Total number of printed pages–23

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 : 1×7=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 ?

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

(g) Name *two* chemistry tools/softwares 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 : 2×4 = 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

(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 : 5×3=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 devises 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 : 10×3=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

A1X + B1Y = C1

A2X + B2Y = C2

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

(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.

(c) What is operator ? Describe the different types of operators with examples in C-language.

(d) 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

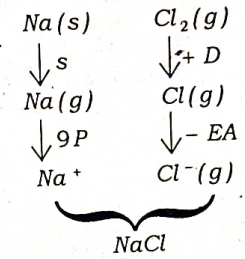
(ii) Determination of vapour pressure

(e) 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

$Na(g) + Cl_2(g) \xrightarrow{-Q} NaCl$ 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

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

Contd.

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

(h) (i) Discuss the advantages of rational 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×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.

Contd.

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 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 $CuSO_4.5H_2O$.

(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 pKa 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

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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 ($kJ\ mol^{-1}$)

(i) 4 - 40

(ii) 40 - 400

(iii) 0.4 - 4.0

(iv) 400 - 4000

(k) Which of the following statements is true ?

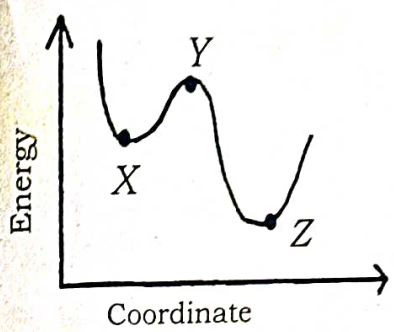
(i) Energy minimization is carried out by using quantum mechanics.

(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 : 2×4=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 representating a molecule by using computer graphics ?

(e) Mention *any two* reputed sources of moleculer 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 π represent in a Q-SAR equation ?

3. Answer ***any three*** questions : 5×3=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 Linnard-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 simulalion 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.

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