PG Even Semester (CBCS) Exam., May—2018

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) Describe the band broadening process of column chromatography. 3

   (b) A chromatographic analysis for the chlorinated pesticide dieldrin gives a peak with retention time of 8·68 min and a baseline width of 0·29 min. How many theoretical plates are involved in this separation? Given that the column used in this analysis is 2·0 meters long. What is the height of a theoretical plate? 3

(c) What are the advantages of using temperature and pressure programming in gas chromatography? 3

(d) What are the basic differences between gas chromatography and high performance liquid chromatography? 3

(e) Write a short note on hyphenated HPLC-ICP-MS. 2

2. (a) What are the essential criteria of an adsorbent required to become an ideal stationary phase in adsorption chromatography? Explain the roles of silica gel and alumina as stationary phase. 2+3=5

   (b) What is partition chromatography? Discuss the factor on which the retention of solute depends in partition chromatography. 1+2=3

   (c) Explain the working principle of HPLC with schematic diagram and mention its application. 6

UNIT—II

3. (a) Define polarography. Briefly explain different types of mass transport process and the respective current in polarography. 1+3=4

(3)

(b) Write down the basic principle and uses of hydrodynamic voltametry.   3+3=6

(c) Draw and explain the cyclic voltammogram of [Pt (p-tap) (tb cat)] in CH_3CN at Pt disk electrode, where p-tap = paratolyl azo pyridine, tb cat= tertiary butyl catechol.   4

4. (a) $Ru(bpy)_2 Cl_2$ shows two redox couples at ~0·3 V and ~1·9 V versus SCE whereas $[Ru(bpy)_2(OH_2)_2]^2$ gives the same couple at ~0·4 V and ~1·6 V versus SCE in CH_3CN at Pt disk electrode, where TBAP was used as supporting electrolyte. Discuss the observation.   4

(b) Write down the advantages and disadvantages of dropping-mercury electrode (DME) over solid electrodes.   3+3=6

(c) Construct Ilkovic equation for the mean diffusion current in polarography from Cottrell equation and explain.   4

UNIT—III

5. (a) What are the optimum conditions to measure TG of a sample?   2

(4)

(b) What are the factors that affect the results of thermogravimetric analytical data?   3

(c) What is the basic difference between atomic absorption spectroscopy (AAS) and flame emission spectroscopy?   2+3=5

(d) Draw the block diagram of X-ray fluorescence system and explain the function of each component.   4

6. (a) Draw the block diagram of the DSC apparatus and discuss their components.   2+3=5

(b) Discuss two types of DSC system.   2+2=4

(c) Explain the terms PGNAA, DGNAA, ENAA and FNAA. How can NAA technique be used in forensic investigations?   2+3=5

UNIT—IV

7. (a) What are different components of hardware? Explain the functioning of a computer system.   4+4=8

(b) Draw the flowchart and write a C program to compute pressure from van der Waals' equation.   3+3=6

(5)

8. *(a)* Explain the salient features of UNIX operating system. 5

(b) Write the important features of C language. Explain different types of constant used in C program. 4+3=7

(c) Draw the symbols to show two-way branching and three-way branching decisions during drawing flowchart. 2

UNIT—V

9. *(a)* What is potential energy surface (PES)? Explain and draw PES of H_2O considering its e_{2v} symmetry. 2+4=6

(b) What is Born-Oppenheimer approximation? Molecular geometry depends only on the mass of the nuclei but not on the charge. Explain. 3+3=6

(c) What is molecular mechanics (MM)? 2

10. *(a)* What is the importance of basis set in DFT calculation? Explain 6-31G basis set. 2+3=5

(b) Explain how ab-initio method is different from semiempirical method. 3

(6)

(c) What are stationary points? Explain the difference between minima and saddle points. What is intrinsic reaction coordinate? 1½+3+1½=6

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