

**FIRST SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY)  
EXAMINATION, NOVEMBER 2021**

(CBCSS)

Chemistry

CHE1C04—THERMODYNAMICS, KINETICS AND CATALYSIS

(2019 Admission onwards)

Time : Three Hours

Maximum : 30 Weightage

**General Instructions**

1. *In cases where choices are provided, students can attend all questions in each section.*
2. *The minimum number of questions to be attended from the Section / Part shall remain the same.*
3. *The instruction if any, to attend a minimum number of questions from each sub section / sub part / sub division may be ignored.*
4. *There will be an overall ceiling for each Section / Part that is equivalent to the maximum weightage of the Section / Part.*

**Section A**

*Answer eight questions.*

*Each question carries a weightage of 1.*

1. Define chemical potential in terms of : (a) internal energy ; and (b) Helmholtz free energy.
2. One mole of toluene is mixed with 0.5 moles of benzene at 300k to form an ideal solution. Find the free energy of mixing.
3. Distinguish between equilibrium and steady state conditions.
4. State and explain onsager reciprocal relation.
5. Define secondary salt effect.
6. Unimolecular gas phase reactions follow first order kinetics at high pressures and second order kinetics at low pressures. Why ?
7. Distinguish between activated and non-activated adsorption.
8. Explain 'catalyst poisoning'.

**Turn over**

9. Define Michaelis-Menton constant. Explain its significance.
10. Nano materials have high surface area. Justify the statement.

(8 × 1 = 8 weightage)

### Section B

*Answer six questions.*

*Each question carries a weightage of 2.*

11. Use third law of thermodynamics to show that absolute zero of temperature is unattainable.
12. Define partial molal volume. How is it evaluated ? Discuss.
13. Derive an equation for the rate of entropy production for one component system with heat and matter transport.
14. What are the conditions under which linear relationship exists between force and flux ? What are the advantages of a linear relationship ?
15. Derive an equation to show primary salt effect.
16. Show that for rigid sphere model of bimolecular reactions. Absolute rate theory agrees with simple collision theory.
17. How would you determine pore size distribution of a solid using mercury porosimetry ?
18. Discuss sol-gel method of preparation of catalysts.

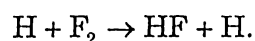
(6 × 2 = 12 weightage)

### Section C

*Answer two questions.*

*Each question carries a weightage of 5.*

19. Discuss Someroff Herishelwood theory of branching chain reactions.
20. Derive BET adsorption isotherm.
21. Compare Langmuier-Hunshelwood surface catalysed reactions. How would you identify the mechanism under a guess set of conditions ?
22. Define potential energy surface with the help of potential energy surface explain 'reaction co-ordinate' for the process :



(2 × 5 = 10 weightage)

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Chemistry

CHE 1C 03—STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS

(2019 Admission onwards)

Time : Three Hours

Maximum : 30 Weightage

**General Instructions**

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**Section A**

Answer any **eight** questions.

Each question carries a weightage of 1.

1. In which of the following solvents benzoic acid is expected to exist as a hydrogen bonded dimer ? Benzene or methanol. Justify.
2. What are cyclodextrins ? Give any *two* applications.
3. Comment on the stability of benzylic carbocations and radicals.
4. *exo*-Halonorbornene reacts faster than its *endo* isomer. Explain.
5. *trans*-Decalin is a conformationally rigid system. Explain.
6. Illustrate bond opposition strain and bond angle strain with appropriate examples, in simple cyclic systems.
7. Define the term enantiomeric excess. How is it determined ?
8. What are prochiral centers ? Predict whether the-CH<sub>2</sub>-hydrogens of ethanol are homotopic, enantiotopic or diastereotopic.

**Turn over**

9. Illustrate substrate controlled asymmetric synthesis with any suitable example.
10. Give an example of an asymmetric hydrogenation reaction with BINAL-H.

(8 × 1 = 8 weightage)

### Section B

*Answer any six questions.*

*Each question carries a weightage of 2.*

11. Write down the structures of cyclopropyl, cyclopentadienyl, and cyclohexadienyl cations. Classify the compounds into aromatic, non-aromatic or anti-aromatic.
12. Comment on the acidity of benzoic acid, 4-nitrobenzoic acid and 4-methoxy benzoic acid. Identify the strongest acid. Justify.
13. Consider the chromic acid oxidation of *cis*- and *trans*-4-*tert*-butylcyclohexanols. Which of these is expected to undergo the reaction faster? Why?
14. Draw the stable conformations of all 2-*tert*-butylcyclohexanols and 3-*tert*-butylcyclohexanols.
15. Explain the stereochemical outcome in pyrolytic elimination of esters.
16. Explain the origin of chirality in organic compounds containing nitrogen and sulfur. Give examples.
17. What are the advantages and disadvantages of chiral pool strategy of asymmetric synthesis?
18. What is 1, 2-asymmetric induction? Predict the stereochemical outcome in an appropriate example.

(6 × 2 = 12 weightage)

### Section C

*Answer any two questions.*

*Each question carries a weightage of 5.*

19. Discuss the stability of various cyclic conjugated pi-systems in organic compounds, based on the concepts of aromaticity and anti-aromaticity.
20. With appropriate examples, describe the terms kinetic and thermodynamic control. Draw structures of the enolate anion of 2-methylcyclohexanone generated under these conditions. Highlight the reagents and conditions used in each case.
21. Discuss the effect of conformation on the course and rate of E1, E2 eliminations illustrated by the following compounds, (i) 4-*t*-butylcyclohexyl tosylate (*cis* and *trans*), (ii) menthyl and neomenthyl chlorides.
22. State and explain the Taft's equation and its application in the mechanistic study of organic reactions with appropriate examples.
23. Differentiate between chiral reagent controlled and chiral catalyst controlled asymmetric synthesis. Give examples. Discuss the advantages and disadvantages of each.

(2 × 5 = 10 weightage)

FIRST SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY)  
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Chemistry

CHE 1C 02—ELEMENTARY INORGANIC CHEMISTRY

(2019 Admission onwards)

Time : Three Hours

Maximum : 30 Weightage

**General Instructions**

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**Section A**

*Answer any eight questions.*

*Each question carries a weightage of 1.*

1. All Bronsted bases may not be Arrhenius bases. Substantiate this statement with suitable example.
2. Classify the following into *closo/nido/arachno* structures :
  - a)  $[B_{12}H_{12}]^{2-}$ .
  - b)  $CB_8H_{12}$ .
  - c)  $C_2B_{10}H_{12}$ .
  - d)  $B_4H_{10}$ .
3. How is polythiazyl prepared ? Comment on the metallic property of this compound.
4. Aluminium can reduce FeO to Fe below  $1500^\circ C$  ; but aluminium will not reduce MgO to Mg below  $1500^\circ C$ . Give reasons.
5. What is the significance of nuclear reaction cross section ?
6. Distinguish between SEM and TEM.
7. 'Bases that are weak in water may appear stronger in more strongly proton donating solvent'. Substantiate this statement with an example.

**Turn over**

8. Arrange the different types of hydrogen atoms present in carboranes in the increasing order of acidity. Justify your answer.
9. Bring out the reasons for water repellent nature of silicones.
10. What information do we get from Latimer diagram ? Explain.

(8 × 1 = 8 weightage)

### Section B

*Answer any six questions.*

*Each question carries a weightage of 2.*

11. Explain leveling effect of solvents with suitable examples.
12. How is tetrasulphur tetranitride prepared ? Give its structure. Comment on the thermochromism exhibited by this compound.
13. How is 1, 2-dicarba-*closo*-dodecaborane(12) prepared ? What happens when it is heated ?
14. Write briefly on the heteropoly and isopoly anions of Mo.
15. Explain how energy is produced in the sun and stars.
16. Explain with suitable examples, the bottom up and top-down approaches for the synthesis of nanomaterials.
17. How XRD is useful in the characterization of nanomaterials ?
18. Compare the differences between 4f and 5f orbitals and the consequences of these on the properties of lanthanides and actinides.

(6 × 2 = 12 weightage)

### Section C

*Answer any two questions.*

*Each question carries a weightage of 5.*

19. Discuss the theoretical basis of classifying acids and bases as 'hard' and 'soft'. Comment on the chemical consequences of this concept in the study of coordination compounds.
20. a) Discuss the importance of icosahedral frame work of boron atoms in boron chemistry.  
b) Write a note on sandwich type metallocarboranes. (3 + 2 = 5 marks)
21. Write an account on the classification of silicates based on their structure giving examples. Discuss the consequences of isomorphous substitution in silicates.
22. Outline the theory and experimental setup involved in neutron activation analysis. Comment on the merits and demerits of this technique.

[2 × 5 = 10 weightage]

**FIRST SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY)  
EXAMINATION, NOVEMBER 2021**

(CBCSS)

Chemistry

CHE 1C 01—QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(2019 Admission onwards)

Time : Three Hours

Maximum : 30 Weightage

**General Instructions**

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**Section A**

Answer **eight** questions.

Each question carries a weightage of 1.

1. Which of the following are well behaved functions. Justify your answer :  
(a)  $A \sin kx$  ; (b)  $A \sin^{-1}x$  ; (c)  $e^{ix}$  ; and (d)  $e^{9x^2}$ .
2. Find the commutator of  $x$  and  $\frac{d}{dx}$ .
3. Explain quantum mechanical tunneling.
4. Write Rodrigue's formula for  $H_{(x)}$  (Simple harmonic oscillator).
5. Explain with example spherical harmonics.
6. Is orbital for H atom is given by  $\psi = Ne^{-r/a_0}$ . Represent graphically. Explain.
7. State and explain variation theorem.

**Turn over**

8. Write Slater determinantal wave function for Li atom.
9. What are the assumptions of molecular mechanics approach of computational chemistry?
10. Explain the term 'split valence' basis set.

(8 × 1 = 8 weightage)

### Section B

Answer **six** questions.

Each question carries a weightage of 2.

11. Show that eigen functions of a Hermitian operator are mutually orthogonal.
12. Apply Schrödinger wave equation for a particle in one dimensional box. Find eigen functions and eigen values.
13. Show that  $\hat{L}_x$  and  $\hat{L}_y$  do not commute.
14. One of the solutions of H atom is  $N(3 \cos^2 \theta - 1)$ . Draw polar plot. Explain.
15. Find the ground state energy of He by perturbation method.
16. What are the modifications suggested by Fock in Hartree's SCF method? Discuss.
17. Compare ab initio and semi empirical methods of computational Chemistry.
18. Write a brief account of classification of basis sets.

(6 × 2 = 12 weightage)

### Section C

Answer any **two** questions.

Each question carries a weightage of 5.

19. Apply Schrödinger wave equation for a non-planar rotator. Find eigen functions and eigen values.
20. Use variation theorem to find the ground state energy of particle in one-dimensional box of length 'a'. Use the trial function  $\Phi = x(a - x)$ .
21. (a) Show that if the operators commute they will have the same set of eigen functions and eigen values. Use the theorem to rationalise Heisenberg uncertainty principle.  
(b) State and discuss expectation value postulate of quantum mechanics.
22. Discuss briefly :
  - (a) Symmetry breaking.
  - (b) Space quantization.

(2 × 5 = 10 weightage)



**FIRST SEMESTER M.Sc. DEGREE (SUPPLEMENTARY) EXAMINATION  
NOVEMBER 2021**

(CUCSS)

Chemistry

CH 1C 04—THERMODYNAMICS, KINETICS AND CATALYSIS

(2015 to 2018 Admissions)

Time : Three Hours

Maximum : 36 Weightage

**Section A**

*Answer all questions.*

*Each question carries a weightage of 1.*

1. Explain with example 'residual entropy'.
2. Define chemical potential in terms of :  
(a) Internal energy ; and (b) Helmholtz free energy.
3. Explain terms forces and fluxes with reference to irreversible thermodynamics.
4. State and explain Glansdorf-pregogine theorem.
5. State and explain steady state approximation.
6. Explain temperature jump method of relaxation spectroscopy.
7. Distinguish between collision cross section and reaction cross section.
8. Unimolecular gas phase reactions follow first order kinetics at high pressures and second order kinetics at low pressures. Why ?
9. Define isotheric heat of adsorption. How is it determined ?
10. How do you distinguish between XPS and AES peaks in the electron spectrum ?
11. Define Michaelis Menton constant. Explain its significance.
12. Distinguish between activated and non-activated adsorption.

(12 × 1 = 12 weightage)

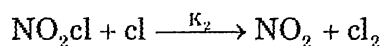
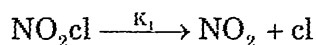
**Turn over**

### Section B

Answer **eight** questions.

Each questions carries a weightage of 2.

13. Using third law of thermodynamics show that absolute zero of temperature is unattainable.
14. Show that solvent obeys Raoult's law in the limit of solute obeying Henry's law.
15. Derive an equation for the rate of entropy production for one component system with heat and matter transport.
16. State and explain Onsager reciprocal relation.
17.  $\text{NO}_2\text{Cl}$  undergoes decomposition according to the mechanism :



Assuming steady state for Cl atom concentration derive the rate law.

18. Derive an equation to show the effect of dielectric constant of the medium on the rate of ionic reactions in solution.
19. With the help of potential energy surfaces explain the term reaction co-ordinate.
20. A first order reaction has a pre-exponential factor of  $5 \times 10^{13} \text{ s}^{-1}$ . Find the entropy of activation at 300K.
21. 160ml of  $\text{N}_2$  is required to form a monolayer on one gram of an adsorbent. Find the surface area. Cross sectional area of  $\text{N}_2$  is  $16.2 \text{ \AA}^2$ .
22. What is ECCA? Discuss its importance in surface characterization.
23. Briefly discuss Lotka Volterra model of oscillating reactions.
24. Discuss kinetics of the reaction  $2\text{CO} + \text{O}_2 \rightarrow 2\text{CO}_2$  on a solid surface.

(8 × 2 = 16 weightage)

**Section C**

*Answer two questions.*

*Each question carries a weightage of 4.*

25. Using irreversible thermodynamics rationalise : (a) thermal osmosis ; (b) any one of the electro kinetic phenomena.
26. Write a brief account of the methods of studying fast reactions.
27. Briefly discuss crossed molecular beam experiment. Discuss its importance.
28. Derive BET adsorption isotherm. Show that it approximates to Langmuir adsorption isotherm under limiting condition. Explain the limiting condition.

(2 × 4 = 8 weightage)

**FIRST SEMESTER M.Sc. DEGREE (SUPPLEMENTARY) EXAMINATION  
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(CUCSS)

Chemistry

CH 1C 03—STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS

(2015 to 2018 Admissions)

Time : Three Hours

Maximum : 36 Weightage

**Section A**

*Answer all questions.*

*Each question has 1 weightage.*

1. Depict the imine-enamine tautomerism.
2. Compare the  $pK_a$  values of maleic acid and fumaric acid.
3. Illustrate the equation of a linear free-energy relationship which explains the relative rates of ester hydrolysis.
4. Draw the most stable conformer for all cis-2-bromo-4-methyl cyclohexanol.
5. Which is the most stable conformation of ethylene glycol and why ?
6. Explain Bredt's rule with an example.
7. Which is the major conformer (alcohol) formed when 4-tert-butyl-cyclohexanone is reduced ?
8. Depict the structure of 2E, 4Z, 6E-octatriene.
9. The observed rotation of a mixture of cholesterol and its enantiomer is  $21^\circ$  at  $20^\circ\text{C}$ . Calculate the % ee of this mixture (natural cholesterol has a specific rotation  $-31.5^\circ$ ).
10. Explain atropisomerism with an example.
11. Depict the homotopic hydrogens in ethanol.
12. What is the product formed when 1-methyl cyclohex-1-ene undergoes hydroboration reaction ?

(12 × 1 = 12 weightage)

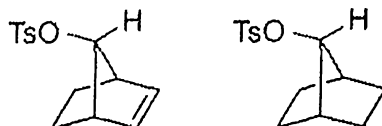
**Turn over**

## Section B

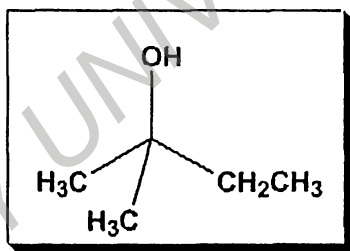
Answer any **eight** questions.

Each question carries 2 weightage.

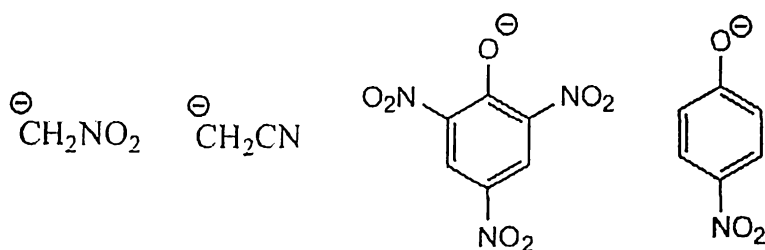
13. The hydrolysis of the unsaturated tosylate occurs  $10^6$  times faster than the saturated analogue. Why ?



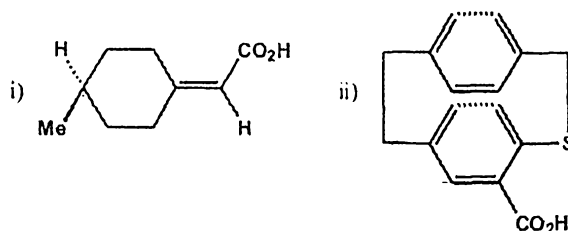
14. Using Cram's rule, illustrate the product formed when  $\text{MeMgBr}$  reacts with 2(R)-phenylpropionaldehyde.
15. Give two examples of non-chiral carbon centered molecules.
16. Explain homoaromaticity with an example.
17. Illustrate the structure of *cis*- and *trans*-decalins.
18. Explain the pro-stereoisomerism of the methyl groups in the following molecule and designate them.



19. The compound 4-t-Bu-N-methyl piperidine on oxidation using *m*-CPBA leads to a mixture of N-oxides in the ratio 95 : 5 (Methyl group equatorial: Methyl group axial). Depict this reaction and explain the product distribution.
20. Explain the type of aromaticity in the following cations : i) Cyclopentadienyl ; ii) Pyrylium ; iii) Cyclopropenyl ; and iv) Tropylium.
21. Arrange the following in the increasing order of basicity .Justify your answer :



22. Illustrate the Sharpless asymmetric epoxidation.
23. Explain helical chirality.
24. Identify the type of chirality and designate whether R or S for the following molecules :



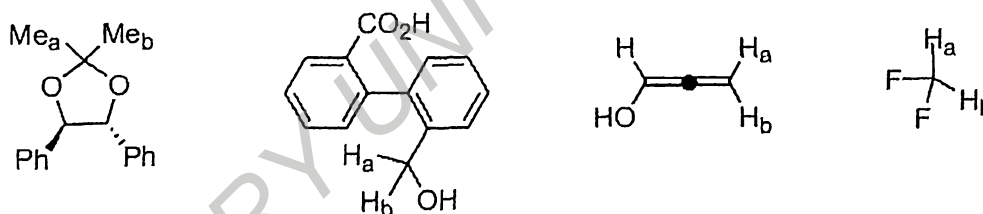
(8 × 2 = 16 weightage)

### Section C

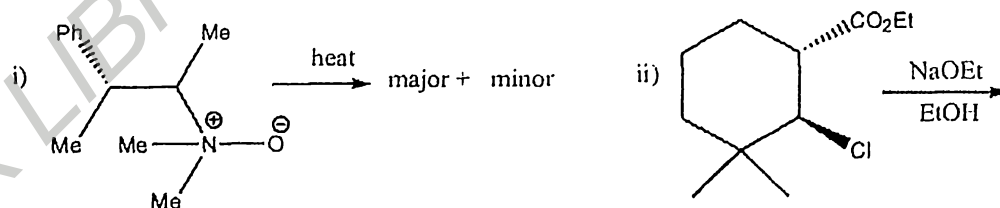
Answer any **two** questions.

Each question carries 4 weightage.

25. Dihydroxylation using OsO<sub>4</sub> and NaOH of (Z)-2-butene leads to meso compound while that of (E)-2-butene leads to racemic mixture. Justify with illustrations.
26. Identify the topicity in each of the labelled atoms or groups :



27. What products do you expect from the following eliminations? Also suggest the mechanisms.



28. Explain the Curtin-Hammett principle with example.

(2 × 4 = 8 weightage)

FIRST SEMESTER M.Sc. DEGREE (SUPPLEMENTARY) EXAMINATION  
NOVEMBER 2021

(CUCSS)

Chemistry

CH 1C 02—ELEMENTARY INORGANIC CHEMISTRY

(2015 to 2018 Admissions)

Time : Three Hours

Maximum : 36 Weightage

**Section A**

*Answer all questions.*

*Each question has 1 weightage*

1. What are Walsh diagrams ? Bring out their significance.
2. Do you find any difference in the geometries of  $\text{ClO}_3^-$  and  $\text{ClO}_4^-$  ions ? Substantiate your answer.
3. Arrange the halide ions  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$  and  $\text{I}^-$  in the increasing order of basicity. Give reasons for your answer.
4. What are Superacids ? Give examples.
5. Zirconium resembles Hafnium in many chemical properties ; why ?
6. What is 'inorganic graphite' ? Why is it called so ?
7. Account for the water repellent nature of silicones.
8. What are Zeolites ? Comment on their acidic nature.
9. What are Frost diagrams ? Mention their utility.
10. What are super heavy elements ? Give examples.
11. What is meant by nuclear reaction cross-section ? Explain.
12. Explain the function of a moderator in nuclear reactors.

(12 × 1 = 12 weightage)

**Turn over**

**Section B**

*Answer any eight questions.*

*Each question carries 2 weightage.*

13. Discuss the principle involved in the determination of molecular structure by X-ray diffraction.
14. Explain the effect of hydrogen bonding on acid strength with suitable examples.
15. Compare the Bronsted-Lowry and Lux-Flood concepts of acids and bases.
16. What is meant by levelling effect and differentiating effect of solvents ?
17. What do you mean by 'diagonal relationship' in the Periodic Table ? Explain.
18. What are Carboranes ? How is 1,2-dicarbido-closo-dodecarborane(12) synthesised ? What happens when it is heated ?
19. Give an account of the classification of silicates on the basis of their structure.
20. How is polythiazyl prepared ? Discuss its properties and structure.
21. What are Ellingham diagrams ? Discuss their applications.
22. Compare the differences between 4f and 5f orbitals and the consequences of these on the properties on lanthanides and actinides.
23. Describe working of a GM counter. What are its merits and demerits ?
24. Write a brief note on stellar energy.

(8 × 2 = 16 weightage)

**Section C**

*Answer any two questions.*

*Each question carries 4 weightage.*

25. Give an account of the 'hard-soft classification' of acids and bases. How this concept is useful in the study of coordination compounds ?
26. Discuss the principle and experimental set up involved in neutron activation analysis. Comment on the merits and demerits of this technique.
27. What are Phosphazenes ? Discuss the preparation, properties and structure of  $(\text{PNCl}_2)_3$ .
28. Write briefly on :
  - a) Bent's rule and energetics of hybridization ;
  - b) Metallocarboranes ; and
  - c) Heteropoly and isopoly anions of Mo.

(2 × 4 = 8 weightage)



**FIRST SEMESTER M.Sc. DEGREE (SUPPLEMENTARY) EXAMINATION  
NOVEMBER 2021**

(CUCSS)

Chemistry

CH 1C 01—QUANTUM CHEMISTRY AND GROUP THEORY

(2015 to 2018 Admissions)

Time : Three Hours

Maximum : 36 Weightage

**Section A**

*Answer all questions.*

*Each question carries a weightage of 1.*

- Using De Broglie relation show that angular momentum of an electron in a circular orbit is an integral multiple of  $\left(\frac{h}{2\pi}\right)$ .
- Write : (a) Time dependent Schrödinger wave equation ; and (b) Hamiltonian for He atom.
- Particle in a cubical box has energy  $\frac{14h^2}{8ma^2}$ . Find the degeneracy of the level.
- Explain the term 'Symmetry breaking'.
- Write  $\uparrow x$  in : (a) Cartesian co-ordinates ; and (b) Spherical polar co-ordinates.
- Explain with example 'Spherical harmonics'.
- The 1s wave function for H atom is  $\psi = Ne^{-r/a_0}$  plot the function against 'r'. Comment on the nature of the plot.
- Explain with example 'spin orbital'.
- Assign Schoenflies symbol of point group for : (a)  $\text{CH}_2\text{Cl}_2$  ; and (b) Cyclohexane. (boat form).
- Generate  $3 \times 3$  matrices for : (a)  $C_3$  ; and (b)  $S_3$ .
- Explain with example 'degenerate representation'.
- Write projection operator for A1 in  $c_{2v}$  point group.

(12 × 1 = 12 weightage)

**Turn over**

### Section B

Answer **eight** questions.

Each question carries a weightage of 2.

13. Define Hermitian operator. Show that kinetic energy operator is Hermitian.
14. Find the commutator of  $\hat{L}_x$  and  $\hat{L}_y$ .
15. Write Hermity polynomial  $H_{(x)}$  for  $\nu = 3$ .
16. Using particle in a box model discuss quantum mechanical tunneling.
17. Solve Schrödinger wave equation for a planar rotor. Find eigen functions and eigen values.
18. Show that spherical harmonics are eigen functions of  $\hat{L}^2$  and  $\hat{H}$  for a rigid rotor. Find the corresponding eigen values.
19. The 1s wave function is  $\psi_{1s} = N e^{-r/a_0}$ . Show that the maximum probability of finding the electron is at  $r = a_0$ .
20. Write Schrödinger wave equation for H atom. Transform into spherical polar co-ordinates separate the variables.
21. Find the similarity transform of any one vertical plane in  $c_{3v}$  molecule.
22. Show that the four symmetry operations E,  $C_{2(z)}$ ,  $\sigma_{vxy}$  and  $i$  form a mathematicla group under multiplication.
23. Taking positional co-ordinates of all atoms in  $H_2O$  generate a reducible representation under  $c_{2v}$ .
24. Write Great Orthogonality theorem. Use the theorem to derive reduction formula.

(8 × 2 = 16 weightage)

### Section C

Answer any **two** questions.

Each question carries a weightage of 4.

25. Solve Schrödinger wave equation for one dimensional simple harmonic oscillator to find eigen functions and eigen values.
26. Discuss postulates of quantum mechanics.

27. (a) Derive  $c_{4v}$  character table.

(b) Reduce the representation T into its IR components :

$C_{2v}$	E	$C_{2z}$	$\sigma_{vz}$	$\sigma'_{vz}$
$A_1$	1	1	1	1
$A_2$	1	1	-1	-1
$B_1$	1	-1	1	-1
$B_2$	1	-1	-1	1
T	9	-1	1	3

28. (a) Show that if two operators commute they will have the same set of eigen functions and eigen values.

(b) What is meant by block diagonalization ? Discuss.

(2 × 4 = 8 weightage)