Reg. No. : ....

Name : ....

First Semester M.Sc. Degree (CBSS – Reg./Supple. (Including Mercy Chance)/Imp.) Examination, October 2020
(2014 Admission Onwards)
CHEMISTRY
CHE 1C.01 : Theoretical Chemistry – I

Time : 3 Hours

Max. Marks : 60

SECTION – A

Answer **all** questions in **one word** or **sentence**. Each question carries 1 mark.

(8×1=8)

1. What is Compton effect ?

2. What is linear operator ? Give one example.

3. Write down the Hamiltonian operator in spherical polar coordinates.

4. What is a node and how it varies with quantum number in Particle in a 1-D box problem ?

5. What is the nature of the wave function proposed by Hartree ?

6. Write down the perturbation term in Helium atom.

7. What is Born Oppenheimer approximation ?

8. Write down the Schrodinger equation for an n-electron, N-nuclei molecule.

SECTION – B

Answer **eight** questions. Answer may be **two** or **three** sentences. **Each** question carries **2 marks**.

(8×2=16)

9. Expand the operator $(x \cdot d/dx)^2$.

10. Prove that Hermitian operators have real eigen values.

11. Give a trigonometric function that is an eigen function of both d/dx and d^2/dx^2.

12. Explain transition moment integral and indicate its importance.

13. What are polar diagrams ?

14. What is the form of Laguerre equation ?

15. Why approximation methods are required to solve the Schrodinger equation of many electron systems ?

16. Write down the ground state term symbol for a) C-atom b) N-atom.

17. Draw the radial distribution functions of 1s, 2s, 3p and 3d.

18. What is meant by 'ab initio method'? Give an example.

19. What is STO ? State its two limitations.

20. How do you calculate free valence index ? Mention its importance.

SECTION – C

Answer **four** questions in short paragraph for **each**. **Each** question carries **3 marks**.

(4×3=12)

21. A system is defined by the wave function $\psi(x) = \cos(2\pi x/L)$ with x varies between $-L/4$ and $L/4$. Normalize the wave function and find out the probability of the particle that will be found between $x = 0$ and $x = L/8$.

22. Prepare the Hermite polynomial, $H_5(x)$ and write down the simple harmonic wave function $\psi_5(x)$.

23. Starting from time dependent Schrodinger equation, arrive at the time independent form by separating the variables.

24. Explain tunneling effect.

25. Explain 'Self consistent field' method.

26. What is a basis set ? Explain the various classifications of basis sets.

27. What are the approximations incorporated in Huckel molecular orbital treatment of conjugated systems.

28. Draw the molecular orbital diagram for O_2 molecule. Extend this to O_2^+ and O_2^- and calculate the bond orders.

SECTION – D

Answer either **a** or **b** of **each** question. **Each** question carries **6 marks**.   (4×6=2

29. a) Explain the main postulates of quantum mechanics.

  OR

  b) Name three experimental phenomena where classical mechanics failed. Also explain, how quantum mechanics explained these satisfactorily.

30. a) Write down the exact wave function form of non planar rigid rotor. With the help of this, justify the various quantum number values of 'l' and 'm'.

OR

b) Starting from the Schrodinger equation of hydrogen atom in spherical polar coordinates, separate the variables and arrive at single variable equations. Also, derive the energy expression.

31. a) Solve for variational parameter α, and energy if the trial wave function proposed for hydrogen atom is $e^{-\alpha r}$.

OR

b) Solve the first order perturbation equation for a non-degenerate system to arrive at first order correction to energy.

32. a) Solve the Schrodinger equation of H_2 molecule under molecular orbital theory.

OR

b) Arrive at the molecular term symbols of O_2 and arrange them in the order of energy.

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I Semester M.Sc. Degree (CBSS-Reg./Suppl./Imp.)
Examination, October - 2019
(2014 Admn. Onwards)
CHEMISTRY
CHE1C.01: THEORETICAL CHEMISTRY - I

Time : 3 Hours   Max. Marks : 60

SECTION-A

Answer **All** questions in one word or sentence. Each question carries 1
mark.   (8x1=8)

1. Write down Hamiltonian operator for an N-particle system.

2. What are stationary states?

3. What are the conditions to be satisfied for the particle to be in a box?

4. Classify the following into even and odd functions: tanx; $(3+x)(3-x)$

5. E_1 and E_2 correspond to the energies of proposed trial functions, φ_1 and φ_2 for a system with latter being the most realistic guess. If E_0 is the real energy, write down these energies in ascending order.

6. What is Pauli's antisymmetry principle?

7. State Born-Oppenheimer approximation.

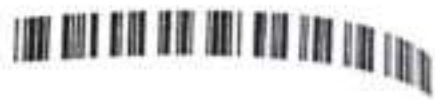8. Calculate the number of basis functions for carbon atom using 6-31 1G basis set.

SECTION - B

Answer **Eight** questions. Answer may be **two** or **three** sentences. Each
question carries **2** marks.   (8 x 2= 16)

9. Normalize the function, $\sin(2\pi x)$ with x varies between 0 and 1.

10. Express $(x+iy)$ in terms of spherical polar coordinates.

11. Explain orthonormalized functions.

P.T.O.

12. Write down the del squared operator in spherical polar coordinates.
13. What is Rodrigues formula?
14. Give the potential energy diagrams of SHO and hydrogen molecule. Why do these differ?
15. Write down possible spin function and orbital functions for the electronic configuration, $1s^1 2s^1$.
16. State two limitations of perturbation methods.
17. Write down the Slater determinant for the ground state of Li atom and show that all three electrons cannot occupy the 1s orbital.
18. What are split-valence basis sets? Give an example.
19. How will you calculate the π- charge density of conjugated molecule?
20. Write down the ground state term symbol of i) C_2; ii) CO

SECTION - C

Answer **Four** questions in short paragraph for each. Each question carries **3 marks**.

$$(4 \times 3 = 12)$$

21. Explain Davisson-Germer experiment. What it demonstrates?
22. What is zero point energy? What are their values for a planar rigid rotor and SHO? Justify that these values are in agreement with Heisenberg's uncertainty principle.
23. Write down the Schrodinger equation of Hydrogen atom in spherical polar coordinates and separate the variables.
24. Write down the explicit form of complete wave function and energy of nonplanar rigid rotor explaining each term.
25. Explain self consistent field method.
26. State and prove variational theorem.
27. Differentiate between STO and GTO.
28. Give the MO and VB approximation for the ground state of H_2 molecule and highlight the basic difference between the two.

SECTION - D

Answer either **a** or **b** of each question. Each question carries **6** marks.

(4x6=24)

29. a) Deduce time dependent Schrodinger equation from classical wave equation.

(OR)

b) Explain the postulates of Quantum mechanics.

30. a) Arrive at the energy and wave function of planar rigid rotor.

(OR)

b) Explain radial distribution functions. Plot these for 1s, 2s, 2p, 3p and 4d.

31. a) Derive first order perturbation correction to energy for a nondegenerate system.

(OR)

b) Derive the various atomic term symbols for carbon atom and arrange them in the order of energy.

32. a) Explain Hartree-Fock theory for molecules.

(OR)

b) Calculate the C-C π-bond order in benzene using Huckel molecular orbital treatment.

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First Semester M.Sc. Degree (CBSS – Reg./Supple.(Including Mercy Chance)/Imp.) Examination, October 2020
(2014 Admission Onwards)
CHEMISTRY
CHE 1C.03 : Organic Chemistry – I

Time : 3 Hours

Max. Marks : 60

SECTION – A

Answer **all** questions in **one** word or **one** sentence. **Each** question carries **one** mark.

(8×1=8)

1. Is cycloheptatrienyl bromide soluble in water ?

2. Which is more basic – imidazole or pyrrole ?

3. Give the structure of a prochiral molecule.

4. Beckmann rearrangement converts a ketone to a _____

5. Nucleophilic aromatic substitution can occur via _____ mechanism.

6. Quaternary ammonium salts can undergo _____ elimination reaction.

7. Which aldehyde is responsible for the human vision ?

8. Give an example for a *cis-trans* isomerization reaction.

SECTION – B

Answer **any eight** questions. Answer may be **two** or **three** sentences. **Each** question carries **two** marks.

(8×2=16)

9. What product is formed when biphenyl azide is heated ?

10. Explain homoaromaticity with an example.

11. Why is 2, 6-dimethyl N, N-dimethyl aniline a better base than N, N-dimethyl aniline ?

12. Explain the axial haloketone rule.

13. Give examples of suitably substituted allenes which are axially chiral and designate them.

14. What is the product formed when 2-methyl cyclohexanone is treated with a peracid ?

15. How is anisole converted to 1, 3-dimethoxy benzene ?

16. How is singlet oxygen generated ? Give an application.

17. What are non-classical carbocations ? Give an example.

18. Predict the product formed when R-2-butanol is treated with thionyl chloride.

19. Depict photo-Fries rearrangement reaction.

20. 2-Bromo fumaric acid undergoes faster elimination than 2-bromo maleic acid. Why ? What is the product formed ?

SECTION – C

Short paragraph questions. Answer **any four** questions. **Each** question carries **three** marks.

(4x½=12)

21. How is NMR spectroscopy helpful to understand the aromaticity of benzene and [18] annulene ?

22. Why are dialkoxy carbenes nucleophilic ?

23. Depict the structures of cis and trans decalins.

24. Depict the mechanism of conversion of dienones to phenols.

25. Illustrate the Favorskii reaction.

26. Illustrate the E1CB mechanism with a suitable example.

27. How are oxetanes photochemically synthesized ?

28. What product is formed when 3, 3-dimethyl 1, 4-pentadiene is heated ?

SECTION – D

Essay type questions. Answer **four** questions. **Each** question carries **six** marks.

(4x6=24)

29. A) Classify the following as aromatic, anti-aromatic or non-aromatic : cyclopropenyl cation, cyclopentadienyl anion, cyclotropylium anion, [16] annulene, cyclooctatetraene and cyclohexadiene.

OR

B) Hyperconjugation can explain the stability of alkenes and carbocations but not carbanions. Justify the statement with suitable illustrations.

30. A) i) Provide examples for molecules having (a) chiral plane (b) non-carbon chiral centre (c) helical structure

    ii) Depict the most stable conformer of (a) ethylene glycol (b) trans-1, 3-dichloro cyclohexane and (c) trans-4-ᵗBu-1-hydroxy cyclohexane.

OR

B) Illustrate the dehydrohalogenation of meso-1, 2-dibromo-1, 2-diphenyl ethane.

31. A) Illustrate the major product formed when the following molecules are treated with a base : i) cis-1-hydroxy-2-tosyloxy cyclohexane and
    ii) trans-1-hydroxy-2-tosyloxy cyclohexane.

OR

B) Illustrate the mechanism of Von Richter reaction.

32. A) Depict the mechanism of i) Norrish Type I and II reactions and ii) Barton reaction.

OR

B) Explain photosensitization and quenching providing examples.

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I Semester M.Sc. Degree (CBSS-Reg./Supple./Imp.)
Examination, October - 2019
(2014 Admission Onwards)
CHEMISTRY
CHE 1C.03 : ORGANIC CHEMISTRY-I

Time : 3 Hours

Max. Marks : 60

SECTION-A

Answer **All** questions in one word or one sentence. Each question carries
One mark.

$(8\times1=8)$

1. Which has higher pKa-O-hydroxy benzoic acid or p-hydroxy benzoic acid?
2. Bromobenzene when treated with_____ generates benzyne.
3. _____ is an example of an enantiotopic molecule.
4. Methylene cyclopropane is synthesized from cyclopropane by the _____ reaction.
5. Reaction of R-2- butanol with _____ yields R-2-chlorobutane.
6. An anti-periplanar geometry favours _____ elimination.
7. What product is formed when cis- diazobenzene is exposed to light?
8. Cis-trans isomerization of _____ is responsible for vision chemistry.

SECTION-B

Answer any **Eight** questions. Answer may be two or three sentences. Each
question carries **Two** marks.

$(8\times2=16)$

9. Depict the structure of DABCO and quinuclidine. Why are they strong bases?
10. Compare the pKa of maleic acid to fumaric acid.
11. Explain homoaromaticity with an example.
12. Depict the structure of an axially chiral allene and a biphenyl derivative.
13. Illustrate the major product formed when 4-tBu cyclohexanone is reduced?

P.T.O.

14. What product is formed when benzyl phenyl ketone is treated with
    a) NH_2OH
    b) PCl_5
    c) Dilute acid.

15. $CH_3CH_2SCH_2CH_2Cl$ can be hydrolyzed much faster that pentyl chlorid Why?

16. Illustrate the Cope elimination reaction.

17. Give examples of two polar aprotic solvents depicting their structure.

18. Illustrate the Paterno Buchi reaction.

19. Mention any one photo reaction of Vitamin D.

20. Explain Di-pi-methane rearrangement.

SECTION-C

Short paragraph questions. Answer any **Four** questions. Each question carries **Three** marks.   **(4×3=12)**

21. Exemplify the following by providing a structure
    a) metallocene
    b) Mesoionic compound
    c) Singlet carbene.

22. How is anisole converted to 1,3-dimethoxy benzene?

23. What is atropisomerism? Provide examples and designate.

24. Illustrate Curtius and Schmidt rearrangement reactions.

25. Cyclohexanol on treatment with mesyl chloride yields A. The latter on treatment with a base and diethyl malonate yields B. Identify A and B.

26. Depict the Hoffmann and Saytzeff elimination reactions.

27. Give an example of a remote functionalization reaction.

28. How is singlet oxygen generated? Give an application.

SECTION-D

Essay type questions. Answer **Four** questions. Each question carries **Six** marks.

                                                                    (4×6=24)

29. a) Compare and explain the aromaticity of thiophene, furan, pyrrole, pyridine, imidazole and pyrazole.

(OR)

b) N, N-dimethyl aminopyridine is more basic than pyridine. Explain.

30. a) Designate the prochiral faces of benzaldehyde. What products are formed when benzaldehyde is treated with methyl magnesium bromide?

(OR)

b) Illustrate the product formation when meso-2, 3-dibromobutane is treated with zinc.

31. a) What is the major product formed when 2-acetyloxy cyclohexane carboxylic acid ethyl ester is heated?

(OR)

b) Illustrate

   i) Demyanov ring expansion and

   ii) Beckmann rearrangement.

32. a) Explain the chemistry behind the vision process.

(OR)

b) Illustrate photo Fries rearrangement and Norrish type II cleavage.

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I Semester M.Sc. Degree (CBSS-Reg./Supple./Imp.)
Examination, October - 2019
(2014 Admission Onwards)
CHEMISTRY
CHE 1C.04 : PHYSICAL CHEMISTRY-I

Time : 3 Hours   Max. Marks : 60

SECTION-A

Answer **All** questions in one word or one sentence. Each question carries 1 mark.   (8×1=8)

1. State third law of thermodynamics.
2. Distinguish between forces and fluxes with reference to irreversible thermodynamics.
3. Define ionic mobility.
4. Explain the term 'asymmetry effect'
5. What is electrode polarization?
6. Define half wave potential.
7. Write electrode reactions under acidic condition.
8. Explain the term 'impedance'.

SECTION-B

Answer **Eight** questions. Answer may be in one or two sentences. Each question carries 2 marks.   (8×2=16)

9. Derive thermodynamic equation of state.
10. State and explain onsager reciprocal relation.
11. State criteria for equilibrium between phases.
12. Write Debye Huckel Onsager equation. How is it verified?
13. Predict the effect of the following on the thickness of the ion atmosphere.
    a) Concentration of electrolyte.
    b) Dielectric constant of the medium.

14. The solubility product of a sparingly soluble salt at 25°c is 8×10^{-15}. Find the solubility of the salt.

15. What are the models of electrical double layer at electrode-electrolyte interface? Explain.

16. What are the advantages of dropping mercury electrode?

17. Explain concentration polarization.

18. Find the EMF of the cell

$Zn / \underset{a=0.1}{Zn^{2+}} // \underset{a=0.01}{Cu^{2+}} / Cu$ the standard electrode potentials of Zn and Cu are 0.767 and +0.334v respectively.

19. Explain 'Passivation'

20. Explain terms
    a) Corrosion current
    b) Corrosion potential.

SECTION-C

Answer **Four** questions. Each question carries 3 marks.   (4×3=12)

21. Derive an equation for the rate of entropy production for one component system with heat and matter transport.

22. Define partial molal volume. How would you find partial molal volume of Nacl in water at room temperature. Discuss.

23. Define mean ionic activity coefficient. Find the activity of the following electrolytes in terms of molal concentration and mean ionic activity coefficient.
    a) MX_3
    b) M_3X_2

24. Write Debye Huckel limiting law. How would you test the validity of the law? Discuss.

25. Derive Loppmann equation.

26. Discuss one of the theories of hydrogen overvoltage.

27. Draw Pourbaix diagram for Fe. Discuss.

28. Discuss the applications of electrochemical Impedance Spectroscopy.

SECTION-D

Answer 'a' or 'b' of each question. Each question carries 6 marks.(4×6=24)

29. a) i) How would you determine third law entropy of a gas? Discuss.

    ii) Define phenomenological coefficients. Show that direct coefficients always dominate indirect coefficients.

(OR)

b) Draw phase diagram for a ternary solution with common ion hydrate formation. Discuss.

30. a) Derive Debye Huckel Onsager equation.

(OR)

b) Discuss briefly.

    i) Osmotic coefficient

    ii) Applications of conductance measurements.

31. a) What is meant by liquid junction potential. How is it measured? Discuss

(OR)

b) Define overvoltage. What are the contribution factors for overvoltage? Discuss

32. a) Discuss kinetics of corrosion.

(OR)

b) Discuss the applications of Electrochemical Impedance spectroscopy in corrosion science.

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Reg. No.: ....

Name : ....

First Semester M.Sc. Degree (CBSS – Reg./Suppl. (Including Mercy Chance)/Imp.) Examination, October 2020
(2014 Admission Onwards)
CHEMISTRY
CHE 1C. 02 : Inorganic Chemistry – I

Time : 3 Hours

Max. Marks : 60

SECTION – A

Answer **all** questions in **one** word or **one** sentence. **Each** question carries 1 mark.

1. What is meant by median value ?

2. Name an organic precipitant used in the gravimetric estimation of nickel (II) from its solution.

3. Give one example each for protic and aprotic solvent.

4. Identify the conjugate bases of $Si(OH)_4$ and H_3PO_4.

5. Give one example for radioactive electron capture reaction.

6. Why do lighter elements generally undergo fusion while heavier elements show nuclear fission ?

7. Classify the following boranes into closo/nido/arachno structure :

    a) B_5H_9 b) $C_2B_{10}H_{12}$

8. How is polythiazyl prepared ?

$(8 \times 1 = 8)$

SECTION – B

Answer **any eight** questions. Answer may be in **two** or **three** sentences. **Each** question carries **2 marks.**

9. Explain the significance of students t-test.

10. What do you mean by precipitation from homogeneous solution ? Explain with an example.

11. Calculate the standard deviation for the following set of analytical data for a sample A : 13.68 mg, 13.70 mg, 13.04 mg, 13.14 mg.

12. Explain the Bronsted-Lowry concept of acids and bases.

13. An acid that is weak in water may appear strong in a solvent that is a strong proton acceptor. Explain.

14. What is symbiosis ? Explain with an example.

15. What is average life of a radioactive element ? How is it related to its half-life ?

16. How do spallation reactions differ from fission reactions ?

17. What is meant by Q-value of a nuclear reaction ? How is it calculated ?

18. The styx code for a boron hydride is 1104. Draw its topological structure.

19. How does diborane react with : a) CO   b) PH_3.

20. How is P_4S_{10} prepared ? Draw its structure.

$(8 \times 2 = 16)$

SECTION – C

Short paragraph questions. Answer **any four** questions. **Each** question carries **3 marks**.

21. Differentiate between co-precipitation and post precipitation giving suitable example.

22. How errors are classified ?

23. What are hard and soft acids and bases ?

24. Write a note on hydrometallurgy.

25. Briefly discuss the Fermi gas model of nucleus.

26. Differentiate between transient equilibrium and secular equilibrium.

27. Give an account of the synthesis, properties and structure of tetrasulphur tetranitride.

28. How is 1,2-dicarba-closo dodecacarborane (12) synthesised ? What happens when it is heated ?

$(4 \times 3 = 12)$

SECTION – D

Essay type questions. Answer **four** questions. **Each** question carries **6** marks.

29. A) Discuss the use of oxine, cupferron and dimethylglyoxime in inorganic analysis.

OR

B) Give an account of the different types of solvent systems used in solvent extraction.

30. A) Give an account of the classification of solvents. Discuss the role of molten salts as non-aqueous solvent system.

OR

B) Discuss the role of H_2SO_4 as a non-aqueous solvent. What are its advantages and disadvantages ?

31. A) Categorise the various types of nuclear reactions on the basis of the nature of bombarding particles. Mention their advantages and disadvantages.

OR

B) Describe the principle and working of GM counter. What are its merits and demerits ?

32. A) How is triphosphonitrilic chloride prepared ? Give an account of its properties, structure and bonding.

OR

B) Explain closo/nido/arachno structures of boranes with suitable examples.

(4×6=24)