C 21008 (Pages : 4) Name.....

Reg. No.....

FOURTH SEMESTER P.G. DEGREE EXAMINATION, APRIL 2022

(CCSS)

Applied Chemistry

ACH 4E 09—CHEMISTRY OF POLYMERS

(2019 Admissions)

Time : Three Hours Maximum : 80 Marks

Section A

Answer **all** *questions.*

Each question carries 1 *mark.*

1. Which of the following is an example for acopolymer ?

   (a) Polyurethane. (b) Polyester.

   (c) Polycarbonate. (d) ABS.

2. Vulcanised natural rubber is ————.

   (a) Less plastic than gum NR. (b) More plastic than gum NR.

   (c) Completely eastic. (d) Completely viscous.

3. In phenolic resins the chain extension is through ————.

   (a) Ortho and para positions. (b) Ortho positions only.

   (c) Para positions only. (d) Ortho and meta positions.

4. N66 has higher melting point than N6 because ————.

   (a) N66 has adipic acid as one monomer.

   (b) N66 has higher possibility of hydrogen bonding per repeat unit.

   (c) Monomer caprolactam for N6 is a weak material.

   (d) Diamine part of N66 is a stronger material.

5. Polyisoprene can exist as a rubber or plastic at room temperature depending on ————.

   (a) Reinforcement. (b) Crosslinking.

   (c) Isomerism. (d) None of these.

6. Which of the following is not a thermoset ?

(a) Unsaturated polyester. (b) Melamine formaldehyde.

(c) Saturated polyester. (d) Urea formaldehyde.

7. Stereospecific polymers are synthesized using ————.

(a) Ziegler Natta catalyst. (b) metallocene catalyst.

(c) Co-ordination catalysts. (d) All of these.

8. Monomer and repeat unit are different in the case of ————.

(a) Step growth polymerization. (b) Chain polymerization.

(c) Ring opening polymerization. (d) None of these.

9. Pick out the odd one :

(a) Solution polymerisation. (b) Bulk polymerization.

(c) Condensation polymerization. (d) Suspension polymerization.

10. A reaction following second order kinetics will show a linear relation between ———— and time.

(a) Concentration of reactant.

(b) Square of concentration of the reactant.

(c) Inverse of concentration of the reactant.

(d) Logarith of concentration of the reactant.

11. Which of the following is true ?

(a) Mn<Mw<Mv<Mz. (b) Mw<Mn<Mw<Mz.

(c) Mz<Mn<Mw<Mz. (d) Mn<Mv<Mw<Mz.

12. Molarity of 1 % (w/v) solution of polystyrene (Mol. Wt = one lakh g per mole) in toluene is ————.

(a) 10^{-4} moles per litre. (b) 10^{-5} moles per litre.

(c) 10^{5} moles per litre. (d) 10^{4} moles per litre.

(12 × 1 = 12 marks)

Section B

Answer **all** *questions.*

Each question carries 2 *marks.*

13. Why does living polymerization give very low polydispersity index ?

14. Describe the basic requirements of monomers used for step growth polymerization.

15. Mention four advantages of bulk polymerization

16. What are short stops ? Give one example

17. State and explain Mark Houwink equation.

18. What is rayon ? How is it made ?

(6 × 2 = 12 marks)

Section C

Answer any **six** *questions.*
Each question carries 6 *marks.*

19. Explain different types of stereospecific polymers. How are they prepared ?

20. What is meant by gelation ? Why does it occur ? How is gel point determined ?

21. Discuss the different methods of stopping the propagation step during polymerisation ? What is the significance such an operation ?

22. Make a comparative evaluation of cationic and anionic polymerizations, taking appropriate examples.

23. What is a miscelle ? Explain its role in a typica emulsion polymerization. Comment on the molecular weight of the product formed.

24. Derive copolymerization equation. How do monomer reactivity ratios affect the copolymer composition ?

25. What is meant by fractionation ? Why is it required ? How is fractionation carried out ?

26. What is interfacial polymerization? How is carried out ? Comment on the advantages, disadvantages and applications.

27. What are different grades of PE ? Describe in detail the preparation, properties and applications of LLDPE.

(6 × 6 = 36 marks)

Section D

Answer any **two** *questions.*
Each question carries 10 *marks.*

28. Make a comparative evalaution of living polymerization by ATRP, RAFT and anionic initiators.

29. Explain the preparation of N6, starting from cyclohexanone. Comment on its properties and applications. How does N6 differ from N66 ?

30. Write notes on :

(i) Kinetic chain length. (ii) Metallocenes.

(iii) Intrinsic viscosity. (iv) Disproportionation.

31. Define glass transition temperature. Explain the determination of Tg using DMA and DSC.

(2 × 10 = 20 marks)

C 2603 (Pages : 3) Name.....

Reg. No.....

FOURTH SEMESTER P.G. DEGREE EXAMINATION, APRIL 2021

(CCSS)

M.Sc. Applied Chemistry

ACH 4E 08—INDUSTRIAL CATALYSIS

(2019 Admissions)

Time : Three Hours Maximum : 80 Marks

Section A

Choose the correct answer.

1. Which of the following is a microporous material ?

   (a) ZSM–5. (b) SBA–15.

   (c) Gamma alumina. (d) Silica.

2. Which of the following is not true for chemisorption on semiconductors ?

   (a) Adsorption of C as C^- on *n*-type semiconductors follow depletive type of chemisorption.

   (b) Adsorption of C as C^- on *n*-type semiconductors follow cumulative type of chemisorption.

   (c) Adsorption of C as C^+ on *n*-type semiconductors follow cumulative type of chemisorption.

   (d) Adsorption of C as C^+ on *n*-type semiconductors follow cumulative type of chemisorption.

3. TPD of ammonia is used to measure :

   (a) Acid strength. (b) Number of acid sites.

   (c) (a) and (b). (d) Thermal stability.

4. In DRIFT ——— radiation is analysed.

   (a) Adsorbed. (b) Transmitted.

   (c) Diffuse reflected. (d) Specular reflected.

5. In photoelectron spectroscopy ——— radiation is used.

   (a) UV. (b) X-rays.

   (c) (a) and (b). (d) Gamma rays.

6. Which of the following spectroscopic techniques makes use of electron energy loss ?

   (a) LEIS. (b) SIMS.

   (c) AES. (d) HREELS.

7. The activity and selecting data of few catalysts are reported. Choose the best catalyst :

Catalyst	A	B	C	D
Activity (%)	60	70	60	50
Selectivity (%)	40	70	80	90

8. Which of the following statements is true for thermal deactivation ?

   (a) It is due to fouling.
   (b) It is due to cocking.
   (c) It is due to sintering.
   (d) It cannot be redegenerated.

9. Which of the following is a shape selective catalyst ?

   (a) ZSM–5.
   (b) SBA–15.
   (c) MCM–41.
   (d) Graphene.

10. Which of the following statements is not true for zeolites ?

   (a) They are alumino Silicates.
   (b) They are acidic catalysts.
   (c) They have shape selectivity.
   (d) They are mesoporous materials.

11. ———— is a cracking catalyst.

   (a) Zeolite–Y.
   (b) ZSM–5.
   (c) Hydrotalcite.
   (d) NiO.

12. Which of the following is not true for Monsanto process ?

   (a) Methanol is converted to acetic acid.
   (b) Rhodium carbonyl is used as catalyst.
   (c) It was developed by BASF.
   (d) CO is converted into hydrocarbons.

(12 × 1 = 12 marks)

Section B

Answer **all** *questions.*
Each question carries 2 *marks.*

13. With the help of suitable examples distinguish between associative and dissociative type of chemisorption.

14. Suggest one method of determining surface basicity. Explain.

15. How do you secure data in STM ? Explain.

16. Explain with example catalyst fouling.
17. What is electro catalysis ? Explain.
18. What is ammoxidation ? Name a catalyst for ammoxidation ?

(6 × 2 = 12 marks)

Section C

Answer any **six** *questions.*
Each question carries 6 *marks.*

19. With the help of potential energy curves discuss activated and non-activated adsorption.
20. Briefly discuss electron band theory of catalysis by metals.
21. Write a brief account of the different types of reactors.
22. What are the sources of deactivation of catalyts ? Discuss.
23. What are the methods of catalyst regeneration ? Discuss.
24. What is Mobil process ? Discuss.
25. Discuss briefly applications of catalysts in pollution control.
26. Discuss applications of Mössbauer spectroscopy in catalysis.
27. How do you study pore volume distribution of a catalyst ? Discuss.

(6 × 6 = 36 marks)

Section D

Answer any **two** *questions.*
Each question carries 10 *marks.*

28. Discuss briefly boundary layer theory of chemisorption on semiconducting oxides.
29. How do you prepare mesoporous materials ? Discuss.
30. Discuss briefly catalytic reactors.
31. Write a brief account of the theory of photocatalysis.

(2 × 10 = 20 marks)

C 2601 (Pages : 5) Name.....

Reg. No.....

FOURTH SEMESTER P.G. DEGREE EXAMINATION, APRIL 2021

(CCSS)

M.Sc. Applied Chemistry

ACH 4E 06—COMPUTATIONAL CHEMISTRY

(2019 Admissions)

Time : Three Hours Maximum : 80 Marks

Section A

Choose the correct answer :

1) Which of the following is *not* a correct aspect of the Born-Oppenheimer approximation ?

   (a) The electrons in a molecule move much faster than the nuclei.

   (b) Excited electronic states have the same equilibrium internuclear distance as the ground electronic state.

   (c) The electronic and vibrational motions of a molecule are approximately separable.

   (d) Electronic energy curves serve as potential energy functions for nuclear vibrational 3 motion.

2) Which of the following abbreviations is *not* likely to be used in quantum chemistry ?

   (a) LCAO. (b) HOMO.

   (c) LUMO. (d) RSVP.

3) How many co-ordinates do you need in order to specify the absolute position in space of all of the nuclei of chlorobenzene, C_6H_5Cl ?

   (a) 12. (b) 30.

   (c) 3. (d) 36.

4) Which of the following statements is *not* correct about Gaussian basis functions used to expand the molecular orbitals ?

   (a) The commonly-used 'Slater-Type Orbital' family of basis sets uses Slater functions.

   (b) For a given number of basis functions, it would be more accurate to use Slater functions instead of Gaussian functions incorrect.

   (c) The integrals over basis functions needed to carry out Hartree-Fock calculations are more difficult to evaluate for Slater functions than for Gaussian functions incorrect.

   (d) Some combinations of multiple Gaussian functions are quite similar to Slater functions.

5) Calculations are carried out on the neon atom and a dimer consisting of two neon atoms separated by 60 Å, at two different levels of theory (i) and (ii). The energies obtained are (i) – 128.7961 and – 257.5924 hartree, and (ii) – 128.7919 and – 257.5688 hartree. What can you conclude from these calculations ?

(a) Total energies of this type tell us lillle beyond the energy required to remove the electrons from the neon nuclei.

(b) Method (i) is better because it returns lower energies in both cases.

(c) Method (ii) returns an energy for the system with two neon atoms that is less negative than twice the energy for two neon atoms; this must be right since we know neon cannot bond to neon.

(d) Method (i) is size-consistent (the energy for two distant neon atoms is exactly twice the energy for one neon atom), while method (ii) is not size-consistent - twice -128.7919 hartree is – 257.5838 hartree.

6) The CCSD(T) method (coupled-cluster theory with single and double excitations, and perturbative treatment of triples) is one of the most accurate quantum chemical methods. Which of the following is *not* a drawback of this method ?

(a) Size-inconsistency.

(b) Huge computational expense, especially for larger molecules.

(c) High requirements on the size of the basis set.

(d) A tendency to yield incorrect energies when significant static correlation is present, as for stretched bonds.

7) Biomolecular simulation using molecular dynamics is one of the major fields of computational science nowadays. Which of the following statements is correct ?

(a) Modelling proteins is harder than modelling simpler systems such as liquid water, as the normal molecular dynamics method cannot be applied to biomolecules.

(b) Only small proteins such as crambin can be simulated, given the huge number of solvent and protein atoms present in larger proteins.

(c) Using state of the art codes and computers, it is possible to carry out simulations of systems containing many millions of atoms.

(d) Proteins are modelled using special forcefields describing secondary structure elements such as α -helices instead of the atoms making up the protein.

8) When designing a computational study, which of the following considerations would typically *not* be relevant ?

(a) The computational resources needed to carry out the intended calculations.

(b) The hazardous nature of the chemical species being modelled.

(c) The appropriate nature of the chosen model in order to be able to describe the experimental property of interest.

(d) The possible accidental nature of the results obtained, due to cancellation of errors.

9) Which of the following does not play an important role in the development of the field of computational chemistry ?

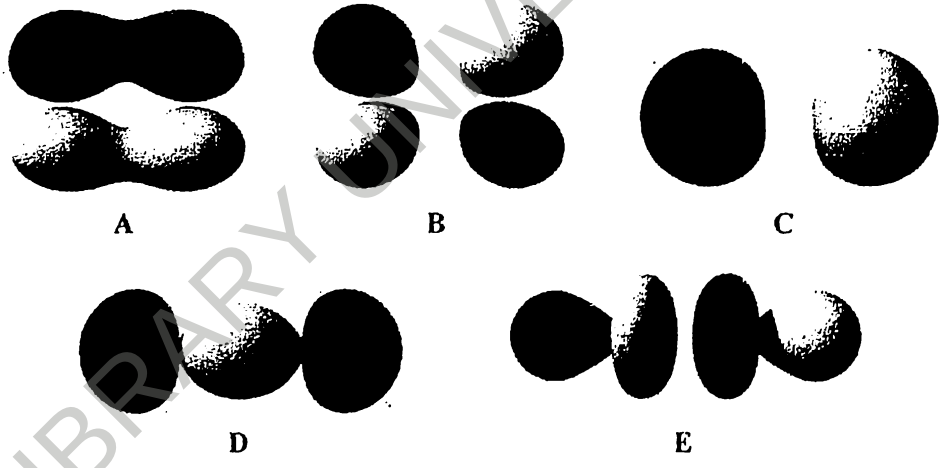
(a) Faster computers.

(b) New discoveries in fundamental quantum mechanics.

(c) New computational methods.

(d) More efficient software implementation.

10) Which of the following is a representation of a σ-bonding molecular orbital ?



(a) A, C and D.

(b) C, D and E.

(c) D.

(d) B.

11) Which of the following terms refers to the molecular modelling computational method that uses equations obeying the laws of classical physics ?

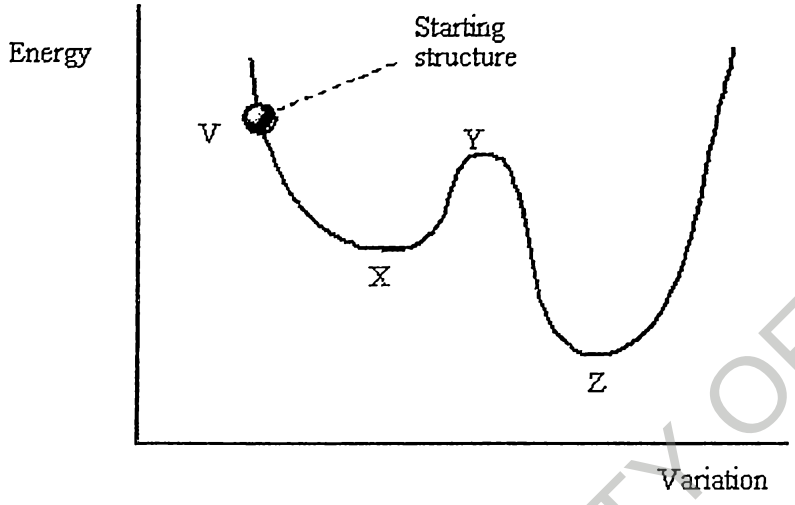
(a) Quantum mechanics.

(b) Molecular calculations.

(c) Molecular mechanics.

(d) Quantum theory.

12) The following graph shows the stability of a molecule as its structure is varied during conformational analysis :



What term is used to describe the point on the graph marked X ?

(a) Global energy minimum. (b) Transition state.

(c) Local energy minimum. (d) Conformational minimum.

(12 × 1 = 12 marks)

Section B

Answer **all** *questions.*
Each question carries 2 *marks.*

13) Why is Kohn-Sham orbitals used in DFT ?

14) What is the difference between transition state and intermediate ?

15) Explain Correlation-consistent basis sets.

16) Comment on the energy obtained after : a) single point energy calculations ; b) optimized geometry calculations.

17) What are the limitations of Gaussian type orbitals ?

18) What is N-representability ?

(6 × 2 = 12 marks)

Section C

Answer any **six** *questions.*
Each question carries 6 *marks.*

19) Briefly explain the problems and challenges of DFT.

20) Discuss how the Hartree approximation can be used to solve for the wavefunctions and energies of multi-electron atoms.

21) Using an illustration, explain what diffuse functions are. Give an example of an oxygen containing molecule that would require diffuse functions in the basis set.

22) Discuss the orbital approach of independent orbitals is an approximation to a multi-electron system with the motions of all electrons coupled together.

23) What is zero-point energy ? How can it be calculated using Gaussian Program package ?

24) Explain the potential energy surface of a diatomic system.

25) What is exchange correlation functional ? Give examples.

26) Explain the different terms involved in force fields.

27) How can you distinguish between local minima and global minima ?

(6 × 6 = 36 marks)

Section D

Answer any **two** *questions.*
Each question carries 10 *marks.*

28) Discuss multiple-zeta basis sets.

29) How is Molecular Mechanical methods different from Quantum Mechanical methods ?

30) What are the advantages of DFT over ab initio theory ?

31) Discuss the different parts of a Gaussian input file for geometry optimization and frequency calculations. Discuss the information that can be obtained from such a calculation.

(2 × 10 = 20 marks)