(b) Write the Flow chart and Algorithm to convert the temperature to Fahrenheit. 2+2=4

(c) Write the Algorithm and Fortran77 Program to calculate the rate constant of a first-order reaction. 3+3=6

Unit-V

9. (a) What are the terms involved in Schrodinger equation of a many body system? How Born-Openheimer approximation is used to solve the Schrodinger equation? Molecular geometry depends on the mass of the nuclei but not on the charge. Explain. 2+3+3=8

(b) What is potential energy surface (PES). Draw and explain PES of H_2O molecule considering its C_{2v} symmetry. 6

10. (a) What are the objectives of computational chemistry? Explain how abinitio method is different from DFT. 2+3= 5

(b) What are the basis sets? Explain the 6-31G basis sets? Calculate the number of basis function and primmitives in the case of CH_2 molecule using 6-31G basis set. 2+3+4=9

★★★

PG (CBCS) EVEN SEMESTER EXAMINATION, 2023

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, selecting one from each unit)

Unit-I

1. (a) In a chromatographic analysis of lemon oil a peak for limonene has a retention time of 8.36 min with a baseline width of 0.96 min. Y-Terpinine elutes at 9.54 min with a baseline width of 0.64 min. The column void time is 0.31 min. What is the resolution between the peaks? Calculate capacity factor of Limonene and Y- Terpinine and selective factor for Limonene and Y- Terpinine. 4

(b) Provide the structures of silica and alumina and explain their role as stationary phase. 4

(c) Give a comparison between normal phase chromatography and reverse phase chromatography. 3

(d) State basic principle and some application of ion exchange chromatography. 3

2) (a) Explain the working principle of GC with suitable schematic diagram and mention its application. 6+2 = 8

(b) What are the main difference between HPLC and GC.
3

(c) Establish Van-Deemter equation with illustration of band broadening process. 3

Unit-II

3. (a) Define polarography. Mention the two important steps for any electrolysis and discuss. 1+3=4

(b) Derive the relation between limiting diffusion current and depolarizer concentration in polarography where DME is used as working electrode. 4

(c) Draw and explain the cyclic voltammogram for $K_3[Fe(CN)_6]$ (Solvent H_2O; Supporting electrolyte, KNO_3; scan rate 50 mV/s, Potential window +0.8 to -0.2 V)
1+3 = 4

(d) Calculate the number of electrons transferred and formal potential for a redox couple in cyclic voltammetry, where E_{pc}= 0.555V and E_{pa}= 0.492. 2

4. (a) Briefly explain the role of supporting electrolyte in polarographic analysis by taking a suitable example. 2

(b) Write a short note on Dropping Mercury electrode (DME).
3

(c) Write down the fundamental principle of amperometric titration. By taking suitable examples, briefly discuss the most common types of curve encountered in amperometric titrations. 2+4= 6

(d) Derive the relation between current vs. time in the controlled potential electrolysis. 3

Unit-III

5. (a) What are the factors that affect the result of a thermogravimetrythermogram? 4

(b) How to calculate mass loss and determine the offset and onset temperature of TG thermogram. 3

(c) Discuss the advantage of DTA over TG. 2

(d) What is differential scanning calorimetry? Discuss the types of differential scanning calorimetry. 1+4 =5

6. (a) What is the basis of neutron activation analysis(NAA)? Explain the terms PGNAA and DGNAA. Explain, how the NAA technique be used in archaeology and forensic investigation. 2+2+4=8

(b) Briefly describe the method of determination of vanadium in lubricating oil by AAS. 3

(c) What are the strength and limitation of XRF? 3

Unit-IV

7. (a) What are the hardware components of a computer? Discuss briefly about them. 3+5=8

(b) Write the Flow chart and Fortran77 Program to calculate the pressure of a real gasusing van der Waal's equation.
3+3=6

8. (a) What is a Flow chart? Why do we need a flow chart?
1+3=4