D 32671 (Pages : 2) Name.....

Reg. No.....

FIRST SEMESTER M.Sc. (CBCSS) REGULAR/SUPPLEMENTARY DEGREE EXAMINATION, NOVEMBER 2022

Chemistry

CHE1C01—QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(2019 Admission onwards)

Time : Three Hours Maximum Weightage : 30

Section A

Answer any **eight** *questions.*
Each question carries a weightate of 1.

1. Which of the following one well behaved functions :

   (a) e^{x};(b) e^{ix}; (c) e^{-ax^2}; (d) $\sin^{-1} x$.

2. Explain with example 'conservative system'.

3. The energy of a particle in cubical box of length 'a' is $\frac{14h^2}{8ma^2}$. What is the degeneracy of the level.

4. Explain the term 'Symmetry breaking'.

5. The solutions of a planar rotor are $\frac{1}{\sqrt{\Pi}} e^{im\phi}$. Express it as a real function.

6. 1s wave function for H atom is Ae^{-r/a_0}. Represent the function graphically. Explain.

7. State and explain independent particle model.

8. What do you mean by 'Slater type of orbitals' ? Write one example.

9. Explain the term 'molecular mechanics' in computational chemistry.

10. Write Z-matrix for NH_3.

(8 × 1 = 8)

Section B

Answer any **six** *questions.*
Each question carries a weightage of 2.

11. Show that eigen functions of a Hermitian operator are mutually orthogonal.

Turn over

12. Write Rogrigue's formula. Use the formulate to find $H_{(X)}$ for $v = 4$ in simple harmonic oscillator.

13. Find the commutator of $\hat{L}_x$ and $\hat{L}_y$.

14. 1s wave function for H atom is Ae^{-r/a_0}. Show that the maximum probability of finding the electron is at $r = a_0$.

15. State and prove Variation theorem.

16. Briefly discuss Fock's modification of Hartree self consistent field method.

17. Compare semi empirical and abinitio methods of computational chemistry.

18. How do you classify basis sets ? Discuss.

(6 × 2 = 12)

Section C

Answer any **two** *questions.*
Each question carries a weightage of 5.

19. Discuss postulates of quantum mechanics.

20. Apply Schrödinger wave equation for a spherical rotor. Find eigen functions and eigen values.

21. Use variation theorem to find the ground state energy of particle in one dimensional box with slanted bottom.

22. (a) Find the ground state energy of He by first order Perturbation method.

    (b) What are the general features of a Gaussian input file ? Discuss.

(2 × 5 = 10)

D 32672 (Pages : 2) Name.....

Reg. No.....

FIRST SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY) EXAMINATION, NOVEMBER 2022

(CBCSS)

Chemistry

CHE 1C 02—ELEMENTARY INORGANIC CHEMISTRY

(2019 Admission onwards)

Time : Three Hours Maximum : 30 Weightage

Section A

Answer any **eight** *questions.*
Each question has 1 *weightage.*

1. Carbon monoxide behaves as a Lewis base towards diborane ; but not towards BF_3. Why ?
2. The acid-base strength is not an inherent property of a substance and it largely depends on the reference solvent ; justify this statement.
3. What is 'inorganic graphite' ? Why is it called so ?
4. Classify the following compounds into *closo, nido* and *arachino* structures :
   a) B_5H_9. b) B_4H_{10}.
   c) B_5H_{11}. d) $C_2B_{10}H_{12}$.
5. Discuss the consequences of isomorphous substitution on silicates.
6. Comment on the metallic property of polythiazyl.
7. What are super heavy elements ? Give examples.
8. Account for the abrupt changes in the Ellingham diagrams.
9. What do you mean by radiation dosimetry ?
10. How do graphenes differ from fullerens ?

(8 × 1 = 8 weightage)

Section B

Answer any **six** *questions.*
Each question carries 2 *weightage.*

11. What do you mean by differentiating and levelling solvents ? Explain with suitable examples.
12. Comment on the acidity of the different types of hydrogen atoms present in carboranes.
13. Describe the synthesis and structure of S_4N_4. Comment on the thermochromism exhibited by this compound.
14. What are Latimer and Frost diagrams ? Mention their uses.
15. Discuss the liquid drop model of nucleus.
16. Describe the bottom-up and top-down approaches for the synthesis of nanomaterials giving examples.
17. Describe the principle involved and working of GM counter.
18. Discuss the applications of XRD in the study of nanomaterials.

(6 × 2 = 12 weightage)

Section C

Answer any **two** *questions.*
Each question carries 5 *weightage.*

19. What are the important characteristics of liquid ammonia as a solvent? Briefly discuss the precipitation reactions taking place in liquid ammonia.
20. Describe the methods of preparation of borazine and substituted borazines. Describe the structure and important reactions of borazine.
21. Give an account of the isopoly and heteropoly anions of W and Mo.
22. Discuss the synthesis, structure and reactivity of $(PNCl_2)_3$. What are the important uses of phosphazines ?

(2 × 5 = 10 weightage)

D 32673 (Pages : 2) Name.....

Reg. No.....

FIRST SEMESTER M.Sc. (CBCSS) [REGULAR/SUPPLEMENTARY] DEGREE EXAMINATION, NOVEMBER 2022

Chemistry

CHE 1C 03—STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS

(2019 Admission onwards)

Time : Three Hours Maximum Weightage : 30

Section A

Answer any **eight** *questions.*
Each question carries a weightage of 1.

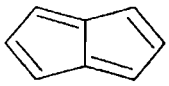
1. Depict the molecular orbitals of ethylene molecule.
2. Illustrate the tautomerism exhibited by nitro compounds.
3. Construct a reaction energy diagram for a slow endothermic reaction.
4. Draw the most stable conformer for ethylene glycol.
5. Arrange the following in increasing order of acditiy : 4-nitro benzoic acid, 4-methoxy benzoic acid, benzoic acid, phthalic acid.
6. Draw the Newman projection of the least stable conformer of 2, 3-dimethylbutane.
7. Will 1-bromo bicyclo [2.2.1] heptane undergo elimination ? Justify your answer with suitable illustration.
8. Depict the structures of (2Z, 4Z)-2, 4-hexadiene and (2E, 4Z, 6E)-2, 4, 6-octatriene.
9. (1R, 2S, 5R)-2-isopropyl-5-methlcyclohexanol is natural menthol. Depict its structure.
10. Illustrate the hydroboration reaction with an example.

(8 × 1 = 8 weightage)

Section B

Answer any **six** *questions.*
Each question carries a weightage of 2.

11. 2-Bromo fumaric acid undergoes dehydrohalogenation 50 times faster than 2-bromo maleic acid. Justify with illustration showing the elimination product also.
12. Specific rotation of a mixture of 2-bromobutanes is – 9.2°. (R)-bromobutane has a specific rotation of –23.1°. How much % R and % S enantiomer is there in the mixture ?

13. Pentalane  has not been isolated, but its dianion is know and stable. Explain.

14. Illustrate the product formed when (S)-2-butanol reacts with $SOCl_2$.

15. Predict the product formed when meso-2,3-dibromobutane is treated with magnesium.

16. Explain the peculiar bonding in cyclopropanes.

17. Illustrate the Sharpless asymmetric epoxidation reaction.

18. Depict the structure of CBS catalyst and mention one application.

(6 × 2 = 12 weightage)

Section C

Answer any **two** *questions.*
Each question carries a weightage of 5.

19. Trans-2-amino cyclohexanol on treatment with nitrous acid yields cyclopentane carbaldehyde alone while the cis isomer yields cyclohexanone as well. Illustrate with mechanism.

20. (-) Lactic acid has a specific rotation of – 3.8°. What is the specific rotation of a solution containing 7.5 g. of (–)-lactic acid and 2.5 g. of (+)-lactic acid.

21. Acetolysis of threo-3-phenyl-2-butyl tosylate gives the threo racemic product while erythro isomer proceeds largely with retention of configuration. Illustrate and explain.

22. Depict examples of (i) non-carbon chiral centred molecule ; (ii) axially chiral molecule ; (iii) atropisomers. Also give R/S designations of the chiral molecules that you have depicted.

(2 × 5 = 10 weightage)

D 32674 (Pages : 2) Name.....

Reg. No.....

FIRST SEMESTER M.Sc. (CBCSS) REGULAR/SUPPLEMENTARY DEGREE EXAMINATION, NOVEMBER 2022

Chemistry

CHE 1C 04—THERMODYNAMICS, KINETICS AND CATALYSIS

(2019 Admission onwards)

Time : Three Hours Maximum Weightage : 30

Section A

Answer any **eight** *questions.*
Each question carries a weightage of 1.

1. State and explain third law of thermodynamics.
2. Explain with example positive and negative deviation from Raoult's law.
3. Distinguish between equilibrium and steady state with reference to irrevertible processes.
4. Explain the term microscopic reversibility.
5. Account for the first and second explosion limits in H_2–O_2 reaction.
6. Explain the term temperature jump method, in relaxation spectroscopy.
7. Explain the term 'transmission co-efficient'.
8. Define threshold energy. How is it related to Arrhenius activation energy ?
9. Explain the term 'surface heterogeneity'.
10. Define Michaelis Menten constant. Explain its significance.

(8 × 1 = 8 weightage)

Section B

Answer any **six** *questions.*
Each question carries a weightage of 2.

11. Define chemical potential. How does it vary with temperature and pressure ? Derive corresponding equations.
12. What are the methods for the determination of activity co-efficient of nonelectrolytes in solution ? Discuss.
13. Define phenomenological co-efficient. Show that direct co-efficients always dominate indirect co-efficent.

Turn over

14. Decomposition of NO_2Cl takes place according to the following mechanism. Derive the rate law :

$$NO_2Cl \xrightarrow{k_1} NO_2 + Cl$$
$$NO_2 + Cl \xrightarrow{k_2} NO_2 + Cl_2$$

(Assume steady-state for Cl. concentration).

15. Compare kinetics of reactions in solution with that of reactions in gas phase. Discuss.
16. Briefly discuss a crossed molecular beam experiment.
17. What are the methods of determination of surface area of solids ? Discuss.
18. Briefly discuss sol-gel method of preparing high surface area material.

(6 × 2 = 12 weightage)

Section C

Answer any **two** *questions.*
Each question carries a weightage of 5.

19. Write mechanism of thermal decomposition of ethane. Derive the rate law. What is the apparent activation energy ?
20. Briefly discuss Lindmann's theory of unimolecular reaction. What are its drawbacks ? How are they modified ? Discuss.
21. Derive Langmuir adsorption isotherm by statistical method.
22. Discuss the importance of nano materials in catalysis.

(2 × 5 = 10 weightage)

D 51518 **(Pages : 2)** **Name.....**

Reg. No.....

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2018

(CUCSS—PG)

Chemistry

CH 1C 02—INORGANIC CHEMISTRY–I

(2010 Syllabus Year)

Time : Three Hours Maximum : 36 Weightage

Part A

Answer **all** *questions.*

Each question carries 1 *weightage.*

1. Which of the following bases is the weakest ?

   Cl, I, Br, F Give reasons.

2. Explain the Lewis concept of acids and bases.

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

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

4. What is hydroboration ? Give an example.

5. What are phosphazenes ? Give an example.

6. How is polythiazyl prepared ? Comment on its metallic property.

7. What are Ellingham diagrams ? Mention their uses.

8. What is meant by passivity ?

9. What is standard deviation ?

10. Distinguish between accuracy and precision.

11. Describe the functioning of a redox indicator.

12. Explain chelate effect with examples.

13. What are the limitations of the valence bond theory ?

14. What is meant by spectrochemical series ? Why is it called so ?

(14 × 1 = 14 weightage)

Turn over

Part B

Answer any **seven** *questions.*
Each question carries 2 *weightage.*

15. Explain levelling effect of solvents giving suitable examples.
16. Discuss the use of *styx* numbers in describing the structure and bonding in boron hydrides.
17. How is tetrasulfur tetranitride prepared ? Mention its important properties.
18. Give an account of the synthesis, structure and uses of silicons.
19. Write a note on metallic corrosion and its prevention.
20. Write briefly on the classification of errors in chemical analysis. How these can be minimized ?
21. Discuss the method of precipitation from homogeneous solution with an example. Comment on the merits of this method.
22. Differentiate between an ambidentate ligand and a macrocyclic ligand. Give examples for each type.
23. With the help of valence bond theory, explain structure and bonding in $[Fe(CN)_6]^{4+}$.
24. State and explain Jahn-Teller effect.

(7 × 2 = 14 weightage)

Part C

Answer any **two** *questions.*
Each question carries 4 *weightage.*

25. Give an account of the important reactions that take place in liquid ammonia. Discuss the advantages and disadvantages of using liquid ammonia as a non-aqueous solvent.
26. How is triphosphonitrilic chloride prepared ? Give an account of its important reactions and its structure.
27. Discuss the factors that affect the stability of metal complexes. Describe the spectrophotometric method for determining the stability of a metal complex.
28. (a) Sketch the molecular orbital diagram for Co (III) low-spin octahedral complex with σ-bonding only and discuss its salient features.

    (b) What are the effects of π-bonding on the stability of metal complexes.

(2 × 4 = 8 weightage)