IMPERIAL COLLEGE LONDON

BSc and MSci DEGREES – JANUARY 2017, for Internal Students of the Imperial College of Science, Technology and Medicine

This paper is also taken for the relevant examination for the Associateship

CHEM40001 Introduction to Chemistry

PAPER ONE

Wednesday 11th January 2017, 14:00-16:15

USE A SEPARATE ANSWER BOOK FOR EACH QUESTION. WRITE YOUR CANDIDATE NUMBER ON EACH ANSWER BOOK.

Q1: Atomic Structure

Answer parts a) **AND** part b), and **EITHER** part c) **OR** part d) of this question.

a) Answer **ALL** parts of this question.

i) What are the four quantum numbers required to specify the state of an electron in a hydrogen atom? What values can they take?

(4 marks)

ii) What is the '*Aufbau Principle*' and explain why the Aufbau sequence for polyelectronic atoms is different from the *hydrogenic* ordering of orbitals.

(5 marks)

iii) It was suggested in 1976 that traces of the element Z = 126 were to be found in a meteorite discovered in Madagascar. What would you predict the electronic configuration of this element to be? You may use the symbol [Rn] to represent the closed inner shell corresponding to the noble gas Radon.

(4 marks)

b) Answer **ALL** parts of this question.

Arrange the ions within each of the groups below in order of **increasing** size, and justify your reasoning:

i) Ba^{2+} ; Al^{3+} ; Mg^{2+} ; Cs^{+}

ii) Cl^{-} ; I^{-} ; O^{2-} ; S^{2-}

(6 marks)

c) Calculate the energy to remove the only remaining electron of a cation X^{Y+} when the limiting wavelength of the highest energy series is $\lambda = 5.69$ nm (ionisation energy of H; $E_{i,H} = 1312$ kJ mol^{-1}). What is the element X?

(6 marks)

d) Define the term *electron affinity* (EA; kJ mol^{-1}) and account for the trends in the values of the following atoms or ions:

C	122	N	–7	O	141	O^{-}	–780
Si	133	P	72	S	200	S^{-}	–590

(6 marks)

Q2: Alkanes, Alkenes & Alkynes

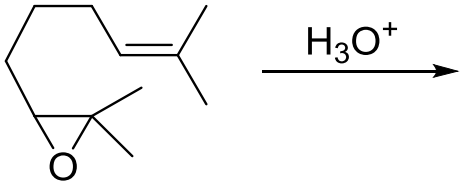
Answer parts a), b), c) **AND** d) of this question.

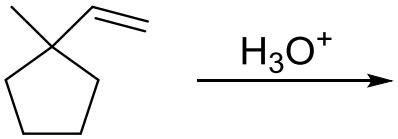
a) Based on your knowledge of related hydrocarbons provide a conformational analysis for propane. Your answer should include a graphical discussion that clearly identifies different conformers and their relative energies.

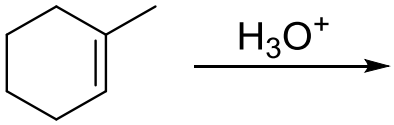
(5 marks)

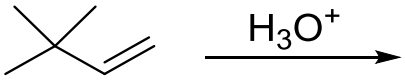
b) Identify the major product(s) formed in **THREE** of the following transformations. Provide full mechanisms and give detailed explanations for any selectivity observed.

(12 marks)

i) 

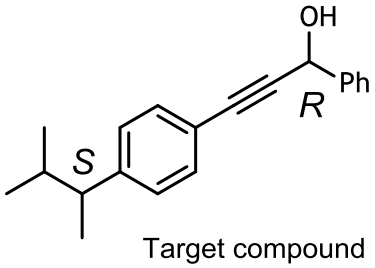
ii) 

iii) 

iv) 

QUESTION CONTINUED OVERLEAF

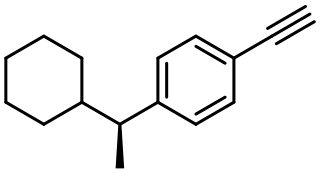
c) The target compound below is an important building block for a potential drug candidate. Showing your workings, redraw the molecule to clearly show the *R* and *S* stereochemistry using the wedge/dash notation.



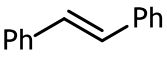
Target compound

(4 marks)

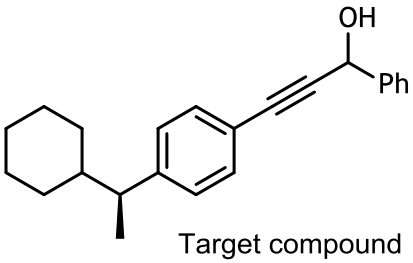
d) Using the two starting materials provided, suggest a route to the second target compound below. This is a multistep process and you should identify the key intermediates and the reagents required for each step. Note that the target compound is a mixture of diastereoisomers, which would be separated later.



Starting material 1



Starting material 2



Target compound

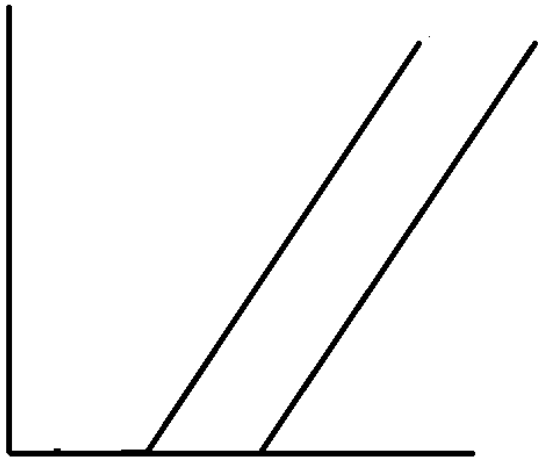
(4 marks)

Q3: Quantum Chemistry

Answer **ALL** of the three parts a), b) and c) of this question.

a) Answer **ALL** parts of this question.

The diagram below may be used to illustrate the photoelectric effect. Reproduce this diagram in your answer booklet and use it to explain the key features and conclusions of the photoelectric effect. You should ensure that your diagram is carefully labelled.



(7 marks)

b) Answer **ALL** parts of this question.

i) A wavefunction is found to take the form shown below. Is this wavefunction acceptable for the range of x values specified? Explain your answer.

$$\psi = \frac{N \exp(-ax^2)}{(x-3)} : 0 < x < 10$$

(4 marks)

ii) The wavefunction for the particle in the box is given by the following expression.

$$\psi = \sqrt{\frac{2}{L}} sin\left(\frac{n\pi x}{L}\right)$$

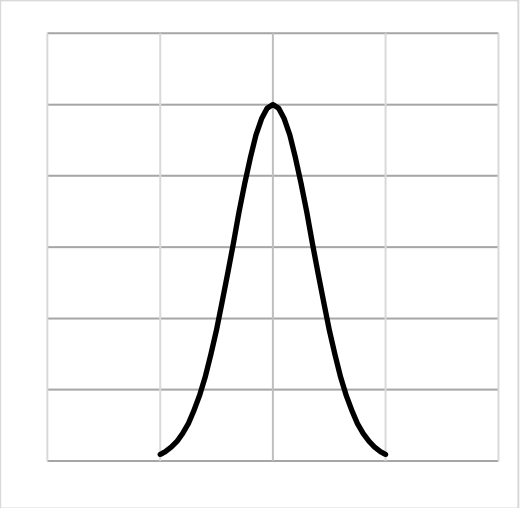
What values is the quantum number n allowed to take? Explain your reasoning.

(4 marks)

QUESTION CONTINUED OVERLEAF

iii) The function depicted below is the wavefunction for the ground state for the vibrating diatomic molecule. What does the function tell us about the kinetic energy of the molecule and how it varies as the bond vibrates?

(4 marks)



c) Answer **EITHER** part i) **OR** part ii) of this question.

i) For the particle in a box of length, L, the probability of finding the particle in a region between 0 and ℓ is given by the expression shown below.

$$\left\{\frac{\ell}{L} - \frac{1}{2n\pi}\sin\frac{2\pi n\ell}{L}\right\}$$

Calculate the probability that the particle occupying the n=1 level in a box of length 1.5 nm will be found in the region between x=0 and x= 0.3nm. What happens to the probability when n becomes very large and what is the significance of this result?

(6 marks)

ii) The wavefunction for a particle on a ring (rotation in a plane) is given by the expression below.

$$\psi(\phi) = \left(\frac{1}{2\pi}\right)^{1/2} \exp(im_l\phi)$$

Does the probability that the particle is found between two angles ϕ_1 and ϕ_2 depend on the value of m_l? Explain your answer

(6 marks)