3 (Sem–5/CBCS) CHE HE 1/2/3

2021

(Held in 2022)

CHEMISTRY

(Honours Elective)

Answer the Questions from any one Option.

OPTION – A

Paper : CHE–HE– 5016

DSE (H) – 1

(Applications of Computers in Chemistry)

Full Marks : 60

Time : Three hours

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

1. Answer **all** questions : 1×7=7

   (a) What is a variable ?

   (b) Convert the number 223 to a binary number.

   (c) What is the full form of ASCII ?

(d) Define debugging.

(e) What is logical operator ?

(f) What is a string ?

(g) What is extrapolation ?

2. Answer **all** questions : 2×4=8

(a) What are the differences between compiled and interpreted languages ?

(b) What is the use of END statement in a BASIC program ?

(c) Find the *two* errors in the following program :

```
10 FOR X = 36 TO 34 STEP 2
20 PRINT X
30 NEXT Y
40 END
```

(d) Write BASIC statements to —

　(i) print square root of a number

　(ii) print absolute value of a number

3. Answer **any three** of the following questions : 5×3=15

(a) What do you mean by computer programming ? Write a BASIC program to print positive even numbers upto 200.

(b) Write short notes on the following :

　(i) IF statement

　(ii) REM and LET statement

(c) Write a BASIC program to calculate the pH of a weak acid.

(d) Write a BASIC program to perform matrix addition.

(e) Write a BASIC program to find the numerical value of the definite integral.

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

(a) Explain Regula-Falsi method for finding roots of a real-valued function.

(b) Write a BASIC program to compute the roots of a system of linear equations using Gauss-Seidel method.

(c) The vapour pressures of liquid acetonitrile CH_3CN at three different temperatures is

i	$T_i(^\circ K)$	$P_i s\,(mm\,Hg)$
1	268.15	20
2	289.05	60
3	300.15	100

Estimate the vapour pressure at $280\cdot15\,K$ using

(i) linear interpolation and

(ii) quadratic interpolation

(d) Write a basic program to compute rate constant of zero-order reaction.

(e) Explain the application of spreadsheet to estimate the following : **(any two)**

(i) Empirical and molecular formula

(ii) Molecular weight

(iii) Vapour pressure

(f) Explain in detail the importance of spreadsheet in statistical analysis of data and data processing with an example.

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OPTION – B

Paper : CHE–HE– 5026

(Analytical Method in Chemistry)

Full Marks : 60

Time : Three hours

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

1. Answer the following questions :   1×7=7

   (a) What is the relation between transmittance and absorbance ?

   (b) What is the difference between accuracy and precision ?

   (c) What is meant by distribution ratio in chromatography ?

   (d) What is the elution order of reverse phase liquid chromatography ?

   (e) In Atomic Absorption Spectroscopy, which of the following is generally used as radiation source ?

      (i) Tungsten lamp

      (ii) Xenon mercury arc lamp

      (iii) Hydrogen or deuterium discharge lamp

      (iv) Hollow cathode lamp

   (f) Why is IR spectra obtained from different sample preparation methods for the same sample looks slightly different from each other ?

   (g) *Cis*-stilbene absorbs at lower wavelength than *trans*-stilbene in the UV-visible region of the electromagnetic spectrum. Why ?

2. Answer the following questions :   2×4=8

   (a) Vibrational frequency of *HF* molecule is found at $845\, cm^{-1}$. If the hydrogen atom of this molecule is substituted with deuterium, what will be the vibrational frequency of the molecule ?

   (b) What are the factors that determine the mobility of a sample in thin-layer chromatography ?

   (c) How are different chormatographic techniques classified based on the mobile phase ? Give *one* example of each class.

(d) What is the function of the monochromator in a spectrophotometer ?

3. Answer *any three* of the following questions :   5×3=15

(a) What are the different mechanisms used in solvent extraction ? What is a chelating reagent ? Discuss its role in solvent extraction by considering a suitable example.   2+1+2=5

(b) What is a chiral shift reagent ? Discuss its role in NMR spectroscopy with a suitable example.   1+4=5

(c) What is the basic principle of atomic absorption spectroscopy ? What are the different atomization processes commonly employed in the atomic absorption spectroscopy (AAS) ?   3+2=5

(d) Explain with a suitable example, how pKa values of an indicator can be determined by UV-visible spectroscopy.   5

(e) How does a silicone photodiode detector work ?   5

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

(a) (i) Discuss the principle used in HPLC.   5

(ii) What are the factors that influence extraction efficiency in solvent extraction ?   2

(iii) A sample of mandelic acid analysed in a polarimeter gave an observed specific rotation of –75 degrees. If the specific rotation of (S)-mandelic acid is +154 degrees, then answer the following :

(A) Which enantiomer (R *or* S) is in excess ?   1

(B) Calculate the enantiomeric excess of the mixture.   1

(C) Calculate the percentage of each enantiomer in the mixture.   1

(b) (i) A mixture of $CaCO_3$ and CaO is analysed using TGA technique. TG curve of the sample indicates that there is a mass change from 145.3 mg to 115.4 mg between 500–900°C. Calculate the percentage of $CaCO_3$ in the sample. 3

(ii) Calculate the percentage mass change (m%) for the following reactions : 2

$$CuSO_4 \xrightarrow{\text{Heat}} CuO + SO_3$$
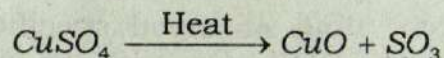
(iii) Discuss the factors on which conductance of an electrolytic solution depends. 5

(c) (i) Discuss with an example, how the strength of an acid can be determined by pH metric titration against a standard base. 5

(ii) Discuss the principle of colorimetric analysis for determination of concentration of an unknown solution. 5

(d) (i) Define systematic and random errors. How can we reduce systematic errors ? 2+3=5

(ii) Discuss the principle of ion exchange chromatography. 5

(e) (i) Analysis of a sample of iron ore gave the following percentage values for the iron content :

7.08, 7.21, 7.12, 7.09, 7.16, 7.14, 7.07, 7.14, 7.18, 7.11

Calculate the mean, standard deviation and coefficient of variation for the values. 1+2+2=5

(ii) What is the fingerprint region in IR spectroscopy ? Why is it called so ? Why is it important ? 1+1+1=3

(iii) What are the limitations of Beer-Lambert's law ? 2

(f) (i) Discuss the principle of conductometric titration for the determination of equivalence points of acid-base reaction. 5

(ii) What are the key components of a thermal analysis system ? Discuss an application of Thermo-gravimetric Analysis (TGA) with a suitable example. 2+3=5

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.***

1. Answer the following questions :
   $1 \times 7 = 7$

   (a) What are different types of models used to describe a molecule ?

   (b) What is a Z-matrix ?

   (c) What do you mean by PES ?

   (d) How is van der Waals surface constructed ?

   (e) What are the conventional units of length and energy in molecular modelling ?

   (f) How will you define a simple molecular mechanics force field ?

   (g) Write the mathematical form of Morse potential.

2. Answer the following questions : $2 \times 4 = 8$

   (a) Describe briefly the Börn-Oppenheimer approximation.

   (b) What types of points on a PES are particularly relevant in understanding a chemical reaction ?

   (c) What are 'hard' degrees of freedom ? Provide schematic illustration of the cross terms believed to be most important in force fields.

   (d) What do you mean by *H*-bonding in molecular mechanics ?

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

   (a) Discuss briefly different types of non-bonded interactions.

   (b) What do you mean by computer hardware and software ? Describe briefly with examples.

   (c) Discuss briefly the solvent dielectric models.

(d) What do you mean by dispersive interactions ? What are exchange forces ? 2½+2½

(e) Discuss briefly the simple water models used for the simulation of liquid water.

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

(a) Give a typical expression for a molecular mechanics potential energy function of the type used for macromolecular simulations. Include intra- and intermolecular terms. Describe, what each energy term represents. Also state briefly the physical origin of each of the energy terms. 10

(b) Describe briefly the following methods for calculating molecular energies and geometries (outline their advantages and disadvantages).

(a) *ab initio* molecular orbital methods

(b) Semiempirical molecular orbital methods 5+5=10

(c) How are different thermodynamic properties calculated using a force field ? Discuss briefly force field parametrisation technique. 5+5=10

(d) Discuss briefly the simplex method and the sequential univariate method used for energy minimisation. 5+5=10

(e) Discuss briefly the Monte Carlo method. State the differences between the MD and Monte Carlo method. 5+5=10

(f) Discuss briefly the different steps involved in running a computer simulation. 10