AC1D Atomic Structure: Depth and Exam Drill

AQA 7405 · Calculator allowed · about 140 minutes

Total Marks

Name: _____ Date: ____ / ____ / _____

Answer ALL questions. Show all your working.

1 This question tests core vocabulary and facts used in mass spectrometry and electron configuration.

(a) Define the term first ionisation energy. **(1)**

(b) State the sub-shell notation and maximum electron capacity of a d sub-shell. **(1)**

(c) State the process, and give its symbol equation using X to represent an atom, that occurs when an atom is ionised in a mass spectrometer to form a singly charged positive ion. **(1)**

(d) State what the mass/charge (m/z) ratio measured by a mass spectrometer represents for a singly charged ion. **(1)**

(Total for Question 1 is 4 marks)

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2 Chlorine gas exists as diatomic molecules, Cl2, and chlorine has two naturally occurring isotopes: 35Cl (75.0% abundance) and 37Cl (25.0% abundance). A sample of chlorine gas was analysed by mass spectrometry.

(a) Calculate the relative atomic mass of chlorine, to 3 significant figures, using the isotopic abundance data given. **(2)**

(b) State the three possible combinations of chlorine isotopes present in a Cl2+ molecular ion, and calculate the m/z value of each. **(3)**

(c) Calculate the expected ratio of the three peaks at m/z = 70, 72 and 74 in the mass spectrum of Cl2, using the isotopic abundances given. Give your answer as a simplified whole-number ratio. **(3)**

(d) Explain why the peak at m/z = 72 is more than twice as tall as the peak at m/z = 74, even though a single 37Cl atom is only three times rarer than a single 35Cl atom. **(1)**

(Total for Question 2 is 9 marks)

3 This question tests the rules governing electron configuration.

(a) Write the full electron configuration of a chromium atom (atomic number 24) in subshell notation, noting that chromium is an exception to the normal filling order. **(2)**

(b) Explain, in terms of electron-electron repulsion and sub-shell stability, why the configuration 3d5 4s1 is more stable for chromium than the configuration 3d4 4s2 predicted by the simple filling order. **(2)**

(c) Write the electron configuration of the Fe2+ ion and the Fe3+ ion (iron, atomic number 26), explaining which sub-shell loses electrons first on ionisation. **(3)**

(d) Suggest why Fe3+ ([Ar] 3d5) is a particularly stable ion compared with Fe2+. **(1)**

(Total for Question 3 is 8 marks)

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4 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 4 is 8 marks)

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5 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 5 is 6 marks)

6 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 6 is 8 marks)

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7 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 $h = 6.63 \times 10^{-34}$ 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 ($N_A = 6.02 \times 10^{23}$ 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 7 is 8 marks)

8 A time-of-flight (TOF) mass spectrometer was used to analyse a sample of an unknown noble gas. Two ions were detected, with times of flight of 1.86×10^{-5} s and 1.97×10^{-5} s respectively, over the same flight tube. All ions entering the flight tube carry the same kinetic energy and the same single positive charge.

(a) Using the relationship time of flight is proportional to the square root of mass (for ions of equal kinetic energy and charge), calculate the ratio of the masses of the two ions detected (mass of ion 2 : mass of ion 1), to 3 significant figures. **(3)**

(b) Given that the lighter ion has a relative mass of 20 (consistent with the isotope 20Ne+), use your ratio from part (a) to calculate the relative mass of the heavier ion, to the nearest whole number, and hence identify this isotope. **(3)**

(c) Explain why, in a time-of-flight mass spectrometer, ions of greater mass take longer to travel the length of the flight tube than ions of smaller mass, given that all ions are accelerated to the same kinetic energy. **(1)**

(Total for Question 8 is 7 marks)

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9 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 Cu2+ ion. **(2)**

(d) Explain why the second electron removed (to form Cu2+ from Cu+) comes from the 3d sub-shell rather than the 4s sub-shell. **(1)**

(Total for Question 9 is 7 marks)

10 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 10 is 8 marks)

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11 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 11 is 9 marks)

Mark scheme · AC1D Atomic Structure: Depth and Exam Drill

Question 1

- (a) **B1** the energy required to remove one electron from each atom in one mole of gaseous atoms, to form one mole of gaseous 1+ ions oe
- **(a) Answer: The energy needed to remove one electron from each atom in one mole of gaseous atoms, forming one mole of gaseous 1+ ions.**
- (b) **B1** a d sub-shell holds a maximum of 10 electrons (5 orbitals, 2 electrons each)
- **(b) Answer: A d sub-shell holds a maximum of 10 electrons.**
- (c) **B1** X(g) -> X+(g) + e-
- **(c) Answer: X(g) -> X+(g) + e-**
- (d) **B1** for a singly (1+) charged ion, m/z is numerically equal to the relative mass of the ion oe
- **(d) Answer: For a singly charged ion, m/z is numerically equal to the ion's relative mass.**

Question 2

- (a) **M1** (35 x 0.750) + (37 x 0.250)
- (a) **A1** 35.5, cao
- **(a) Answer: 35.5**
- (b) **B1** 35Cl-35Cl, m/z = 70
- (b) **B1** 35Cl-37Cl, m/z = 72
- (b) **B1** 37Cl-37Cl, m/z = 74
- **(b) Answer: 70 (35Cl-35Cl), 72 (35Cl-37Cl), 74 (37Cl-37Cl).**
- (c) **M1** probability of 70 (35-35) = 0.750 x 0.750 = 0.5625; probability of 74 (37-37) = 0.250 x 0.250 = 0.0625
- (c) **M1** probability of 72 (35-37, either combination) = 2 x 0.750 x 0.250 = 0.375
- (c) **A1** ratio 70:72:74 = 0.5625 : 0.375 : 0.0625, which simplifies to 9 : 6 : 1, cao
- **(c) Answer: 9 : 6 : 1 (m/z 70 : 72 : 74)**
- (d) **B1** there are two distinct ways of forming a 35-37 combination (35Cl paired with a second-position 37Cl, or 37Cl paired with a second-position 35Cl), so the probability of m/z=72 is doubled relative to a single fixed combination, whereas m/z=74 requires both atoms to be the rarer 37Cl isotope, so its probability is reduced further still oe
- **(d) Answer: There are two distinct ways to form a mixed 35Cl-37Cl molecule (doubling the m/z=72 probability), whereas m/z=74 requires both atoms to be the rarer 37Cl isotope, compounding its low probability, so 72 ends up more than twice as tall as 74.**

Question 3

- (a) **M1** 1s2 2s2 2p6 3s2 3p6 as the core configuration
- (a) **A1** 3d5 4s1 (not 3d4 4s2), giving the full configuration 1s2 2s2 2p6 3s2 3p6 3d5 4s1, cao
- **(a) Answer: 1s2 2s2 2p6 3s2 3p6 3d5 4s1**
- (b) **B1** a half-filled 3d sub-shell (5 electrons, one in each of the 5 d orbitals) has extra stability because electron-electron repulsion between paired electrons in the same orbital is minimised/electrons are more spread out oe
- (b) **B1** moving one electron from 4s to 3d achieves this half-filled, lower-energy arrangement, so the atom as a whole has lower overall energy (is more stable) than the 3d4 4s2 arrangement oe
- **(b) Answer: A half-filled 3d sub-shell minimises electron-electron repulsion (each of the 5 d orbitals holds one unpaired electron), giving a lower-energy, more stable overall configuration than 3d4 4s2.**
- (c) **B1** Fe2+: 1s2 2s2 2p6 3s2 3p6 3d6
- (c) **B1** Fe3+: 1s2 2s2 2p6 3s2 3p6 3d5
- (c) **B1** the 4s electrons are lost before the 3d electrons, because once occupied the 4s sub-shell is at a higher energy than the (now occupied) 3d sub-shell, so 4s electrons are lost first on ionisation oe
- **(c) Answer: Fe2+: [Ar] 3d6. Fe3+: [Ar] 3d5. The 4s electrons are always lost before 3d electrons.**
- (d) **B1** Fe3+ has a half-filled 3d sub-shell (3d5), which has extra stability due to minimised electron-electron repulsion, as in part (b) oe
- **(d) Answer: Fe3+ has a half-filled, extra-stable 3d5 configuration, analogous to the stability seen in chromium.**

Question 4

- (a) **M1** identify the large jump in ionisation energy between the 2nd (1451) and 3rd (7733) ionisation energies
- (a) **A1** Group 2, cao
- (a) **B1** 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
- **(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) **M1** correct substitution: (7733 - 1451)/1451 x 100
- (b) **A1** 433% (accept 430-435%), awrt
- **(b) Answer: Approximately 433%**
- (c) **B1** 1s2 2s2 2p6 3s2 (magnesium's configuration; Y is identified as magnesium), cao
- **(c) Answer: 1s2 2s2 2p6 3s2**
- (d) **B1** 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
- (d) **B1** 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
- **(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 5

- **Level 3** (5-6): 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.
- **Level 2** (3-4): 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.
- **Level 1** (1-2): Limited response; may state the trend without correct explanation, or identify only one relevant factor (e.g. atomic radius) with little development.
- **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 6

- (a) **B1** 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
- (a) **B1** 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
- **(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) **B1** 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
- (b) **B1** the 2p electron is also slightly shielded by the 2s electrons, further reducing the effective nuclear attraction it experiences oe
- (b) **B1** these effects outweigh the increased nuclear charge, so less energy is needed to remove boron's 2p electron than beryllium's 2s electron oe
- **(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) **B1** 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
- (c) **B1** the two electrons paired in the same oxygen orbital repel each other more strongly than electrons in separate orbitals would oe
- (c) **B1** 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
- **(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 7

- (a) **B1** electron energy levels get closer together in energy as n increases (they converge towards a limit) oe
- (a) **B1** 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
- **(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) **M1** $E = hf = 6.63 \times 10^{-34} \times 3.28 \times 10^{15}$
- (b) **A1** 2.17×10^{-18} J, awrt
- **(b) Answer: 2.17×10^{-18} J**
- (c) **M1** energy per mole = $2.17 \times 10^{-18} \times 6.02 \times 10^{23}$, ft from (b)
- (c) **M1** = 1.306×10^{6} J/mol
- (c) **A1** 1310 kJ/mol (1.31×10^{3} kJ/mol), awrt
- **(c) Answer: 1.31×10^{3} kJ/mol (1310 kJ/mol)**
- (d) **B1** 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
- **(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 8

- (a) **M1** recognise t is proportional to $\sqrt{m}$, so m is proportional to t^2
- (a) **M1** mass ratio = $(1.97 \times 10^{-5})^2 / (1.86 \times 10^{-5})^2$
- (a) **A1** 1.12 : 1 (accept 1.12-1.13 : 1), awrt
- **(a) Answer: Approximately 1.12 : 1 (ion 2 : ion 1)**
- (b) **M1** mass of heavier ion = 20 x 1.122, ft from (a)
- (b) **A1** 22 (to the nearest whole number), cao
- (b) **B1** identified as the isotope 22Ne+ (neon-22)
- **(b) Answer: Relative mass approximately 22; this is the isotope 22Ne+ (neon-22).**
- (c) **B1** since kinetic energy ($1/2\ m\ v^2$) is the same for all ions, an ion of greater mass must have a smaller velocity, so it takes longer to travel the fixed length of the flight tube oe
- **(c) Answer: Because kinetic energy is the same for all ions, a heavier ion must have a lower velocity, so it takes longer to cross the flight tube.**

Question 9

- (a) **M1** core configuration 1s2 2s2 2p6 3s2 3p6
- (a) **A1** 3d10 4s1, giving 1s2 2s2 2p6 3s2 3p6 3d10 4s1, cao
- **(a) Answer: 1s2 2s2 2p6 3s2 3p6 3d10 4s1**
- (b) **B1** 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
- (b) **B1** 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
- **(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) **B1** Cu+: 1s2 2s2 2p6 3s2 3p6 3d10 ([Ar] 3d10)
- (c) **B1** Cu2+: 1s2 2s2 2p6 3s2 3p6 3d9 ([Ar] 3d9)
- **(c) Answer: Cu+: [Ar] 3d10. Cu2+: [Ar] 3d9.**
- (d) **B1** 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
- **(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.**

Question 10

- (a) **M1** percentage abundance = (peak height / total height) x 100 = (78.9/100.0) x 100
- (a) **A1** 78.9%, cao
- **(a) Answer: 78.9%**
- (b) **M1** percentage uncertainty = (0.5 / 78.9) x 100
- (b) **A1** 0.63%, awrt
- **(b) Answer: 0.63%**
- (c) **M1** absolute uncertainty = percentage uncertainty x value = 0.63% x 78.9%, ft
- (c) **A1** ± 0.50 percentage points (accept 0.49-0.50), awrt
- **(c) Answer: ± 0.50 percentage points, i.e. 78.9% ± 0.5%**
- (d) **B1** 3 significant figures (e.g. 24.3)
- (d) **B1** 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
- **(d) Answer: 3 significant figures (e.g. 24.3), because the measurement uncertainty does not justify greater precision than this.**

Question 11

- (a) **M1** correct method: (54 x 0.058) + (56 x 0.917) + (57 x 0.022) + (58 x 0.003)
- (a) **M1** = 3.132 + 51.352 + 1.254 + 0.174
- (a) **A1** 55.9, cao
- **(a) Answer: 55.9**
- (b) **M1** 1s2 2s2 2p6 3s2 3p6 as the core configuration
- (b) **A1** 3d6 4s2, giving 1s2 2s2 2p6 3s2 3p6 3d6 4s2, cao
- **(b) Answer: 1s2 2s2 2p6 3s2 3p6 3d6 4s2**
- (c) **B1** 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
- (c) **B1** 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
- (c) **B1** instead, ionisation energies increase relatively steadily as successive electrons are removed from the 3d sub-shell of an increasingly positively charged ion oe
- **(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) **B1** (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
- **(d) Answer: Approximately 105% increase, consistent with both electrons coming from the same 4s sub-shell.**