First Semester M Sc Chemistry

AN1C01/AP1C01/ CH1C01/ PH1C01/ POH1C01
Organometallics and Nuclear Chemistry

(common to all branches of Chemistry)

Model Question Paper

Time: 3 Hrs Max. Weight: 30

Section A

(Answer any 10 questions. Each question carries a weight of 1)

01. Give the structures of $Mn_2(Co)_{10,}$ $Co_2(CO)_6$ and $Fe_2(CO)_9$.
02. What is isolobal concept? Explain with one example.
03. Give one typical method of synthesis of butadiene complex of transition metals.
04. Compare the sigma and pi bonding abilities of CO and PR_3 ligands.
05. Give one evidence to show that $[Co(NH_3)_6]^{3+}$ follow a dissociative mechanism in its substitution reaction.
06. What is meant by hydroformylation reaction or oxo process? Give one example.
07. Give two examples of organometallic condensation polymers based on rigid polyynes.
08. Discuss the classification of micronutrients?
09. What are cytochromes? Give two examples.
10. Explain the role of Carboxy Peptidise A in the synthesis of proteins.
11. What are the general features of enzymes? What is an apoenzyme?
12. Write down the criteria for a spontaneous nuclear reaction to occur.
13. Explain the synthesis of transuranic elements Curium, Berkelium, Einsteinium and Lawrencium.

(10 x 1 =10)

Section B

(Answer 5 questions. Each question carries a weight of 2)

14. What are metal carbynes? How these will be synthesized?
15. Discuss the structure and bonding in Ferrocene.
16. What is the difference between oxidative addition and insertion reactions with suitable examples?
17. What are π-acceptor ligands? Discuss in detail the nature of bonding involved in metal carbonyls.
18. Describe the Wacker Process for the synthesis of Acetaldehyde.
19. What are organometallic dendrimers. How they are prepared?

20. Explain the function of PSII in photosynthesis.

21. Explain the principles underlying the various types of counters used in radioactive counting.

(5 x 2 =10)

Section C

(Answer any 2 questions. Each question carries a weight of 5)

22. (a) Discuss briefly the mechanism of ligand displacement reaction in octahedral complexes.

    (b) Explain clearly LNCCS and HNCCS.

23. Write briefly on

    (a) Catalysis by Platinum pop photodehydrogenation catalyst in the conversion of secondary alcohols to ketones.

    (b) fluxional isomerism.

24. (a) Give an account of iron storage and transport in biological systems.

    (b) Explain how cytochrome P-450 enzymes catalyse the addition of oxygen to a hydrocarbon substrate.

25. Write briefly on

    (a) Analytical applications of radioisotopes.

    (b) Radiochemistry of water and aqueous solutions.

(2 x 5 =10)

AN1C02/AP1C02/ CH1C02/ PH1C02/ POH1C02
Structural and Molecular Organic Chemistry

(common to all branches of Chemistry)

Model Question Paper

Time: 3 Hrs Max. Weight: 30

Section A

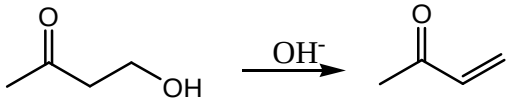
(Answer any 10 questions. Each question carries a weight of 1)

01. Draw the *pi*-MO diagrams of (a) 1,3-butadiene and (b) allyl cation and explain their characteristic features

02. Draw the line diagram of hex-5-en-2-yne, label each carbon and predict the hybridization and geometry of each carbon centre.

03. Explain the mechanism with curved arrow notations:

(a)



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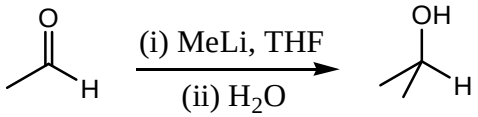


04. Treatment of cyclooctatetraene with potassium metal has been found to yield a stable aromatic compound. Justify.

05. How is γ-hydrogen abstractin established in Norrish type II reaction?

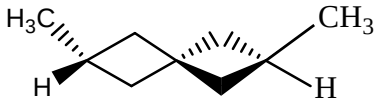
06. Explain the mechanism of esterification of acid by AAL^1 mechanism.

07. Give an example of Di-π-methane rearrangement.

08. Predict the major stereoisomer formed in the following reaction:
R-2-phenyl propanal+phenyl magnesium bromide → ?

09. Assign the configuration as R or S for the following:

(a)



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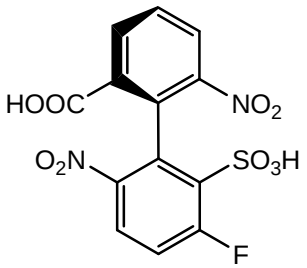


10. What are ansa compounds? Illustrate with examples.

11. Draw the stable conformations of cis and trans t-butyl cyclohexanols. Which one is esterified easily? Why?

12. What are the structural factors supporting Hofmann elimination products over Saytzeff elimination products? Illustrate with examples.

13. Briefly explain the conformational aspects of dehalogenations with a specific example.

(10×1=10 weights)

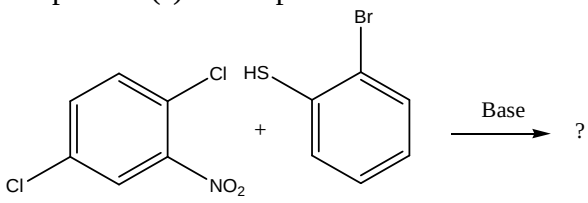
Section B

(Answer 5 questions by attempting not more than 3 questions from each bunch. Each question carries a weight of 2)

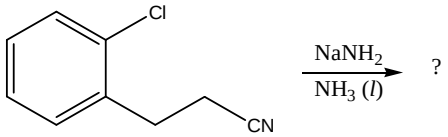
Bunch 1(Problem Type)

14. Predict the product(s) and explain the mechanism of the following reactions:

(a)

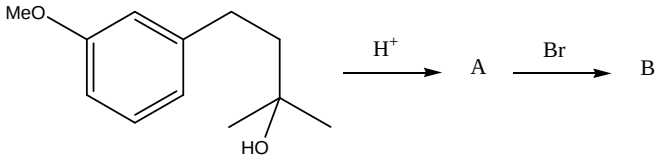


(b)

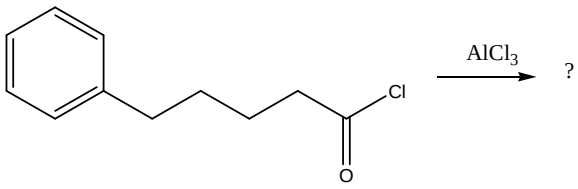


15. Predict the product(s) and explain the mechanism of the following reactions:

(a)

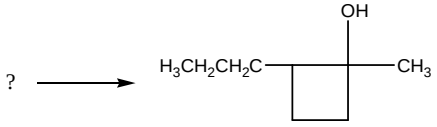


(b)



16. Complete the following reactions and explain the mechanisms:

(a)



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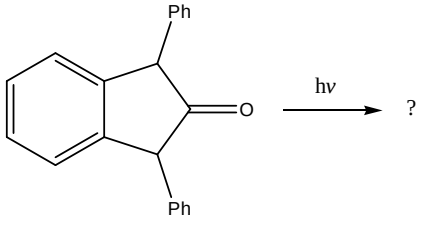
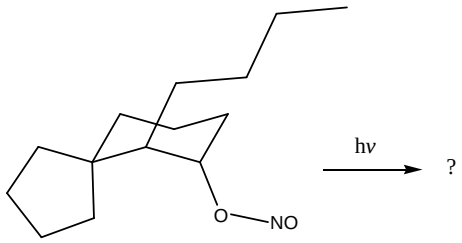
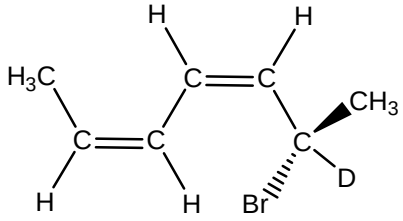


(c)



17. How many isomers are possible for the following structure? Draw them.



Bunch 2(Short Essay Type)

18. The relative rates of reactions of the following nucleophiles with MeBr in EtOH is:

F^-	Br^-	I^-
0.0	5×10^3	1.2×10^5

Explain using HSAB concept.

19. Write briefly on the stereochemistry of spirans.

20. Describe the conformational analysis of decalines.

21. Using Curtin-Hammet principle, explain the consequences of conformational equilibrium.

(5×2=10 weights)

Section C

(Answer any 2 questions. Each question carries a weight of 5)

22. Using HMO theory explain aromaticity. Describe the applications of NMR spectroscopy as a tool for distinguishing aromatic and antiaromatic compounds.

23. Give a detailed account of the different mechanisms of ester hydrolysis with experimental evidences.

24. Write an essay on the rules of R-S and E-Z nomenclature in stereochemistry.

25. Illustrate the conformational studies of cyclic and acyclic systems such as:

(a) cyclohexane, (b) adamantine, and (c) ethane.

(2×5=10 weights)

AN1C03/AP1C03/ CH1C03/ PH1C03/ POH1C03
Quantum Chemistry and Group Theory

(common to all branches of Chemistry)

Model Question Paper

Time: 3 Hrs Max. Weight: 30

Section A

(Answer any 10 questions. Each question carries a weight of 1)

01. Explain tunneling.

02. What are Hermite polynomials? Write the Hermite polynomial for n=2 and n=3.

03. When a particle of mass 9.1×10^{-31}kg in a one dimensional box goes from n=3 to n=1 level it emits a photon of frequency 3.4×10^{14} s^{-1}. Calculate the length of the box.

04. Which of the following are eigenfunctions of d/dx ? a) Ae^{-ax}, b) x^2, c) B cos nx, d) cosx + sinx

05. a) Find the spherical polar coordinates corresponding to the Cartesian coordinates (1, 2, 0), and

    b) Find the Cartesian coordinates corresponding to the spherical polar coordinates $(0, \pi/4, \pi/3)$.

06. State whether true or false:

    a) the probability density for a particle in a box stationary states is constant along the length of the box.

    b) x cos x is an even function

    c) when two operators have a common complete set of eigenfunctions then they commute.

    d) the lowest energy state of a particle in a three dimensional box is triply degenerate.

07. Explain ladder operators.

08. Show whether the following matrices commute:

$$\begin{bmatrix} 2 & 0 \\ 1 & 1 \end{bmatrix} \text{ and } \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix}.$$

09. Differentiate between reducible and irreducible representations.

10. Assign point group to each of the following:

    a) CH_2Cl_2, b) allene, c) HCl, d) FeF_6^{3-}

11. What is meant by space group? List the space groups in the triclinic crystal system.

12. Explain the relationship between molecular dissymmetry and optical activity. The absence of which symmetry element implies molecular dissymmetry?

13. What are the distinct operations generated by S_5 axis ?

(10 x 1 =10)

Section B

(Answer 5 questions. Each question carries a weight of 2)

14. Find the eigenvalues and eigenfunctions of a particle on a ring.
15. Compare the cartesian and spherical polar coordinates.
16. Derive the commutator of the following

    a) $[L_x, L_y]$ b) $[P_x, x]$.
17. Discuss the important features of the quantum mechanical treatment of one dimensional harmonic oscillator.
18. What are the symmetry elements and symmetry operations of C_{3v} point group? Group the symmetry operations into different classes by similarity transformation.
19. State and explain Great orthogonality theorem. What are the important rules that can be deduced from the theorem?
20. Derive the matrix representation of S_4 operation using the vector (x,y,z) as coordinates.
21. Determine the symmetry of the normal modes of NH_3 molecule using internal coordinates.

(5 x 2 =10)

Section C

(Answer any 2 questions. Each question carries a weight of 5)

22. State and explain the postulates of quantum mechanics.
23. Setup the Schrodinger equation for hydrogen atom and separate the variables to obtain r, θ and ϕ equations. Write the general solution of these equations.
24. What are character tables? Construct the character table for C_{2v} point group. Discuss the significance of each area of the table.
25. Using group theory obtain the selection rules for vibrational transitions in IR and Raman spectroscopy. Examine the IR and Raman activities of the vibrations of trans-N_2F_2 molecules.

(2 x 5 =10)

AN1C04/AP1C04/ CH1C04/ PH1C04/ POH1C04
Classical and Statistical Thermodynamics

(common to all branches of Chemistry)

Model Question Paper

Time: 3 Hrs Max. Weight: 30

Section A

(Answer any 10 questions. Each question carries a weight of 1)

01. Derive the Clausius inequality applicable to irreversible processes.
02. What is meant by chemical affinity? Derive the relation between enthalpy and chemical affinity.
03. What are thermodynamic excess functions? Derive an expression for the excess entropy of a binary mixture.
04. Apply Stirlings approximation if $N = 6.023 \times 10^{23}$.
05. Derive an expression for the variation of fugacity with pressure.
06. Sketch and explain the graphical representation of a three component system having three partially miscible pairs.
07. Explain the exergonic nature of ATP hydrolysis.
08. Explain coupled reactions.
09. Derive Konovalov's first law.
10. Distingush between reversible and irreversible processes. How does irreversibility arise in chemically reacting and flow systems?
11. Derive Gibbs-Duhem equations.
12. Distinguish between Seebeck effect and Peltier effect. Define ε and π.
13. Differentiate between flux and force in phenomenological relations.

Section B

(Answer 5 questions by attempting not more than 3 questions from each bunch. Each question carries a weight of 2)

Bunch 1 (Short Essay Type)

14. Derive Gibbs Duhem Margules Equation and explain whether the equation is applicable to both ideal and non ideal systems.
15. Derive the Maxwell's relation $\left(\frac{\partial P}{\partial T}\right)_V = \left(\frac{\partial S}{\partial V}\right)_T$. What is the significance of Maxwell's relations?
16. Derive Sackur - Tetrode equation applicable to monoatomic gases.
17. Get expressions for internal energy and entropy in terms of partition functions.

Bunch 2 (Problem Type)

18. The intermolecular separation in hydrogen molecule is 0.074 nm. Calculate the molecular rotational partition function at 300K.
19. Calculate with reference to v = 0 the molecular vibrational partition function for H_2 at 300K and 3000K if the characteristic temperature θ_{vib} is 6210K.
20. a) 2 moles of compound A and 5 moles of compound B mix together to form an ideal solution. Evaluate the entropy, enthalpy, volume and free energy of mixing of the solution, if it happens at 300K.

    b) For a reaction, ΔG^o =187.1kJ/mol and ΔH^o = 184.7kJ/mol at 298K. Calculate ΔG and Kp at 498K assuming that ΔH^o remain constant during that temperature range.
21. Calculate the translational entropy of one mole of atomic chlorine at 350K and 1atm pressure.

(5 x 2 =10)

Section C

(Answer any 2 questions. Each question carries a weight of 5)

22. Taking an example each, explain the phase behaviour of the following three component systems using suitable diagrams;

    a) Solid- liquid system with hydrate formation

    b) liquid system with two pairs of partially miscible liquids
23. Using the principle of microscopic reversibility show that the cross coefficients are equal.
24. a) Derive an expression for Bose-Einstein statistics.

    b) Give a comparative account of Maxwell-Boltzman, Bose-Eienstein and Fermi-Dirac statistics.
25. Derive Debye theory of heat capacity of solids. How does it differ from Einstein theory?

(2 x 5 =10)