

Question one

a) What is the physical significance of a radial wave function $R(r)$? [1 mark]

b) If a wave function of a hydrogen atom is given by

$$\psi = (27-18b + 2b^2)\exp(-b/3)$$

where $b=Zr/a_0$, give the expression for each of the following:

- i) radial part
- ii) angular part
- iii) radial distribution function.

[4 marks]

c) For the wavefunction of a $6d_{x^2-y^2}$ orbital, sketch the diagram corresponding to

- i) radial part
- ii) radial distribution function
- iii) angular part

[6 marks]

d) For each of the following species, write the electron configuration and determine the number of unpaired electrons present:

- i) Re^{2+}
- ii) Nd^{2+}

[8 marks]

e) Briefly state the de Broglie hypothesis. Your answer should include the appropriate equation. Briefly explain how the hypothesis has contributed to understanding of the properties of an electron.

[6 marks]

Question Two

- a) Consider the species Ga, Ga⁺ and Ga²⁺.
- For each of the species above, calculate the effective nuclear charge for an electron in the valence shell [12 marks]
 - Based on your calculated effective nuclear charges, which of the species is expected to have the lowest ionization energy? Explain. [2 marks]
- b) Consider the molecule IO₂F₃, where iodine, I, is the central atom.
- Draw at least three non-equivalent Lewis structures of the molecule
 - Use formal charges to determine which one of the structures you have drawn is the most reasonable.
 - Calculate the average I-O bond order.

[11 marks]

Question Three

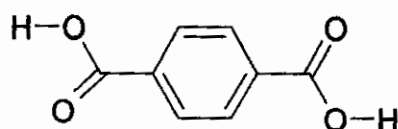
- a) For each of the following species, determine the molecular geometry and suggest an appropriate hybridization scheme for the central atom:
- F₂O (O is the central atom)
 - SF₄
 - BrF₅ (Br is the central atom)

[12 marks]

[13 marks]

Question Four

- a) With the help of appropriate structures, suggest the nature of hydrogen bonding present in the following species:
- Ethanol, $\text{CH}_3\text{CH}_2\text{OH}$
 - $[\text{NH}_4][\text{BH}_4]$
 - A compound containing H-bonds between RCOOH and RCOO^-
 - 1,4-benzene dicarboxylic acid:



1,4-benzene dicarboxylic acid

[9 marks]

- b) Use balanced equations to illustrate what happens when the following species are dissolved in water:
- Diborane, B_2H_6
 - Al_4C_3
 - Mg_3N_2

[6 marks]

- c) For each of the following, sketch the structure and indicate the coordination number around the Lewis acid:
- $[\text{BF}_4]^-$
 - $\text{Be}^{2+}(\text{aq})$
 - SiF_6^{2-}
 - $\text{Na}^+(\text{aq})$

[10 marks]

Question Five

- a) For each of the groups (of the periodic table) given below, state the common oxidation state(s) which occur in oxides, and give the formula, M_xO_y , of each of such oxides:
- group 1
 - group 2
 - group 13
 - group 14
 - group 15

[10 marks]

b) Give a balanced equation for a reaction that is expected to take place when each of the following chlorides is added to water:



[6 marks]

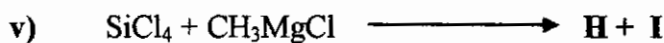
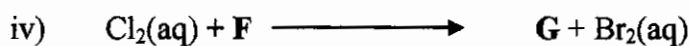
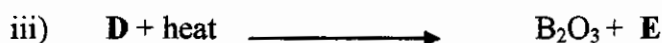
c) Give one example of an oxide and write a balanced reaction equation to illustrate its property as indicated below.

- i) An acidic oxide that is soluble in water and show how it reacts with water
- ii) A basic oxide that is soluble in water and show how it reacts with water
- iii) An amphoteric oxide and show how it reacts with an acid and a base

[9 marks]

Question Six

a) Identify the species **A, B, C, D, E, F, G, H, I, J** and **K**:



[11 marks]

b) Give an outline of the Born-Haber cycle for the formation of indium chloride, $\text{InCl}_3(\text{s})$.

[6 marks]

c) A sodium chloride structure has 4 formula units per unit cell. A unit cell length of 564 pm for NaCl has been determined by x-ray diffraction studies. Determine the inter-ionic distance for NaCl, and calculate the volume, the mass and the density of the unit cell.

[8 marks]

Slater's Rules:

1) Write the electron configuration for the atom using the following design;

(1s)(2s,2p)(3s,3p) (3d) (4s,4p) (4d) (4f) (5s,5p) etc

**2) Any electrons to the right of the electron of interest contributes no shielding.
(Approximately correct statement.)**

3) All other electrons in the same group as the electron of interest shield to an extent of 0.35 nuclear charge units

4) If the electron of interest is an *s* or *p* electron: All electrons with one less value of the principal quantum number shield to an extent of 0.85 units of nuclear charge. All electrons with two less values of the principal quantum number shield to an extent of 1.00 units.

5) If the electron of interest is an *d* or *f* electron: All electrons to the left shield to an extent of 1.00 units of nuclear charge.

6) Sum the shielding amounts from steps 2 through 5 and subtract from the nuclear charge value to obtain the effective nuclear charge.

Derived SI Units

Physical quantity	Name of unit	Symbol for unit	Definition of unit
Energy	Joule	J	$\text{kg m}^2\text{s}^{-2}$
Force	Newton	N	$\text{kg m s}^{-2} = \text{J m}^{-1}$
Power	Watt	W	$\text{kg m}^2\text{s}^{-3} = \text{J s}^{-1}$
Pressure	Pascal	Pa	$\text{kg m}^{-1}\text{s}^{-2} = \text{N m}^{-2}$
Electric charge	Coulomb	C	A s
Electric potential difference	Volt	V	$\text{kg m}^2\text{s}^{-3}\text{A}^{-1} = \text{J A}^{-1}\text{s}^{-1}, \text{J/C}$
Electric resistance	Ohm	Ω	$\text{kg m}^2\text{s}^{-3}\text{A}^{-2} = \text{V A}^{-1}$
Electric capacitance	Farad	F	$\text{A}^2\text{s}^4\text{kg}^{-1}\text{m}^{-2} = \text{A s V}^{-1}$
Magnetic flux	Weber	Wb	$\text{kg m}^2\text{s}^{-2}\text{A}^{-1} = \text{V s}$
Inductance	Henry	H	$\text{kg m}^2\text{s}^{-2}\text{A}^{-2} = \text{V s A}^{-1}$
Magnetic flux density	Tesla	T	$\text{kg s}^{-2}\text{A}^{-1} = \text{V s m}^{-2}$
Frequency	Hertz	Hz	$\text{Hz} = \text{s}^{-1}$
Customary temperature, <i>t</i>	Degree Celsius	$^{\circ}\text{C}$	$t[^{\circ}\text{C}] = T[\text{K}] - 273.15$

Fundamental Constants

Quantity	Symbol	Value	SI unit
Speed of light in vacuum	<i>c</i>	$2.997\,925 \times 10^8$	m s^{-1}
Elementary charge	<i>e</i>	$1.602\,189 \times 10^{-19}$	C
Planck constant	<i>h</i>	$6.626\,18 \times 10^{-34}$	J s
Avogadro constant	<i>N_A</i>	$6.022\,04 \times 10^{23}$	mol^{-1}
Atomic mass unit	<i>u</i>	$1.660\,566 \times 10^{-27}$	kg
Electron rest mass	<i>m_e</i>	$0.910\,953 \times 10^{-30}$	kg
Proton rest mass	<i>m_p</i>	$1.672\,649 \times 10^{-27}$	kg
Neutron rest mass	<i>m_n</i>	$1.674\,954 \times 10^{-27}$	kg
Faraday constant	<i>F</i>	$9.648\,46 \times 10^4$	C mol^{-1}
Rydberg constant	<i>R_∞</i>	$1.097\,373 \times 10^7$	m^{-1}
Bohr radius	<i>a₀</i>	$0.529\,177 \times 10^{-10}$	m
Electron magnetic moment	<i>μ_e</i>	$9.284\,83 \times 10^{-24}$	J T^{-1}
Proton magnetic moment	<i>μ_p</i>	$1.410\,617 \times 10^{-26}$	J T^{-1}
Bohr magneton	<i>μ_B</i>	$9.274\,08 \times 10^{-24}$	J T^{-1}
Nuclear magneton	<i>μ_N</i>	$5.050\,82 \times 10^{-27}$	J T^{-1}
Molar gas constant	<i>R</i>	8.314 41	$\text{J mol}^{-1} \text{K}^{-1}$
Molar volume of ideal gas (stp.)	<i>V_m</i>	0.022 413 8	$\text{m}^3 \text{mol}^{-1}$
Boltzmann constant	<i>k</i>	$1.380\,662 \times 10^{-23}$	J K^{-1}

Conversion Factors

1 cal	= 4.184 joules (J)
1 eV/molecule	= 96.485 kJ mol ⁻¹
	= 23.061 kcal mol ⁻¹
1 kcal mol ⁻¹	= 349.76 cm ⁻¹
	= 0.0433 eV
1 kJ mol ⁻¹	= 83.54 cm ⁻¹
1 wavenumber (cm ⁻¹)	= 2.8591×10^{-3} kcal mol ⁻¹
1 erg	= 2.390×10^{-11} kcal
1 centimeter (cm)	= 10^8 Å
	= 10^7 nm
1 picometer (pm)	= 10^{-2} Å
1 nanometer (nm)	= 10 Å

App

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Definit
the proces

Older che
which is -

- 1 H
- 2 He
- 3 Li
- 4 Be
- 5 B
- 6 C
- 7 N
- 8 O
- 9 F
- 10 Ne
- 11 Na
- 12 Mg
- 13 Al
- 14 Si
- 15 P
- 16 S
- 17 Cl
- 18 Ar
- 19 K
- 20 Ca
- 21 Sc
- 22 Ti
- 23 V
- 24 Cr

Periodic Table of the Elements

GROUP
1

1 H 1.0079	2 He 4.0026																
3 Li 6.941	4 Be 9.0122	5 B 10.811	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180	11 Na 22.990	12 Mg 24.305	13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.066	17 Cl 35.453	18 Ar 39.948		
19 K 39.098	20 Ca 40.078	21 Sc 44.956	22 Ti 47.867	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.933	28 Ni 58.693	29 Cu 63.546	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.468	38 Sr 87.62	39 Y 88.906	40 Zr 91.224	41 Nb 92.906	42 Mo 95.94	43 Tc 98.906*	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.29
55 Cs 132.91	56 Ba 137.33	57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm 146.92*	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97	
87 Fr 223.02	88 Ra 226.03*	89 Ac 227.03	90 Th 232.04*	91 Pa 231.04*	92 U 238.03	93 Np 237.05*	94 Pu 239.05*	95 Am 241.06*	96 Cm 244.06*	97 Bk 249.08*	98 Cf 252.08*	99 Es 252.08*	100 Fm 257.10*	101 Md 258.10*	102 No 259.10*	103 Lr 262.11*	
112 Cn (294)	113 Nh (294)	114 Fl (294)	115 Mc (294)	116 Lv (294)	117 Ts (294)	118 Og (294)	119 Uu (294)	120 Uub (294)	121 Uut (294)	122 Uuq (294)	123 Uuq (294)	124 Uuq (294)	125 Uuq (294)	126 Uuq (294)	127 Uuq (294)	128 Uuq (294)	

*Lanthanide series

▲Actinide series

Note: Atomic masses shown here are the 1993 IUPAC values with a maximum of five significant figures (T. B. Coplen *et al.*, *Inorg. Chim. Acta* 1994, 217, 217). An asterisk indicates the mass of a commonly known radioisotope. Numbers in parentheses are the mass numbers of the corresponding longer-lived isotope.