

**UNIVERSITY COLLEGE LONDON**

University of London

**EXAMINATION FOR INTERNAL STUDENTS**

For The Following Qualifications:-

*B.Sc.*    *M.Sc.*

**Physics 2B24: Atomic and Molecular Physics**

**COURSE CODE            :    PHYS2B24**

**UNIT VALUE             :    0.50**

**DATE                     :    17-MAY-06**

**TIME                     :    10.00**

**TIME ALLOWED         :    2 Hours 30 Minutes**

Answer ALL questions from Section A and THREE questions from Section B.

The following data may be used:

Speed of light,  $c = 2.998 \times 10^8 \text{ ms}^{-1}$

Planck's constant,  $h = 6.626 \times 10^{-34} \text{ Js}$

Bohr magneton,  $\mu_B = 9.274 \times 10^{-24} \text{ JT}^{-1}$

1 atomic unit of energy =  $219475 \text{ cm}^{-1} = 27.2 \text{ eV} = 2 \text{ Rydberg}$

Fundamental electronic charge,  $e = 1.602 \times 10^{-19} \text{ C}$

Mass of a nucleon (proton or neutron),  $m_u = 1.66 \times 10^{-27} \text{ kg}$

Mass of an electron,  $m_e = 9.11 \times 10^{-31} \text{ kg}$

*The numbers in square brackets show the provisional allocation of maximum marks per question or part of question.*

### Section A

1. Briefly describe the Rutherford scattering experiment, the results obtained and what can be deduced about the structure of the atom. [6]
2. Sketch the spectrum of X-rays that is produced when a heavy metal target is bombarded with energetic electrons. [3]  
Indicate which parts change when the target material is changed, and which are independent of the target. Briefly explain why. [4]
3. Describe the central field approximation as applied to an alkali atom that has a single optically active electron. [3]  
Give an expression for the energy (in atomic units) of the outer electron in terms of an effective nuclear charge  $Z_{\text{eff}}$ , the principal quantum number  $n$ , and the quantum defect  $\Delta_{nl}$ . [2]  
The alkali metal lithium has nuclear charge  $Z = 3$ , and a quantum defect for the 2s electron  $\Delta_{2s} = 0.40$ . Calculate the energy of the electron. [2]
4. State the electric dipole selection rules for the quantum numbers  $J, M_J$  and  $l$  for a multi-electron atom. [4]  
Hence explain why the 1s2s ( $^3P$ ) excited state of helium is metastable. [4]
5. Sketch the form of the symmetric and antisymmetric wavefunctions for the ground state of the hydrogen molecular ion  $\text{H}_2^+$  in the linear combination of atomic orbitals (LCAO) approximation. [2]  
Now sketch the corresponding electron probability densities. [2]  
Which combination is energetically stable and why? [2]
6. Explain what sort of transitions in an ideal diatomic molecule give rise to absorption lines in the microwave region, and hence which molecules will not have a microwave absorption spectrum. What determines the energy spacing of the lines? [4]  
Which, if any, of the following molecules will not absorb energy in the microwave region?

$\text{O}_2, \text{OH}^-, \text{CO}$ .

[2]

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## Section B

7. State without proof the Rydberg formula for the wavelength of light emitted when an electron in a hydrogen atom makes a transition from a state with quantum number  $n$  to one with quantum number  $m$ . [2]

With reference to the Rydberg formula, explain why the lines in the emission spectrum of atomic hydrogen occur in series, the lines within each series converging towards a short wavelength limit. [4]

The table below shows the wavelengths of consecutive lines in the Balmer series in the emission spectrum of hydrogen.

label	$\lambda/\text{nm}$
$\alpha$	656.3
$\beta$	486.1
$\gamma$	434.0
$\delta$	410.2
$\epsilon$	397.0
$\zeta$	388.9
$\eta$	383.5

By plotting a suitable graph determine the Rydberg constant for Hydrogen and the short wavelength limit of the Balmer series. [8]

Why can the spectrum of singly ionised helium ( $\text{He}^+$ ) be fitted to a formula similar to that you have written for atomic hydrogen? What is this formula? [3]

The Pickering series in  $\text{He}^+$  contains several lines that are almost coincident with lines of the Balmer series in hydrogen. [3]

8. Explain the notation of the Russell-Saunders term symbol:

$$^{2S+1}L_J.$$

[3]

When determining the term from a given electronic configuration which electrons must be considered and which may be neglected? Explain why. [2]

State Hund's Rules for the ordering of terms in increasing energy according to their value of  $S$ ,  $L$  and  $J$ . [6]

What restriction is placed on the symmetry of the wavefunction of a multi-electron atom by the Pauli Exclusion Principle? [2]

Explain qualitatively how this gives rise to the ordering of terms according to their value of  $S$  described by Hund's Rules. [4]

Samarium (Sm) has electronic configuration  $[\text{Xe}]6s^24f^6$ . The ground state has total spin  $S = 3$  and total orbital angular momentum  $L = 3$ . What values of  $J$  are possible? Hence write down the lowest energy term of the ground state. [3]

9. Give an expression for the magnetic moment,  $\underline{\mu}_L$ , associated with the orbital angular momentum  $\underline{L}$  of an electron, in terms of  $\underline{L}$ , the Bohr magneton  $\mu_B$  and a g-factor  $g_L$ .

Do the same for the spin magnetic moment  $\underline{\mu}_S$ , in terms of  $\underline{S}$ ,  $\mu_B$  and  $g_S$ . [2]

Give a formula for the interaction energy between the total magnetic moment and a magnetic field  $\underline{B}$  in terms of the quantum numbers  $m_l$  and  $m_s$ . You may take  $g_L = 1$  and  $g_S = 2$ . [4]

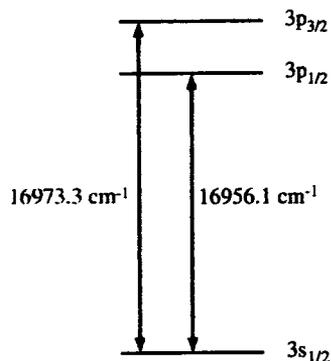
What is the magnetic moment of neutral silver in its ground state  $^2S_{1/2}$ ? [2]

If a beam of neutral silver atoms travels along the  $x$ -direction through a region of non-uniform magnetic field with gradient in the  $z$ -direction  $\frac{dB}{dz} = b$ , obtain an expression for the force acting on the silver atoms. [2]

Describe what you would observe when the silver atoms are incident on a screen placed perpendicular to the initial direction of propagation and explain how this provides evidence for the quantisation of spin. [4]

The experiment is repeated with neutral lithium and with singly ionised lithium. Give the term symbols for each species, describe what you would expect to see in the experiment for each case, and compare the results with those for silver. [6]

10. A sketch of the first few energy levels of the sodium atom is shown below.



Explain *qualitatively* the physical origin of the splitting of the 3p state into two energy levels labelled by  $j = \frac{3}{2}$  and  $j = \frac{1}{2}$ . Include in your explanation a justification for the change in energy from the 3p state being of the form:

$$\Delta E_{LS} = \frac{1}{2}A(j(j+1) - l(l+1) - s(s+1)),$$

where  $A$  is a constant. [9]

What happens to the energy levels if a weak magnetic field is applied? What are the good quantum numbers in this case? What if a strong magnetic field is applied? What are the good quantum numbers now? [6]

Sketch the energy levels of sodium in a *strong* magnetic field, labelled by the appropriate quantum numbers, and indicate the electric dipole allowed transitions. How many spectral lines will be observed? [5]

11. For many covalent diatomic molecules the effective potential in which the nuclei move is well described by the Morse potential:

$$V(R) = D_e \left( e^{-2\alpha(R-R_e)} - 2e^{-\alpha(R-R_e)} \right)$$

Sketch the form of  $V(R)$ , marking clearly on your sketch the parameters  $D_e$  and  $R_e$ . [4]

Show that for small displacements from  $R_e$  the Morse potential is approximately harmonic (You may use the expression  $e^{-ax} \simeq 1 - ax + \frac{1}{2}(ax)^2 \dots$  valid for small  $x$ ).

Hence obtain a relation between the energy required to dissociate the molecule in its lowest vibrational state,  $D_0$ , and the energy  $D_e$ . [5]

From your approximation to  $V(R)$ , find an expression for the spring constant,  $k$ , of the bond in terms of  $\alpha$  and  $D_e$ . [2]

Given that for the hydrogen molecule  $H_2$ ,  $D_e = 4.75$  eV and  $\alpha = 1.94 \times 10^{10} \text{ m}^{-1}$ , calculate the vibrational frequency near the bottom of the potential well, and thus the energy  $D_0$ . [5]

Hence calculate  $D_0$  for the deuterium molecule,  $D_2$ . [4]

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4. State the electric dipole selection rules for the quantum numbers  $J, M_J$  and  $S$  for a multi-electron atom. [4]  
Hence explain why the  $1s2s$  ( $^3P$ ) excited state of helium is metastable. [4]