2.1 Atomic Structure: 1-hour Pack

AQA 7405 · Calculator allowed · about 60 minutes

Total Marks

Name: _____ Date: ____ / ____ / _____

Answer ALL questions. Show all your working.

1 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 1 is 8 marks)

© Revision Library | revisionlibrary.co.uk

2 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 x m x 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 2 is 10 marks)

---

3 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 3 is 6 marks)

© Revision Library | revisionlibrary.co.uk

4 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 4 is 7 marks)

© Revision Library | revisionlibrary.co.uk

5 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, $N_A = 6.02 \times 10^{23}$ 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 5 is 7 marks)

---

6 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 6 is 7 marks)

© Revision Library | revisionlibrary.co.uk

Mark scheme · 2.1 Atomic Structure: 1-hour Pack

Question 1

(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 2

(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: $v = 3.47 \times 10^{5}$ 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: $t = 5.76 \times 10^{-6}$ s

Question 3

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.

© Revision Library | revisionlibrary.co.uk

Question 4

(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 5

(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 6

(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)

© Revision Library | revisionlibrary.co.uk