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

**2022**

**CHEMISTRY**

(Honours Elective)

**Answer the Questions from any one Option.**

**OPTION-A**

**(Applications of Computers in Chemistry)**

Paper : CHE-HE-5016

**OPTION-B**

**(Analytical Method in Chemistry)**

Paper : CHE-HE-5026

**OPTION-C**

**(Molecular Modelling and Drug Design)**

Paper : CHE-HE-5036

Full Marks : 60

Time : Three hours

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

Contd.

## OPTION-A

### (Applications of Computers in Chemistry)

Paper : CHE-HE-5016

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

- (a) CD-ROM is a
- (i) Semiconductor memory
  - (ii) Memory register
  - (iii) Magnetic memory
  - (iv) None of the above

(Choose the correct answer)

- (b) Standard ANSIC recognizes \_\_\_\_\_ number of keywords. (Fill in the blank)
- (c) Define the terms OMR and OCR related to computer system.
- (d) Convert the binary number  $(11001)_2$  into decimal system.
- (e) What is an interface ?

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- (f) What do you mean by an interpolation method ?
- (g) Name *two* chemistry tools/software that are useful in drawing chemical structures, reaction schemes etc.
- (h) Define linear programming.
- (i) Explain the use of DEF statement.
- (j) Explain debugging.
- (k) Differentiate between compiler and interpreter.
- (l) Which one of the following is suitable for drawing infrared spectrum (IR) of a molecule ?

ISIS Draw, Origin, BASIC

2. Answer **any four** questions :  $2 \times 4 = 8$
- (a) Write *any four* features of MS Excel.
- (b) Write a program in BASIC to plot five concentric circles using For ..... Next loop.
- (c) Correct the errors in the following statements :
- (i) LS=Len (AS)
  - (ii) A1=8
- (d) Differentiate between bug and virus.
- (e) What are the applications of the following library functions ?
- (i) RND
  - (ii) LOG

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Contd.

- (f) Define cheminformatics with an application.
- (g) Mention *any two* search engines and explain.
- (h) Define *any four* programming languages.
3. Answer **any three** questions :  $5 \times 3 = 15$
- (a) Explain the CPU and its working in computer.
- (b) What is the use of GOTO statement in BASIC programming?
- (c) Write a BASIC program to compute pressure form van der Waals' equation.

**Or**

Write an algorithm to find the largest of three numbers.

- (d) 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.

- (e) Write short notes on the following :  
**(any two)**

- (i) Variables and dimensions
- (ii) Simpson's numerical integration method
- (iii) ANOVA

- (f) Draw a BASIC program for determination of electronegativity or bond length.
- (g) How many types of INPUT devices are generally used? Explain them.
- (h) Write a program in BASIC to find the product of first ten natural numbers.

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

- (a) (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.

- (b). 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	0.333	0.500	0.667	0.833
$y$ :	0.320	0.550	0.710	0.830	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

- visual inspection of the best straight line through the points.
- the method of averages.
- the method of least square.

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

- What is operator ? Describe the different types of operators with examples in C-language.
- Explain Newton-Raphson method for roots of a real valued function.

**Or**

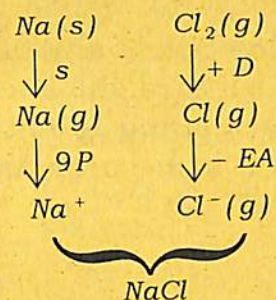
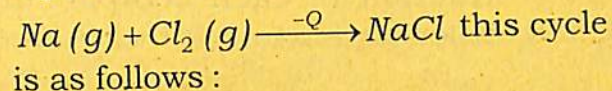
Explain in detail the uses of spreadsheet in chemistry by taking the following examples :

- Determination of empirical and molecular formula
- Determination of vapour pressure

- Draw a flowchart for calculation of lattice energy of  $\text{NaCl}$  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



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

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

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

- (f) 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 :

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

- (g) 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 : ( $\text{kJmol}^{-1}$ )	630	650	824	851	875	1050	1110	1200
Temperature : ( $^{\circ}\text{C}$ )	-200	-100	0	100	200	300	400	500

- (h) (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

## OPTION-B

### (Analytical Method in Chemistry)

Paper : CHE-HE-5026

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

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

- (a) 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.
- (b) Name different gases that can be used as fuel and oxidant in Flame-AAS.
- (c) 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  $2886\text{ cm}^{-1}$ . Calculate the ratio of the zero-point energy of  $H^{35}Cl$  to that of  $D^{35}Cl$ .
- (d) Draw a probable TG curve for  $CuSO_4 \cdot 5H_2O$ .
- (e) Describe the source of pH dependence in a glass membrane electrode.
- (f) What are the different types of paper chromatography?
- (g) What do you mean by synergistic extraction?
- (h) What is the role played by a masking agent in the extraction of metal ions?

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

- (a) What is the difference between accuracy and precision? Discuss the methods for determining the accuracy.  $1+4=5$
- (b) Describe briefly *two* different sample preparation methods for IR measurement.
- (c) Discuss the working principle of atomic absorption spectrometer.
- (d) 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?  $2+3=5$
- (e) Explain the basic working principle and the applications of the TGA technique. What are the factors that affect the TGA curve?  $3+2=5$
- (f) What is conductometry? How will you determine the  $pK_a$  value of an acid with the help of conductometric titration?  $1+4=5$

(g) Discuss the factors on which conductance of a solution depends.

(h) What is chromatogram? Write shortly about *any two* chromatogram development methods? 1+4=5

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

(a) (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

(b) 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

(c) (i) Match the following : 1

(A) Near IR region (A) Rotation

(B) Middle IR region (B) Overtone

(C) Far-IR region (C) 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

(d) 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

(e) 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

(f) 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  $NaOH$ .

10

(g) (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

(h) (i) Describe the qualitative and quantitative aspects of gas chromatography. 5

(ii) How can NMR spectroscopy be used to determine the enantiomeric composition? 5



## OPTION-C

### (Molecular Modelling and Drug Design)

Paper : CHE-HE-5036

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

- (a) Define the term 'molecular modelling'.
- (b) Which of the following is not an electronic parameter ?
- (i) Dipole moment
  - (ii) Hammett substituent constant
  - (iii) Molecular connectivity
  - (iv) HOMO/LUMO
- (c) 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

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

(j) The energies of hydrogen bonds typically lie in the range of ( $\text{kJ mol}^{-1}$ )

(i) 4 - 40

(ii) 40 - 400

(iii) 0.4 - 4.0

(iv) 400 - 4000

(k) Which of the following statements is true?

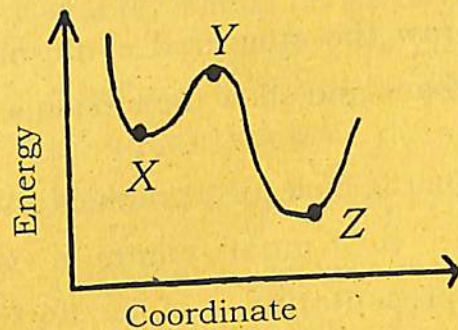
(i) Energy minimization is carried out by using quantum mechanics.

(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.

(l) 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

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

(a) What are the *two* most common types of errors in molecular simulation? Give an example of each.

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

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

- (a) How is temperature controlled in MD and MC simulations? Briefly explain.
- (b) Briefly describe the advantages and disadvantages of doing computer simulations.
- (c) Describe two techniques that are used to reduce computational time in molecular dynamics simulations.
- (d) Explain how an energy minimization problem can be stated.
- (e) Discuss the importance of hydrogen bonding in molecular mechanics.
- (f) Describe how a protein structure can be predicted by using 'threading'.
- (g) What is a potential energy surface (PES)? Draw a diagram of a PES and explain the significance of various points in the curve.

- (h) 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

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

- (a) Describe briefly about the various steps involved while performing a computer simulation.
- (b) Discuss the force field models for the simulation of liquid water.
- (c) Give an account of the first-order energy minimization method.
- (d) Give an account of the molecular dynamics simulation at constant temperature and pressure.
- (e) Describe the steps involved in Monte-Carlo simulation.
- (f) Explain the concept of Q-SAR. Write about the different electronic and steric parameters to be considered in Q-SAR analysis.  
4+6=10

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

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