidence for the existence of discrete electron shells.
- Within a shell, smaller step changes in successive ionisation energies can reflect the existence of sub-shells, for example a somewhat bigger increase when electrons start being removed from an s sub-shell after a p sub-shell is emptied.
- The general trend of increasing first ionisation energy across a period occurs because nuclear charge increases while shielding remains roughly constant, so atomic radius decreases and outer electrons are held more strongly.
- Two anomalies interrupt this general increase: a decrease from Group 2 to Group 3 (e.g. Mg to Al), and a decrease from Group 5 to Group 6 (e.g. P to S).
- The Group 2 to Group 3 dip occurs because the outer electron moves from a stable, full s sub-shell into a higher energy p sub-shell, which is easier to remove despite the increased nuclear charge; this is evidence for the s and p sub-shells having different energies.
- The Group 5 to Group 6 dip occurs because a p orbital becomes occupied by a pair of electrons, and the extra repulsion between paired electrons in the same orbital makes one easier to remove; this is evidence for the existence of individual orbitals within a sub-shell.
- Together, the repeating (periodic) pattern of these features in every period provides strong, consistent evidence for a shell and sub-shell model of electron arrangement, rather than electrons being arranged randomly or singly around the nucleus.

Question 8

(a) this peak arises from molecules containing the heavier chlorine isotope, 37Cl, in place of 35Cl oe **B1**

(a) the C_3H_7 part of the molecule has mass 43, so 43 + 37 = 80, two mass units higher than the 78 peak (43 + 35) **B1**

(a) Answer: The m/z = 80 peak is from molecules containing 37Cl instead of 35Cl (43 + 37 = 80).

(b) 35Cl is approximately three times as abundant as 37Cl oe **B1**

(b) i.e. natural chlorine is approximately 75% 35Cl and 25% 37Cl **B1**

(b) Answer: 35Cl is about 3 times as abundant as 37Cl (approximately 75% : 25%).

(c) Mr = (3 x 12.0) + (7 x 1.0) + 35.5 **M1**

(c) Mr = 78.5 **A1**

(c) Mr uses the weighted-average Ar of chlorine (accounting for both isotopes' abundances), whereas each mass spectrum peak corresponds to molecules containing one specific integer-mass isotope, so neither integer peak equals the non-integer average Mr oe **B1**

(c) Answer: Mr = 78.5. Neither peak equals this because each peak is from molecules with one specific chlorine isotope, while Mr uses the weighted-average Ar.

Question 9

(a) E = h f = 6.63 x 10^{-34} x 3.29 x 10^{15} **M1**

(a) E = awrt 2.18 x 10^{-18} J **A1**

(a) Answer: E = 2.18 x 10^{-18} J

(b) energy per mole = (their answer to (a)) x 6.02 x 10^{23} (ft/ecf from (a)) **M1**

(b) converts J to kJ (divides by 1000) **M1**

(b) awrt 1310 kJ/mol (accept 1300-1320 kJ/mol) **A1**

(b) Answer: 1.31 x 10^3 kJ/mol (approx 1310 kJ/mol)

(c) energy is quantised: each photon carries a fixed, discrete amount of energy, E = h f, determined by its frequency and not by the intensity of the light oe **B1**

(c) ionisation requires a single photon to transfer at least the ionisation energy to one electron in a single interaction; a lower-frequency photon carries less energy than this threshold regardless of how many photons arrive per second (intensity affects only the number of photons, not the energy of each one), so it cannot ionise the atom oe **B1**

(c) Answer: Photon energy depends only on frequency (E=hf); a single low-frequency photon cannot supply enough energy to ionise the atom no matter how intense the beam is.

Question 10

(a) general trend is an increase in first ionisation energy from Na to Ar (with two dips, at Al and at S) **B1**

(a) nuclear charge (number of protons) increases across the period while the number of occupied shells, and therefore shielding by inner shells, stays approximately constant oe **B1**

(a) atomic radius decreases across the period, so the outer electrons are held more strongly, meaning more energy is needed to remove one oe **B1**

(a) Answer: First IE generally increases Na to Ar because nuclear charge increases with roughly constant shielding, so atomic radius falls and outer electrons are held more strongly.

(b) in magnesium the outer electron removed is from the full 3s sub-shell (3s2), which has extra stability oe **B1**

(b) in aluminium the outer electron removed is from the 3p sub-shell, which is at a higher energy than the 3s sub-shell (and/or experiences extra shielding from the full 3s2 sub-shell) oe **B1**

(b) so the 3p electron in aluminium is easier to remove than a 3s electron in magnesium, despite aluminium's higher nuclear charge oe **B1**

(b) Answer: Mg's outer electron is in a stable, full 3s sub-shell; Al's outer electron is in the higher-energy 3p sub-shell, so it is easier to remove despite Al's greater nuclear charge.

(c) phosphorus (3p3) has one electron in each of the three 3p orbitals (unpaired), which minimises electron-electron repulsion oe **B1**

(c) sulfur (3p4) has one 3p orbital containing a pair of electrons oe **B1**

(c) extra repulsion between the two paired electrons in the same orbital makes one of them easier to remove, lowering sulfur's first ionisation energy despite its greater nuclear charge oe **B1**

(c) Answer: P's 3p3 electrons are all unpaired (low repulsion); S's 3p4 has a pair in one orbital, and the extra repulsion makes an electron easier to remove.

Question 11

(a) after each electron is removed, the resulting ion has one fewer electron but the same number of protons, so there is less repulsion between the remaining electrons and a greater effective nuclear attraction per electron oe **B1**

(a) more energy is therefore required to remove each successive electron oe **B1**

(a) Answer: Each successive ion has one fewer electron but the same nuclear charge, so remaining electrons are attracted more strongly, needing more energy to remove.

(b) IE4 / IE3 = 25026 / 3660 = awrt 6.8 **M1**

(b) compares with other ratios, e.g. IE2/IE1 approx 3.0 and IE3/IE2 approx 1.5, both much smaller, confirming a genuinely large jump between IE3 and IE4 oe **A1**

(b) Answer: IE4/IE3 = 6.84, much larger than IE2/IE1 (approx 3.03) or IE3/IE2 (approx 1.51), confirming a large jump.

(c) the large jump between IE3 and IE4 shows that the 4th electron removed comes from an inner shell (closer to the nucleus, with less shielding) than the first three electrons oe **M1**

(c) this means Y has 3 electrons in its outer shell, so Y is in Group 3 (Group 13) **A1**

(c) Answer: Group 3 (Group 13).

(d) 1s2 2s2 2p1 (ft from (c): Period 2, Group 3 = boron) **B1**

(d) Answer: 1s2 2s2 2p1 (boron, Z = 5)

Question 12

(a) percentage abundance = (peak height / total height) x 100 = (78.9/100.0) x 100 **M1**

(a) 78.9%, cao **A1**

(a) Answer: 78.9%

(b) percentage uncertainty = (0.5 / 78.9) x 100 **M1**

(b) 0.63%, awrt **A1**

(b) Answer: 0.63%

(c) absolute uncertainty = percentage uncertainty x value = 0.63% x 78.9%, ft **M1**

(c) ± 0.50 percentage points (accept 0.49-0.50), awrt **A1**

(c) Answer: ± 0.50 percentage points, i.e. 78.9% ± 0.5%

(d) 3 significant figures (e.g. 24.3) **B1**

(d) because the uncertainty in the abundance data (of the order of a few tenths of a percentage point) only justifies confidence in the calculated relative atomic mass to about 1 decimal place/3 significant figures; quoting further figures would imply a precision not supported by the measurement uncertainty oe **B1**

(d) Answer: 3 significant figures (e.g. 24.3), because the measurement uncertainty does not justify greater precision than this.

Question 13

(a) correct method: (54 x 0.058) + (56 x 0.917) + (57 x 0.022) + (58 x 0.003) **M1**

(a) = 3.132 + 51.352 + 1.254 + 0.174 **M1**

(a) 55.9, cao **A1**

(a) Answer: 55.9

(b) 1s2 2s2 2p6 3s2 3p6 as the core configuration **M1**

(b) 3d6 4s2, giving 1s2 2s2 2p6 3s2 3p6 3d6 4s2, cao **A1**

(b) Answer: 1s2 2s2 2p6 3s2 3p6 3d6 4s2

(c) Z is a transition metal, and after the 2 electrons in the 4s sub-shell are removed, further electrons are removed from the 3d sub-shell, which is at a similar energy to (not dramatically lower than) the 4s sub-shell oe **B1**

(c) the 3d and 4s sub-shells are both part of the same (n=3/4) region of similar shielding, so there is no sudden jump into a completely different, much less shielded inner shell as there would be after removing all outer-shell electrons in a simple main-group element oe **B1**

(c) instead, ionisation energies increase relatively steadily as successive electrons are removed from the 3d sub-shell of an increasingly positively charged ion oe **B1**

(c) Answer: As a transition metal, Z's third and later ionisation energies come from removing 3d electrons, which are similar in energy/shielding to the 4s electrons, so there is no dramatic jump into a very different inner shell as seen in main-group elements; instead ionisation energies rise fairly steadily.

(d) (1562-762)/762 x 100 = 105% increase; this relatively modest increase (roughly doubling, not several-fold) is consistent with both electrons being removed from the same, similarly shielded 4s sub-shell oe **B1**

(d) Answer: Approximately 105% increase, consistent with both electrons coming from the same 4s sub-shell.

Question 14

(a) identify the large jump in ionisation energy between the 2nd (1451) and 3rd (7733) ionisation energies **M1**

(a) Group 2, cao **A1**

(a) a large increase occurs when an electron is removed from a full inner shell (closer to the nucleus, less shielded), which happens after the 2 outer-shell electrons have been removed, showing Y has 2 electrons in its outer shell oe **B1**

(a) Answer: Group 2. There is a very large jump in ionisation energy between the 2nd and 3rd values, showing that the 3rd electron is removed from a full inner shell, so Y has 2 outer-shell electrons.

(b) correct substitution: (7733 - 1451)/1451 x 100 **M1**

(b) 433% (accept 430-435%), awrt **A1**

(b) Answer: Approximately 433%

(c) 1s2 2s2 2p6 3s2 (magnesium's configuration; Y is identified as magnesium), cao **B1**

(c) Answer: 1s2 2s2 2p6 3s2

(d) each successive electron is removed from an ion with an increasingly large positive charge, so the remaining electrons are held more strongly (greater electrostatic attraction to the nucleus) oe **B1**

(d) since these electrons are all in the same inner shell/similarly shielded, the increases are steady/gradual rather than a sudden very large jump, which only occurs when a new (closer, less-shielded) shell begins to be emptied oe **B1**

(d) Answer: Each successive ionisation removes an electron from an ion of increasing positive charge, so the remaining same-shell electrons are held more strongly, causing a steady increase rather than the sudden large jump seen when a new inner shell begins to be emptied.

Question 15

Level 3 A detailed, well-structured evaluation that correctly states the trend (first ionisation energy decreases down Group 2), identifies all three relevant factors (increasing nuclear charge, increasing atomic radius/distance of outer electron from nucleus, increasing shielding by additional inner shells), and correctly explains which factors dominate to give the overall observed trend, with clear, logical reasoning throughout. **5-6**

Level 2 A reasonably clear account that states the correct trend and identifies at least two of the three relevant factors, with some explanation of how they combine, but the reasoning about which factor dominates is incomplete or not fully justified. **3-4**

Level 1 Limited response; may state the trend without correct explanation, or identify only one relevant factor (e.g. atomic radius) with little development. **1-2**

Indicative content:

- First ionisation energy decreases going down Group 2, from beryllium to barium.
- Going down the group, nuclear charge increases (more protons in the nucleus of each successive element), which alone would be expected to increase ionisation energy by increasing nuclear attraction for outer electrons.
- However, going down the group, atomic radius also increases because electrons occupy additional principal quantum shells (energy levels) further from the nucleus.
- Additionally, the number of inner (complete) shells of electrons between the nucleus and the outer electron increases down the group, increasing the shielding (screening) effect on the outer electron from the full nuclear charge.
- The combined effect of increased distance and increased shielding outweighs the effect of increased nuclear charge, so the effective nuclear attraction experienced by the outer electron actually decreases down the group.
- As a result, less energy is needed to remove the outer electron as you go down the group, so first ionisation energy decreases, despite the larger nuclear charge.
- A strong answer explicitly weighs all three factors against one another and states clearly why shielding and distance 'win' over the increasing nuclear charge.

Question 16

(a) nuclear charge increases across the period (more protons), while the outer electrons are added to the same principal shell/quantum shell, so shielding by inner electrons stays roughly constant oe **B1**

(a) the increasing nuclear charge therefore attracts the outer electrons more strongly (atomic radius also decreases), so more energy is needed to remove an electron, increasing ionisation energy oe **B1**

(a) Answer: Nuclear charge increases across the period while shielding stays roughly constant, so the outer electrons are pulled in more strongly, increasing the energy needed to remove one.

(b) in boron, the outer electron removed comes from the 2p sub-shell, which is at a slightly higher energy than the 2s sub-shell oe **B1**

(b) the 2p electron is also slightly shielded by the 2s electrons, further reducing the effective nuclear attraction it experiences oe **B1**

(b) these effects outweigh the increased nuclear charge, so less energy is needed to remove boron's 2p electron than beryllium's 2s electron oe **B1**

(b) Answer: Boron's outer electron is in the higher-energy 2p sub-shell and is partly shielded by the 2s electrons, so despite boron's greater nuclear charge, less energy is needed to remove this electron than beryllium's 2s electron.

(c) in oxygen, the electron removed comes from a doubly occupied 2p orbital, whereas in nitrogen all three 2p electrons are unpaired, each in a separate orbital oe **B1**

(c) the two electrons paired in the same oxygen orbital repel each other more strongly than electrons in separate orbitals would oe **B1**

(c) this extra electron-electron repulsion makes the paired electron in oxygen easier to remove than an unpaired electron in nitrogen, despite oxygen's greater nuclear charge oe **B1**

(c) Answer: Oxygen's removed electron is one of a repelling pair sharing the same 2p orbital, so extra electron-electron repulsion makes it easier to remove than nitrogen's unpaired 2p electron, despite oxygen's greater nuclear charge.

Question 17

(a) electron energy levels get closer together in energy as n increases (they converge towards a limit) oe **B1**

(a) so the energy (and therefore frequency) difference between adjacent transitions to n = 1 gets smaller as the starting energy level (n) increases, causing the spectral lines to converge oe **B1**

(a) Answer: Energy levels get closer together as n increases, so the energy (and frequency) gaps between successive transitions to n=1 shrink, causing the lines to converge.

(b) $E = hf = 6.63 \times 10^{-34} \times 3.28 \times 10^{15}$ **M1**

(b) 2.17×10^{-18} J, awrt **A1**

(b) Answer: 2.17×10^{-18} J

(c) energy per mole = $2.17 \times 10^{-18} \times 6.02 \times 10^{23}$, ft from (b) **M1**

(c) = 1.306×10^{6} J/mol **M1**

(c) 1310 kJ/mol (1.31×10^{3} kJ/mol), awrt **A1**

(c) Answer: 1.31×10^{3} kJ/mol (1310 kJ/mol)

(d) the convergence frequency can be measured very precisely using spectroscopy, and it corresponds directly and exactly to the energy needed to completely remove the electron (n = infinity), giving a direct physical measurement rather than an indirect estimate oe **B1**

(d) Answer: The convergence frequency is measured directly and precisely by spectroscopy and corresponds exactly to complete removal of the electron, giving a direct physical measurement rather than an indirect estimate.

Question 18

(a) core configuration 1s2 2s2 2p6 3s2 3p6 **M1**

(a) 3d10 4s1, giving 1s2 2s2 2p6 3s2 3p6 3d10 4s1, cao **A1**

(a) Answer: 1s2 2s2 2p6 3s2 3p6 3d10 4s1

(b) a fully-filled 3d sub-shell (10 electrons, each of the 5 orbitals doubly occupied) has extra stability compared with a 3d9 arrangement, due to a more symmetrical, lower-energy distribution of electrons oe **B1**

(b) moving one electron from 4s to 3d achieves this fully-filled, more stable arrangement, giving the atom as a whole a lower overall energy than the 3d9 4s2 arrangement oe **B1**

(b) Answer: A fully-filled 3d10 sub-shell gives a more symmetrical, lower-energy arrangement than 3d9, so moving one electron from 4s to 3d lowers the atom's overall energy.

(c) Cu^{+}: 1s2 2s2 2p6 3s2 3p6 3d10 ([Ar] 3d10) **B1**

(c) Cu^{2+}: 1s2 2s2 2p6 3s2 3p6 3d9 ([Ar] 3d9) **B1**

(c) Answer: Cu^{+}: [Ar] 3d10. Cu^{2+}: [Ar] 3d9.

(d) the 4s sub-shell is already empty in Cu^{+} (all 4s electrons removed first, since 4s is higher in energy than an occupied 3d once electrons are present); the only electrons left to remove are in the 3d sub-shell oe **B1**

(d) Answer: The 4s electron has already been removed to form Cu^{+}, so the only electrons available for further removal are in the 3d sub-shell.