2019

PG Even Semester (CBCS) Exam., May—2019

CHEMISTRY

(4th Semester)

Course No. : CHMCC–401

(Analytical and Computational Chemistry)

Full Marks : 70
Pass Marks : 28

Time : 3 hours

The figures in the margin indicate full marks for the questions

Answer **five** questions, taking **one** from each Unit

UNIT—I

1. *(a)* Define capacity factor of a solute. Establish the relation between capacity factor and fraction of solute present in mobile phase. How can solute's capacity factor be measured from chromatogram? ½+2½+2=5

(b) What are the factors that affect the ion-exchange equilibria in ion-exchange chromatography? 2

(c) What do you mean by isocratic elution and gradient elution? 2

(d) Explain the working principle of GC with schematic diagram and mention its application. 5

2. *(a)* What do you mean by hyphenated techniques in analytical chemistry? Discuss the working principle of GC-MS with proper schematic diagram. 2+4=6

(b) Discuss plate theory of column chromatography. 2

(c) Distinguish between adsorption and partition chromatography. 2

(d) Discuss about the forces acting in adsorption chromatography. 2

(e) Write some applications of ion-exchange chromatography. 2

UNIT—II

3. *(a)* Summarize the different features of the cyclic voltammogramic response for reversible and quasi-reversible systems. 3

(b) Explain the use of cyclic voltammetry for estimating the value of formal potential ($E°$) and number of electron transfer (n) for a reversible system. 3

(c) Draw a block diagram of typical controlled potential coulometry apparatus. Deduce current-time behaviour of controlled potential electrolysis. In bulk electrolysis, find out the time needed for 99·9% completion of electrolysis (where m_0 10 ^{2} cm/s). 2+4+2=8

4. *(a)* In cyclic voltammetry *cis* $[Ru(bpy)_2Cl_2]$ shows two redox couples at 0·3 V and 1·9 V whereas *cis* $[Ru(bpy)_2(H_2O)_2]^{2}$ shows two redox couples at 0·4 V and 0·6 V with respect to SCE in CH_3CN at Pt-disk working electrode ($^{t}BuNClO_4$ used as supporting electrolyte). Elucidate the observation. 3

(b) Deduce the relationship between diffusion current and concentration of an analyte in polarography. 4

(c) Discuss the current versus potential relationship for the reduction of metal ion in solution at dropping mercury electrode. 2

(d) What does amperometry refer to? Describe the most common types of curve encountered in amperometric titration. 1+4=5

UNIT—III

5. *(a)* Explain the fundamental principle of X-ray fluorescence spectroscopy (XRF). How does this principle differ from the principle of scanning electron microscopy (SEM)? Draw a schematic diagram of wavelength dispersive X-ray fluorescence (WDXRF) instrument and explain the function of detector used in XRF instrument. 2+2+5=9

(b) Depict and explain the block diagram of thermal gravimetric analyzer. 5

6. *(a)* What is differential thermal analysis (DTA)? How does it differ from differential scanning calorimetry (DSC)? 3+2=5

(b) Discuss the Curie point calibration method of TGA instrument. 3

(c) Briefly describe the advantages of neutron activation analysis (NAA). 3

(d) Give a schematic representation of the atomization process in a flame for magnesium sulfate heptahydrate solution. 3

UNIT—IV

7. *(a)* What do you mean by memory of a computer? Delineate the differences between RAM and ROM. 2+4=6

(b) Discuss the various symbols used for drawing flowchart. How is flowchart helpful in writing program? Draw the flowchart to compute decay constant. 4+2+2=8

8. *(a)* What do you mean by softwares? Delineate the differences between application software and system software. 2+4=6

(b) Write the flowchart and C program to compute rate constant of a second-order chemical reaction, $k \quad \frac{x}{at(a \quad x)}$. 3+3=6

(c) What is algorithm? 2

UNIT—V

9. *(a)* What is 2D potential energy surface (PES)? Draw and explain the potential energy surface to represent the variation of energy during the conversion of ozone to isozone. 2+4=6

(b) What are the objectives of molecular modelling? Explain the difference between molecular mechanics and ab initio methods. Why is DFT preferred over other methods? 2+4+2=8

10. *(a)* What is Hartree-Fock approximation? 2

(b) What is hypersurface? Explain why, higher-order potential energy surface cannot be drawn in a paper. How can hypersurface be explained mathematically? 1+2+3=6

(c) Explain two principles of Kohn-Sham theorem of DFT. 3

(d) What is parametrization? What is its utility in semiemperical method? 1+2=3

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