

Total number of printed pages-15

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 ?

Contd.

- (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 :

$$5 \times 3 = 15$$

(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 (mm Hg)
1	268.15	20
2	289.05	60
3	300.15	100

Estimate the vapour pressure at 280.15K 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 : $1 \times 7 = 7$
 - (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 : $2 \times 4 = 8$

(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 chromatographic 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

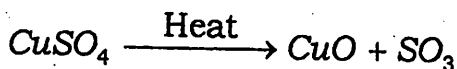
(iii) A sample of mandelic acid analysed in a polarimeter gave an observed specific rotation of -75 degrees. If the specific rotation of (S)-mandelic acid is +154 degrees, then answer the following :

(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 145.3mg to 115.4mg between $500\text{--}900^\circ\text{C}$. Calculate the percentage of CaCO_3 in the sample. 3
- (ii) Calculate the percentage mass change ($m\%$) for the following reactions : 2



- (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 Thermogravimetric 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 :

1×7=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.

(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 ? $2\frac{1}{2}+2\frac{1}{2}$

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

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

(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.
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3 (Sem-5/CBCS) CHE HE 4/HE 5/HE 6

2021

(Held in 2022)

CHEMISTRY

(Honours Elective)

Answer the Questions from any one Option.

OPTION-A

Paper : CHE-HE-5046

(Novel Inorganic Solids)

Full Marks : 60

Time : Three hours

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

1. Answer the following as directed : $1 \times 7 = 7$

(a) The colour of gold nanoparticles is

(i) yellow

(ii) orange

(iii) red

(iv) variable

(Choose the correct answer)

Contd.

(b) Carbon nanotubes are also known as _____.
(Fill in the blank)

(c) What is the basis of classification of composite materials ?

(d) Quartz is an acidic refractory.
(State True or False)

(e) What are fullerides ?

(f) Give an example of a magnetic material used in data storage devices.

(g) What is solid electrolyte made of ?

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

(a) What are inorganic pigments ? How are they different from organic pigments ?

(b) What is the amount (%) of carbon in pure iron, cast iron and steel ?

(c) What are superalloys ? Mention *two* important applications of superalloy.

(d) Distinguish between natural and artificial nanoparticles.

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

(a) What are solid-state electrolytes (SSEs) ? In which batteries SSEs are used ?
 $3 + 2 = 5$

(b) Discuss a method for the synthesis of silver nanoparticles. What is the colour of silver nanoparticles ? $4+1=5$

(c) What is the role of matrix in a composite material ? Discuss the advantages of composite materials. $2+3=5$

(d) What are polymer matrix materials ? Mention their important applications. Why are polymer matrix materials better than metals ? $1+2+2=5$

(e) Based on the composition, how are ceramic materials classified ? Discuss each of them. $2+3=5$

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

(a) (i) Discuss the top-down and bottom-up approach in nanomaterial synthesis. $2\frac{1}{2} + 2\frac{1}{2} = 5$

(ii) What is the molecular structure of carbon nanotubes ? What are their uses in carbon nanotechnology ? $3+2=5$

(b) Write notes on the following : $2\frac{1}{2} \times 4 = 10$

(i) Hydrothermal synthesis

(ii) Thermoplastics

- (iii) Molecular magnets
 - (iv) Green synthesis of nanoparticles
 - (c) (i) Discuss the effects of environmental factors on composite materials. 5
 - (ii) What are fibre-reinforced composites ? Discuss their applications. 2+3=5
 - (d) What are alloying elements ? Discuss the various types of aluminium alloys and their uses. 2+8=10
 - (e) What is DNA nanotechnology ? Write a brief note on biological applications of DNA nanomaterials. 3+7=10
 - (f) Discuss the various methods used in the synthesis of inorganic solids. 10
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OPTION-B

Paper : CHE-HE-5056

(Polymer Chemistry)

Full Marks : 60

Time : Three hours

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

1. Answer the following as directed : $1 \times 7 = 7$

(a) What do you mean by degree of polymerization ?

(b) What is an inorganic polymer ?

(c) Arrange the following polymers in increasing order of intermolecular forces :

Buna-S, Polythene, Nylon 6,6

(d) What is super fibre ?

(e) Which of the following natural products is not a polymer ?

(i) DNA

(ii) Cellulose

(iii) ATP

(iv) Urease

(Choose the correct answer)

(f) Example of addition polymer is —

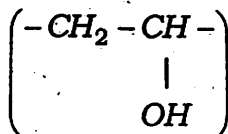
(i) Buna-S

(ii) Bakelite

(iii) Nylon-6

(iv) Dacron

(g) Write the IUPAC name of



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

(a) Draw the structure of the monomers of the following polymers

(i) Teflon

(ii) Polythene

(b) What is Ziegler-Natta catalysts ?

(c) Describe the classification of polymers on the basis of structure. Give examples.

(d) Define the term 'oriented polymers'.

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

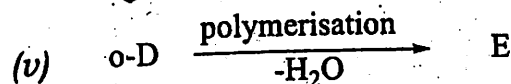
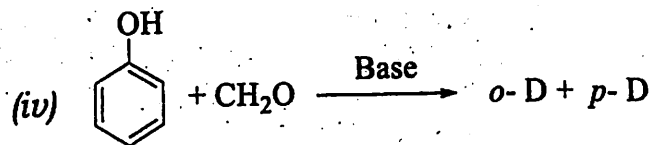
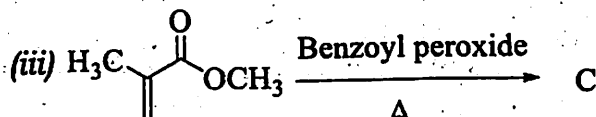
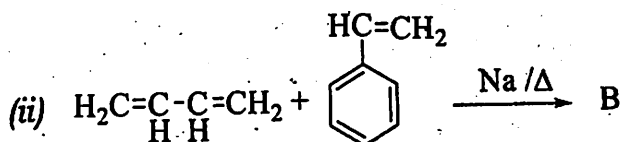
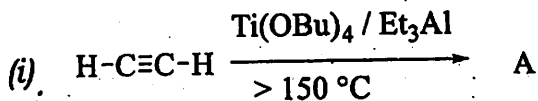
$5 \times 3 = 15$

(a) (i) 'All polymers are macromolecules but all macromolecules are not polymers' — Justify the statement.

3

(ii) Write the importance of plasticizer in polymer chemistry with an example. 2

(b) Identify A-E in the following polymeric reactions : 5



(c) Briefly discuss the preparation, properties and uses of the following polymers : 2.5×2=5

(i) Polyamides

(ii) Polyvinyl chloride (PVC)

(d) Write short note on thermodynamics of polymer solutions. What are *two* main factors which helps crystallization of polymers ? $3+2=5$

(e) Differentiate between copolymerization and homopolymerization. Give *one* example of each. What is graft and block copolymer ? $2+1+2=5$

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

$10 \times 3 = 30$

(a) What are natural and synthetic polymer. Give examples. How do you explain the functionality of a monomer and how does it affect the polymer formation ? Give an account of synthetic criteria of polymer formation.

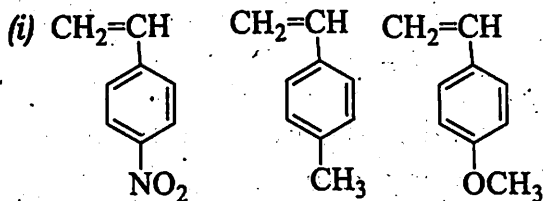
$3+4+3=10$

(b) What are the basic differences between addition and condensation polymer ? How will you distinguish between free radical and ionic polymerization ? Write the free radical mechanism for the polymerisation of ethene.

$3+3+4=10$

(c) Name *any two* initiators used in anionic polymerization. Describe the polymerization of 2,2-dimethyloxirane by an anionic and cationic mechanism. List the following groups of monomers in order of decreasing ability to undergo anionic polymerization.

$2+3+3+2=10$



(d) What is glass transition temperature (T_g) ? Discuss various factors affecting glass transition temperature. Which of the polymers in each pair is expected to have higher T_g and why ?

(i) polyethylene and polypropylene

(ii) poly(but-1-ene) and poly(but-2-ene).

Write a short note on Conducting polymer. 1+3+3+3=10

(e) Define living polymerization. Mention *two* benefits of living polymerization in general over conventional non-living polymerizations. Mention *two* techniques of living radical polymerization. Give an example of block co-polymer that is usually synthesized by living anionic polymerization. 2+3+3+2=10

(f) Why is molecular weight of polymers taken as 'average'? Explain viscometry methods of determining molecular weight of polymers. Why is M_v measured by viscosity method not an absolute molecular weight? Explain the term Polydispersity index. 2+4+2+2=10

OPTION-C

Paper : CHE-HE-5066

(Instrumental Methods of Chemical Analysis)

Full Marks : 60

Time : Three hours

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

1. Answer **all** the questions as directed :

1×7=7

- (a) What is the source of visible light used in a modern UV-visible spectrophotometer ?
- (b) The reference compound use in $^1\text{H-NMR}$ spectroscopy is _____.
- (c) Which of the following is used as the source of radiation in atomic absorption spectroscopy ?
- (A) Tungsten lamp
(B) Xenon-mercury arc lamp
(C) Deuterium lamp
(D) Hollow cathode lamp

(Fill in the blank)

(Choose the correct answer)

(d) Which of the following statements is wrong ?

- (A) A mass spectrometer uses high energy UV radiation.
- (B) A mass spectrometer does not use a spectrophotometric detector.
- (C) Mass spectrometry does not always require samples of high purity.
- (D) A mass spectrum does not show signals due to uncharged radicals.

(e)

Column-1	Column-2
(a) Mass spectrometry	(i) Deuterium lamp
(b) NMR	(ii) Michelson Interferometer
(c) FT-IR	(iii) Base peak
(d) UV-visible	(iv) Chemical shift

Choose the correct option for the matching pairs from both the columns:

- (A) (a) → (iii); (b) → (iv); (c) → (ii); (d) → (i)
- (B) (a) → (iii); (b) → (i); (c) → (iv); (d) → (ii)
- (C) (a) → (iv); (b) → (iii); (c) → (ii); (d) → (i)
- (D) (a) → (ii); (b) → (iii); (c) → (iv); (d) → (i)

- (d) Which of the following statements is wrong ?
- (A) A mass spectrometer uses high energy UV radiation.
- (B) A mass spectrometer does not use a spectrophotometric detector.
- (C) Mass spectrometry does not always require samples of high purity.
- (D) A mass spectrum does not show signals due to uncharged radicals.

(e) Column-1	Column-2
(a) Mass spectrometry	(i) Deuterium lamp
(b) NMR	(ii) Michelson Interferometer
(c) FT-IR	(iii) Base peak
(d) UV-visible	(iv) Chemical shift

Choose the correct option for the matching pairs from both the columns:

- (A) (a) → (iii); (b) → (iv); (c) → (ii); (d) → (i)
- (B) (a) → (iii); (b) → (i); (c) → (iv); (d) → (ii)
- (C) (a) → (iv); (b) → (iii); (c) → (ii); (d) → (i)
- (D) (a) → (ii); (b) → (iii); (c) → (iv); (d) → (i)

(f) Which of the following statements is wrong ?

- (A) UV light absorption causes electronic transitions.
- (B) UV spectra provide information about valence electrons.
- (C) IR absorption causes transitions between rotational energy levels of a molecule.
- (D) NMR spectrometers use radiofrequency electromagnetic radiation.

(g) Consider the following instrumental methods :

- (i) IR spectroscopy
- (ii) UV-visible spectroscopy
- (iii) Mass spectrometry
- (iv) Chromatography

Which method(s) can give structural information regarding a molecule ?

- (A) (i) and (ii)
- (B) (ii) and (iii)
- (C) (i), (ii) and (iii)
- (D) All of the above

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

(a) Give *two* advantages of using tetramethyl silane (TMS) as the reference standard in $^1\text{H-NMR}$ spectroscopy.

(b) Mention *two* requirements of a carrier gas in gas chromatography. Why is O_2 unsuitable as a carrier gas ?

(c) (i) What quantities are usually displayed in a typical FT-IR spectrum ?

(ii) Convert 20000 cm^{-1} to nm .

$1 + 1 = 2$

(d) Two analysts determined the percentage of silver in a coin and reported the following results :

Analyst 1 : 100.00, 99.60, 99.70, 99.10

Analyst 2 : 98.80, 98.82, 98.84, 98.81

If the true value is 100.00, comment on the accuracy and precision of the measurements of both the analysts.

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

(a) Briefly discuss about the working principle of a double-beam UV-visible spectrometer by using a neat diagram.

(b) Discuss the advantages and limitations of instrumental methods in chemical analysis.

- (c) Discuss the methods of sample preparation in IR spectroscopy.
- (d) Briefly discuss about the importance of column chromatography in the separation of mixtures.
- (e) The electronic absorption spectrum of a molecule recorded in a solution phase is typically broad in appearance. Explain using appropriate diagram.

4. Answer the following questions : $10 \times 3 = 30$

- (a) Discuss the principle and instrumentation of atomic absorption spectroscopy (AAS). $5+5=10$

Or

- (i) Briefly discuss the principle of NMR spectroscopy. 5
- (ii) What is chemical shift ? What are the factors that affect chemical shift ? $1+4=5$

- (b) Discuss the principle, instrumentation and applications of gas chromatography. $4+4+2=10$

Or

Discuss the principle and instrumentation of mass spectrometry.

10

(c) Answer **either** (i) to (iii) **or** (iv) to (vii) :

(i) Discuss the instrumentation of FT-IR spectroscopy. 5

(ii) Discuss the advantages of FT-IR spectrometers over dispersive instruments. 4

(iii) What is fingerprint region in IR spectroscopy ? 1

Or

(iv) Write down the mathematical form of the Beer-Lambert law and explain the various terms involved. 2

(v) Give *two* important causes of deviations from the Beer-Lambert law. 2

(vi) What is the significance of the molar extinction coefficient ? 1

(vii) Radiation of wavelength 280 nm is passed through 1 cm of an aqueous solution of the amino acid tryptophan present at a concentration of 0.50 mol dm⁻³. The light intensity is reduced to 54% of its initial value. Calculate the absorbance and the molar extinction coefficient of tryptophan at 280 nm. What would be the transmittance through a cell of thickness 2 cm ? 2+2+1=5