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3 (Sem-5/CBCS) CHE HE 1/2/3

2025

CHEMISTRY

(Honours Elective)

Answer the Questions from any one Option.

OPTION-A

Paper : CHE-HE-5016

(Applications of Computers in Chemistry)

OPTION-B

Paper : CHE-HE-5026

(Analytical Method in Chemistry)

OPTION-C

Paper : CHE-HE-5036

(Molecular Modelling and Drug Design)

Full Marks : 60

Time : Three hours

The figures in the margin indicate full marks for the questions.

OPTION-A

Paper : CHE-HE-5016

(Applications of Computers in Chemistry)

1. Answer **any seven** questions : $1 \times 7 = 7$

(a) Which one of the following is suitable for drawing infrared spectrum (IR) of a molecule ?

ISIS Draw, Origin, BASIC

(b) Differentiate between compiler and interpreter.

(c) Explain debugging.

(d) Explain the use of DEF statement.

(e) Define linear programming.

(f) Name *two* chemistry tools/software that are useful in drawing chemical structures, reaction schemes etc.

(g) What do you mean by an interpolation method ?

(h) What is an interface ?

(i) Convert the binary number $(11001)_2$ into decimal system.

(j) Define the terms OMR and OCR related to computer system.

(k) Standard ANSIC recognizes — number of keywords. (Fill in the blank)

(l) CD-ROM is a

(i) Semiconductor memory

(ii) Memory register

(iii) Magnetic memory

(iv) None of the above

(Choose the correct answer)

2. Answer **any four** questions : $2 \times 4 = 8$

(a) Define *any four* programming languages.

(b) Mention *any two* search engines and explain.

(c) Define cheminformatics with an application.

(d) What are the applications of the following library functions ?

(i) RND

(ii) LOG

(e) Differentiate between bug and virus.

(f) Correct the errors in the following statements :

(i) LS=Len (AS)

(ii) A1=8

(g) Write a program in BASIC to plot five concentric circles using For Next loop.

(h) Write *any four* features of MS Excel.

3. Answer **any three** questions : $5 \times 3 = 15$

- (a) Write a program in BASIC to find the product of first *ten* natural numbers.
- (b) How many types of INPUT devices are generally used? Explain them.
- (c) Draw a BASIC program for determination of electronegativity *or* bond length.
- (d) Write short notes on the following :
(any two)
 - (i) Variables and dimensions
 - (ii) Simpson's numerical integration method
 - (iii) ANOVA
- (e) Explain the method of averages in data analysis.

Or

A stream of nitrogen gas contains 0.2 wt% water vapour. Determine the mole fraction of water.

- (f) Write a BASIC program to compute pressure form van der Waals' equation.

Or

Write an algorithm to find the largest of *three* numbers.

- (g) What is the use of GOTO statement in BASIC programming?
- (h) Explain the CPU and its working in computer.

4. Answer **any three** questions : $10 \times 3 = 30$

- (a) (i) Discuss the advantages of relational database management. 4
- (ii) Discuss on the design and development of simple data bases on chemical and physical properties of substances. 6
- (b) Develop a flowchart and a BASIC program to fit a straight line for the following data relating to enthalpy of methane at 1 atm. pressure with temperature :

Data:

Enthalpy : (kJmol^{-1}) 630 650 824 851 875 1050 1110 1200

Temperature : ($^{\circ}\text{C}$) -200 -100 0 100 200 300 400 500

- (c) Calculate the value of the integral by using Simpson's 1/3 and 3/8 rules and also calculate the approximate value of *z* in each case.

Or

Draw a flowchart using spreadsheet for determining the mass fraction and mole fraction of each component in the following mixture of hydrocarbons :

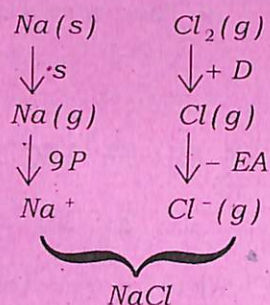
125g of methane, 125g of ethane and 250g of propane.

- (d) Draw a flowchart for calculation of lattice energy of NaCl on the basis of the Born-Haber cycle given below :

Lattice energy on the basis of Born-Haber cycle can be calculated for a reaction as follows :

e.g., for the reaction

$\text{Na}(g) + \text{Cl}_2(g) \xrightarrow{-Q} \text{NaCl}$ this cycle is as follows :



So, $-Q = S + IP + \frac{1}{2}D - EA - U$, where S is the

heat of sublimation, IP is the ionization potential of Na , D is the dissociation energy, EA is the electron affinity, U is the lattice energy and Q is the heat of formation. On rearranging it

$$-U = -Q - S - IP - \frac{1}{2}D + EA \quad \text{or,} \quad U = Q + S + IP + \frac{1}{2}D - EA.$$

- (e) Explain Newton-Raphson method for roots of a real valued function.

Or

Explain in detail the uses of spreadsheet in chemistry by taking the following examples :

- (i) Determination of empirical and molecular formula
 - (ii) Determination of vapour pressure.
- (f) What is operator ? Describe the different types of operators with examples in C-language.
- (g) Write a BASIC program to calculate pH of acidic, basic and neutral solutions.

Or

For the vapour-liquid equilibrium of a binary mixture of benzene and toluene, the following results are reported :

$$x : 0.167 \quad 0.333 \quad 0.500 \quad 0.667 \quad 0.833$$

$$y : 0.320 \quad 0.550 \quad 0.710 \quad 0.830 \quad 0.930$$

where, x and y represent mole fraction of benzene in liquid and vapour respectively. Indicate how these data might be plotted to give a straight line if the relative volatility were constant. Fit the best straight line to point on such a graph by

- (i) visual inspection of the best straight line through the points

- (ii) the method of averages
- (iii) the method of least square

Determine the average relative velocity of the mixture by using the straight line obtained.

- (h) (i) Discuss the various symbols used for drawing flowchart. 4
- (ii) Write on program testing and execution. 4
- (iii) What is batch processing system ? 2

Or

Systems of simultaneous equations are given as

$$A_1X + B_1Y = C_1$$

$$A_2X + B_2Y = C_2$$

Write a BASIC program to compute the values of X and Y. 10

OPTION-B

Paper : CHE-HE-5026

(Analytical Method in Chemistry)

1. Answer **any seven** of the following questions :
1×7=7
- (a) Name the binder that is present in silica gel G.
 - (b) Define the term 'specific rotation'.
 - (c) When is batch extraction used for extraction process?
 - (d) Name the *two* light sources used in UV-visible spectrophotometer.
 - (e) A sample exhibited an absorbance 1.0 in UV-visible spectroscopy. What will be its percentage of transmittance?
 - (f) What is the function of Nernst glower ?
 - (g) What is meant by thermogravimetric analysis ?
 - (h) What is meant by Nernstian behaviour in an indicator electrode ?
 - (i) What is potentiometry ?
 - (j) Why is source modulation used in atomic absorption spectroscopy ?
 - (k) Why is IR spectrum considered 'finger print' of a molecule ?
 - (l) How is standard deviation related to accuracy ?

2. Answer **any four** of the following questions :

$$2 \times 4 = 8$$

- (a) What is the role played by a masking agent in the extraction of metal ions?
- (b) What do you mean by synergistic extraction?
- (c) What are the different types of paper chromatography?
- (d) Describe the source of pH dependence in a glass membrane electrode.
- (e) Draw a probable TG curve for $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$.
- (f) The force constant for H^{35}Cl and D^{35}Cl are the same and both can be considered as harmonic oscillators. H^{35}Cl has a fundamental vibrational transition at 2886 cm^{-1} . Calculate the ratio of the zero-point energy of H^{35}Cl to that of D^{35}Cl .
- (g) Name different gases that can be used as fuel and oxidant in Flame-AAS.
- (h) The standard deviation from one set of 11 determinations was 0.210, and the standard deviation from 13 determinations was 0.641. Is there any significant difference between the precision of these *two* sets of results at the 10% level? Given the value of F for 10 and 12 degrees of freedom at 10% probability level is 2.28.

3. Answer **any three** of the following questions :

$$5 \times 3 = 15$$

- (a) What is chromatogram? Write shortly about *any two* chromatogram development methods. 1+4=5
- (b) Discuss the factors on which conductance of a solution depends.
- (c) What is conductometry? How will you determine the pKa value of an acid with the help of conductometric titration? 1+4=5
- (d) Explain the basic working principle and the applications of the TGA technique. What are the factors that affect the TGA curve? 3+2=5
- (e) Describe the basic differences between atomic emission and atomic absorption spectroscopy. Among atomic emission and atomic absorption, which one is more sensitive to flame instability and why. 2+3=5
- (f) Discuss the working principle of atomic absorption spectrometer.

- (g) Describe briefly *two* different sample preparation methods for IR measurement.
- (h) What is the difference between accuracy and precision? Discuss the methods for determining the accuracy. 1+4=5

4. Answer **any three** of the following questions :
10×3=30

- (a) (i) Describe the qualitative and quantitative aspects of gas chromatography. 5
- (ii) How can NMR spectroscopy be used to determine the enantiomeric composition? 5
- (b) (i) What is meant by solvent extraction? State the law on which it is based on. Define the term 'distribution ratio'. How is it different from distribution coefficient? 1+1+1+2=5
- (ii) Describe briefly the continuous extraction technique used in solvent extraction. 5

(c) Discuss the basic features of conductometric titration curves obtained from the reactions between —

- (i) HCl and $NaOH$;
- (ii) $H_2C_2O_4$ and Na_2CO_3 ;
- (iii) Na_2CO_3 and HCl ;
- (iv) CH_3COOH and $NaOH$.

(d) What is potentiometric titration? How one reveals the end point of a potentiometric titration? Describe the features of a potentiometric titration curve. Discuss the use of potentiometry in food industry and pharmaceutical industry. 1+1+3+5=10

(e) What are the factors that influence the vibrational frequency? Discuss with the help of example. Distinguish between the *two* isomers having molecular formula, C_3H_6O namely CH_3COCH_3 and CH_3CH_2CHO in terms of their IR frequencies. 6+4=10

(f) (i) Match the following : 1

- (A) Near IR region (I) Rotation
(B) Middle IR region (II) Overtone
(C) Far-IR region (III) Vibration-rotation

(ii) How many stretching modes of vibration are there for H_2O and HCl molecule ? 2

(iii) Diagrammatically show the bending modes of vibration for H_2O and CO_2 molecule. 2

(iv) In an IR spectrophotometer, diffraction gratings have displaced prisms as the main source of monochromation. Why ? 1

(v) What type of detectors is preferred in IR spectrophotometer for measurements that must be made rapidly ? 1

(vi) What are the advantages of FT-IR over continuous wave spectrophotometer ? 2

(vii) How will you distinguish between propanone and propan-2-ol using IR spectroscopy ? 1

(g) Describe the working principle of single beam and double beam UV-visible spectrophotometers. Mention *two* advantages of double beam spectrophotometer over the single beam. $8+2=10$

(h) (i) Mention *two* advantages of spectrophotometric analysis. 2

(ii) UV-visible spectroscopy can be used to distinguish keto-enol tautomers. Explain with the help of a suitable example. 3

(iii) Explain with an example how Job's method of continuous variation can be used to determine the composition of a metal complex. 5

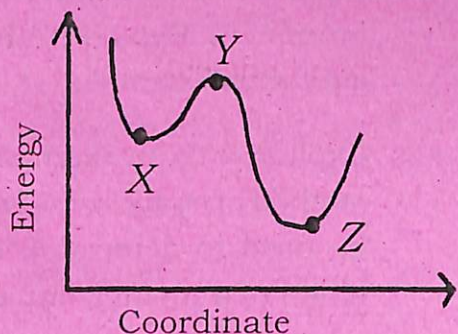
OPTION-C

Paper : CHE-HE-5036

(Molecular Modelling and Drug Design)

1. Answer **any seven** of the following questions :
1×7=7

(a) The following graph shows the stability of a molecule as its structure is varied during conformational analysis :



Which term is used to describe the point marked 'Z' ?

- (i) Global energy minimum
- (ii) Transition state
- (iii) Conformation energy minimum
- (iv) Lowest energy minimum

(b) Which of the following statements is true ?

- (i) Energy minimization is carried out by using quantum mechanics.
- (ii) Energy minimization is used to find a stable conformation of a molecule.
- (iii) Energy minimization is carried out by varying only bond lengths and bond angles.
- (iv) Energy minimization stops when a structure is found with a much greater stability than the previous one in the process.

(c) The energies of hydrogen bonds typically lie in the range of (kJ mol^{-1})

- (i) 4 - 40
- (ii) 40 - 400
- (iii) 0.4 - 4.0
- (iv) 400 - 4000

- (d) CoMFA method is used for
- (i) 4D - QSAR
 - (ii) 3D - QSAR
 - (iii) 6D - QSAR
 - (iv) 5D - QSAR
- (e) Which of the following software programmes is used for automated de novo drug design?
- (i) DOCK
 - (ii) LUDI
 - (iii) CHEM3D
 - (iv) CoMFA
- (f) What is chemoinformatics?
- (g) What is meant by 'molecular docking'?
- (h) Koopmans theorem helps in correct prediction of — by relating it to the energy of HOMO. (Fill in the blank)
- (i) Which is the computationally most expensive part of a molecular dynamics simulation?

- (j) Which of the following is not used by molecular modelling software packages?
- (i) Relative molar mass
 - (ii) Bond angle
 - (iii) Bond length
 - (iv) Torsion angle
- (k) Which of the following is not an electronic parameter?
- (i) Dipole moment
 - (ii) Hammett substituent constant
 - (iii) Molecular connectivity
 - (iv) HOMO/LUMO
- (l) Define the term 'molecular modelling'.

2. Answer **any four** questions : $2 \times 4 = 8$

- (a) What do the symbols P and π represent in a Q-SAR equation?

- (b) Mention *any two* common types of non-bonded interactions that can exist amongst molecules.
- (c) What is 6 - 31G basis set ?
- (d) Mention *any two* reputed sources of molecular modelling literatures.
- (e) What is molecular graphics ? What are the *two* most common ways of representing a molecule by using computer graphics ?
- (f) Draw the staggered conformation of ethane and show the torsion angle.
- (g) What is the difference between molecular dynamics (MD) and Monte Carlo (MC) approaches ?
- (h) What are the *two* most common types of errors in molecular simulation ? Give an example of each.

3. Answer **any three** questions : $5 \times 3 = 15$

- (a) What is Lennard-Jones 12-6 potential ? Write down the equation and explain the meanings of the terms involved. How can we calculate the distance corresponding to the potential energy minimum in the curve ? $1+3+1=5$
- (b) What is a potential energy surface (PES) ? Draw a diagram of a PES and explain the significance of various points in the curve.
- (c) Describe how a protein structure can be predicted by using 'threading'.
- (d) Discuss the importance of hydrogen bonding in molecular mechanics.
- (e) Explain how an energy minimization problem can be stated.
- (f) Describe *two* techniques that are used to reduce computational time in molecular dynamics simulations.

(g) Briefly describe the advantages and disadvantages of doing computer simulations.

(h) How is temperature controlled in MD and MC simulations? Briefly explain.

4. Answer **any three** questions : $10 \times 3 = 30$

(a) Discuss about the various sources of errors in computer simulation methods.

(b) Give an account of structure based de novo ligand design.

(c) Explain the concept of Q-SAR. Write about the different electronic and steric parameters to be considered in Q-SAR analysis. $4+6=10$

(d) Describe the steps involved in Monte-Carlo simulation.

(e) Give an account of the molecular dynamics simulation at constant temperature and pressure.

(f) Give an account of the first-order energy minimization method.

(g) Discuss the force field models for the simulation of liquid water.

(h) Describe briefly about the various steps involved while performing a computer simulation.