2018/EVEN/08/22/CHM–401 (C)/040

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

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)* Discuss the basic principles of normal-phase and reversed-phase chromatographies and mention the various types of stationary and mobile phases employed for these processes. Provide the structures of neutral, acidic and basic alumina and explain their role as stationary phase. 2+3+3=8

(b) What is the advantage of using temperature and pressure programming in gas chromatography? 3

(c) What are the basic differences between gas chromatography and high-performance liquid chromatography? 4

2. *(a)* What is partition chromatography? Mention some of its applications. Mention three features to distinguish adsorption chromatography from partition chromatography. 1+2+3=6

(b) What do you mean by 'hyphenated techniques' in analytical chemistry? 2

(c) Explain the working principle of gas chromatography with schematic diagram. 7

UNIT—II

3. *(a)* Discuss the principles and uses of hydrodynamic voltametry. 6

(b) Write down the principle of amperometric titration of Pb^{2} ion by SO_4^{2} and explain. 2+3=5

(c) Extract quantitatively the standard state potential for the redox reaction of

$$O_x \quad ne \rightleftharpoons \text{Red at DME surface}$$ 4

4. *(a)* Write down the principle of polarography and deduce Ilkovic equation for the diffusion current in polarographic work. 2+4=6

(b) Draw and explain the cyclic voltammogram of $Fe(\ ^{5}\text{-}C_5H_5)_2$ in CH_2Cl_2, where $[NBu_4][PF_6]$ is used as supporting electrolyte and Pt electrode as working electrode. 5

(c) In a controlled potential bulk electrolysis, find out current vs. time behaviour. 4

UNIT—III

5. *(a)* Depict and explain the block diagram of thermal gravimetric analyzer. Mention the basic differences among TGA, DTA and DSC. Discuss the application of DSC. 4+2+3=9

(b) Explain nuclear-activation analysis and its advantages. 6

6. *(a)* Explain the principle of X-ray fluorescence spectroscopy (XRFS). Briefly describe the instrumentation with block diagram. 6

(b) Explain the differences between atomic absorption spectroscopy and flame-emission spectroscopy. Write the application of AAS. 3+2=5

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

UNIT—IV

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

(b) What do you understand by the programming languages? Define any four programming languages. 3+2=5

(c) How many different types of constant are known in FORTRAN? 2

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

(b) Write the important features of C language. Explain different types of constants used in C program. 4+4=8

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

UNIT—V

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

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

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

10. *(a)* What are objectives of computational chemistry? 3

(b) What are basis sets? Explain in detail the 6-31G basis set. 2+3=5

(c) What are stationary points? Explain the difference between minima and saddle points. What is intrinsic reaction coordinate? 2+3+2=7

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