PG Even Semester (CBCS) Exam., May—2017

CHEMISTRY

(4th Semester)

Course No. : CH–401 (C)

(Analytical and Computational Chemistry)

Full Marks : 75
Pass Marks : 30

Time : 3 hours

The figures in the margin indicate full marks for the questions

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

UNIT—I

1. *(a)* What is the basic principle of chromatography? What are the three structural components of alumina as a stationary phase? Provide structural representation. 2+2+1=5

(b) Give a comparison between normal phase chromatography and reverse phase chromatography. 4

(c) Outline the principles of ion-exchange chromatography with an illustrative example of the process, highlighting the mode of action. What is pearl polymerization? 4+2=6

2. *(a)* Explain the working principle of gas chromatography with schematic diagram and mention its application. 7+3=10

(b) What are the essential features of HPLC? What are the advantages of HPLC over conventional column chromatography? 3+2=5

UNIT—II

3. *(a)* Write down the principle of polarography and deduce Ilkovic equation for the diffusion current in polarographic work. 3+4=7

(b) What is dropping mercury electrode (DME)? Discuss the advantages and disadvantages of DME. Show the polarogram with respect to drop size / drop lifetime. 1+3+1=5

(c) Describe the most common types of curve encountered in amperometric titration. 3

4. *(a)* Illustrate the linear sweep polarography for the redox reaction of 0·5 m $M\,CdCl_2$ in 1 M HCl. Explain the nature of currents with respect to the applied potential. 6

(b) Discuss the principles and use of hydrodynamic voltametry. 6

(c) In a controlled potential bulk electrolysis, find out the current vs. time behaviour. 3

UNIT—III

5. *(a)* Write down the principle of AAS. Draw the block diagram of its instrumentation and explain the function of each component. 10

(b) Describe the analytical application of XRF. What elements can be detected by XRF spectroscopy? 3+2=5

6. *(a)* What is the principle of thermo-gravimetric analysis? 3

(b) Provide the instrumentation of DSC. 4

(c) What is differential thermal analysis (DTA)? How does it differ from DSC? 3+2=5

(d) Describe the application of NAA in brief. 3

UNIT—IV

7. *(a)* What are different components of hardware? 5

(b) What do you mean by the memory of a computer? Explain different types of memory. 2+3=5

(c) Write the flowchart of C program to compute radioactive decay constant. 2+3=5

8. *(a)* Write the important features of C program. Explain different types of constant used in C program. 5+5=10

(b) Explain the salient features of UNIX operating system. 5

UNIT—V

9. *(a)* What are the objectives of computational chemistry? Explain the differences between molecular mechanism and ab initio methods. 2+4=6

(b) What is 2D potential energy surface? Draw the potential energy surface to represent the variation of energy during the conversion of ozone to isoozone. 2+4=6

(c) Explain Hartree-Fock approximation. 3

10. *(a)* What are the basic differences between density functional theory and molecular mechanics? 4

(b) What is hypersurface? Explain why higher-order hypersurface cannot be drawn. How will you explain hyper-surface mathematically? 1+2+3=6

(c) What is stationary point? How will you differentiate between the energy minima and transition state? 2+3=5

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