2.1 Atomic Structure: Test Pack

AQA 7405 · Calculator allowed · about 50 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)

2 This question is about calculating relative atomic mass from isotopic abundance data.

(a) Bromine consists of two isotopes: 79Br (55.0% abundance) and 81Br (45.0% abundance). Calculate the relative atomic mass of bromine, giving your answer to 1 decimal place. **(2)**

(b) Neon consists of three isotopes: 20Ne (90.5% abundance), 21Ne (0.3% abundance) and 22Ne (9.2% abundance). Show that the relative atomic mass of neon is 20.2 (to 1 decimal place). **(3)**

(c) The relative atomic mass of chlorine is 35.5. Explain why this value is not a whole number, even though the mass number of every individual isotope of chlorine is always a whole number. **(2)**

(Total for Question 2 is 7 marks)

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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 Fe^{2+} ion and the Fe^{3+} ion (iron, atomic number 26), explaining which sub-shell loses electrons first on ionisation. **(3)**

(d) Suggest why Fe^{3+} ([Ar] 3d5) is a particularly stable ion compared with Fe^{2+}. **(1)**

(Total for Question 3 is 8 marks)

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4 Chlorine gas exists as diatomic molecules, Cl_2, 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 Cl_2, 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 4 is 9 marks)

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5 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 5 is 7 marks)

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Mark scheme · 2.1 Atomic Structure: Test Pack

Question 1

(a) 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 **B1**

(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) a d sub-shell holds a maximum of 10 electrons (5 orbitals, 2 electrons each) **B1**

(b) Answer: A d sub-shell holds a maximum of 10 electrons.

(c) X(g) -> X+(g) + e- **B1**

(c) Answer: X(g) -> X+(g) + e-

(d) for a singly (1+) charged ion, m/z is numerically equal to the relative mass of the ion oe **B1**

(d) Answer: For a singly charged ion, m/z is numerically equal to the ion's relative mass.

Question 2

(a) (79 x 0.550) + (81 x 0.450) or equivalent correct method **M1**

(a) 79.9 cao **A1**

(a) Answer: 79.9

(b) correct substitution: (20 x 0.905) + (21 x 0.003) + (22 x 0.092) **M1**

(b) evaluates to 20.187 **M1**

(b) = 20.2 (1 dp), as required, cso **A1**

(b) Answer: 20.2 (cso, as given)

(c) chlorine exists naturally as a mixture of isotopes (35Cl and 37Cl), each with an integer mass number oe **B1**

(c) relative atomic mass is the weighted mean (average) of the isotopic masses, weighted by their relative abundance, so the result is not necessarily a whole number oe **B1**

(c) Answer: Chlorine is a mixture of isotopes; relative atomic mass is a weighted mean of these, so it need not be an integer.

Question 3

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

(a) 3d5 4s1 (not 3d4 4s2), giving the full configuration 1s2 2s2 2p6 3s2 3p6 3d5 4s1, cao **A1**

(a) Answer: 1s2 2s2 2p6 3s2 3p6 3d5 4s1

(b) 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 **B1**

(b) 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 **B1**

(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) Fe^{2+}: 1s2 2s2 2p6 3s2 3p6 3d6 **B1**

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

(c) 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 **B1**

(c) Answer: Fe^{2+}: [Ar] 3d6. Fe^{3+}: [Ar] 3d5. The 4s electrons are always lost before 3d electrons.

(d) Fe^{3+} has a half-filled 3d sub-shell (3d5), which has extra stability due to minimised electron-electron repulsion, as in part (b) oe **B1**

(d) Answer: Fe^{3+} has a half-filled, extra-stable 3d5 configuration, analogous to the stability seen in chromium.

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Question 4

(a) (35 x 0.750) + (37 x 0.250) **M1**

(a) 35.5, cao **A1**

(a) Answer: 35.5

(b) 35Cl-35Cl, m/z = 70 **B1**

(b) 35Cl-37Cl, m/z = 72 **B1**

(b) 37Cl-37Cl, m/z = 74 **B1**

(b) Answer: 70 (35Cl-35Cl), 72 (35Cl-37Cl), 74 (37Cl-37Cl).

(c) probability of 70 (35-35) = 0.750 x 0.750 = 0.5625; probability of 74 (37-37) = 0.250 x 0.250 = 0.0625 **M1**

(c) probability of 72 (35-37, either combination) = 2 x 0.750 x 0.250 = 0.375 **M1**

(c) ratio 70:72:74 = 0.5625 : 0.375 : 0.0625, which simplifies to 9 : 6 : 1, cao **A1**

(c) Answer: 9 : 6 : 1 (m/z 70 : 72 : 74)

(d) 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 **B1**

(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 5

(a) recognise t is proportional to $\sqrt{m}$, so m is proportional to t^2 **M1**

(a) mass ratio = $(1.97 \times 10^{-5})^2 / (1.86 \times 10^{-5})^2$ **M1**

(a) 1.12 : 1 (accept 1.12-1.13 : 1), awrt **A1**

(a) Answer: Approximately 1.12 : 1 (ion 2 : ion 1)

(b) mass of heavier ion = 20 x 1.122, ft from (a) **M1**

(b) 22 (to the nearest whole number), cao **A1**

(b) identified as the isotope 22Ne+ (neon-22) **B1**

(b) Answer: Relative mass approximately 22; this is the isotope 22Ne+ (neon-22).

(c) 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 **B1**

(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.

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