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

2023

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

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) Which one of the following is not a computer language ?
Python, Java, Rust, GOTO
- (b) Computer can perform arithmetic operations on the data automatically as per set of instructions which is known as _____ (command/language/program).
(Fill in the blank from the given options)
- (c) What is debugging ?
- (d) In a flowchart, what operation is symbolized by a "Rectangle" ?
- (e) What is the method of averages in data analysis ?
- (f) Convert the real number 52.6 to binary.
- (g) Define a string constant.

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

(a) Write the expanded forms of the following :

QBASIC, ROM, End, LCD

(b) What is the application of REM statement ?

(c) What is a time dependent differential equation ? Which one of the following includes a time dependent differential equation ?

Chemical Reactions (evolution of concentrations with time); Vibrational frequencies

(d) What is interpolation of data analysis ?

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

(a) Identify the errors in the following constants:

(i) "MO-theory"

(ii) "X+Y"

(iii) 453R7

(b) Describe the different types of operators used in C-language with examples.

(c) Write the output of the following :

```
10 SCREEN 1
20 WINDOW(0,0) - (50, 50)
30 PSET (30,40)
40 LINE (0,0)-(10,10)
50 END
```

(d) Differentiate between the following :

- (i) RAM and ROM
- (ii) Low level language and High level language

(e) Write a BASIC program for determination of electronegativity or bond length.

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

- (a) (i) What are the basic components of a digital computer? Briefly describe their functions. 6
- (ii) Mention **any four** applications of computers in chemistry. 4

(b) (i) Write a BASIC program to calculate pH of acidic, basic and neutral solution. 6

(ii) For the vapor-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 represents mole fraction of benzene in liquid and vapor, 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 points on such a graph by the method of averages.

4

(c) Write a BASIC program to calculate the following :

$$u_{av} = \sqrt{\frac{8RT}{\pi M}} \quad \text{and} \quad u_{ms} = \sqrt{\frac{2RT}{M}}$$

For various gases, $R = 8.314$, $T = 350$,
 $M = 32 \times 10^{-4}$

- (d) (i) Explain the functions of the following keywords : 4

PSET, GOSUB, DIM, LET

- (ii) For any weak acid like acetic acid when C is the concentration and α is the degree of ionization of acid, the K_a value can be predicted on the basis of Ostwald's dilution law as

$$K_a = \frac{C\alpha^2}{(1-\alpha)}$$

Write a BASIC program for computation of K_a of this acid. 6

- (e) Write a program in BASIC to find the value of Mean, Variance, and Standard Deviation of a set of N numbers. Provide the data using Input statement :

$$\text{Mean} = 1/N \sum X_i$$

$$\text{Variance} = 1/N \sum (X_i - \bar{X})^2$$

$$\text{Standard Deviation} = (\text{Variance})^{1/2}$$

- (f) Write a program in BASIC to find the root of the following equation using Iterative method or Newton Raphson method.

$$X^5 - 6X^2 + 8 = 0$$

Or

Draw a flow chart 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

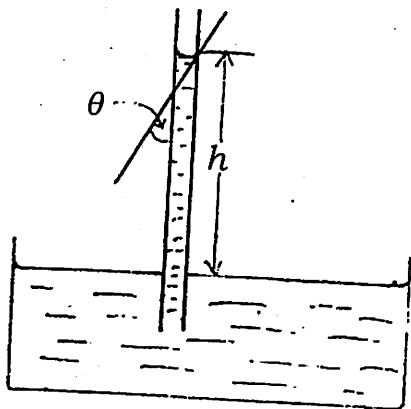
- (g) (i) Explain the different features of the chemistry software ChemDraw and its applications. 6
- (ii) Write a BASIC program to calculate the pressure required to compress O_2 gas to a density of 0.4 g/cm^3 at 10°C . 4

- (h) Make a flowchart to calculate the value of surface tension of a liquid on the basis of capillary action as per the given expression.

For capillary action

$$\gamma = \frac{r h \rho g}{2 \cos \theta}$$

where r is the radius of capillary, h is the height, ρ is the density of the liquid, g is the acceleration due to gravity and θ is the angle that the liquid makes with the walls of capillary.



OPTION-B

(Analytical Method in Chemistry)

Paper : CHE-HE-5026

1. Answer the following questions : $1 \times 7 = 7$
- (a) What is the applicability of Q-test in data analysis ?
 - (b) Why quartz cuvettes are used for UV-visible spectroscopy ?
 - (c) What is the mid-IR wavelength range ?
 - (d) Why is atomic absorption spectroscopy (AAS) more sensitive than atomic emission spectroscopy ?
 - (e) State *true or false* :
Thermal analysis gives information about changes in material properties as function of temperature.
 - (f) How does the change in temperature affect the end-point of conductometric titration ?

(g) Give an example of chelating agent used in solvent extraction process.

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

- (a) The mean of four determinations of the copper content of a sample of an alloy was 8.27% with a standard deviation 0.17%. Calculate the 95% confidence limit for the true value. Given, from the *t*-tables, the value of *t* for the 95% confidence level with three degrees of freedom is 3.18.
- (b) What are the limitations of Beer-Lambert's law?
- (c) What is Potentiometry? Mention *one* application of potentiometry.
- (d) Mention *two* advantages of thin layer chromatography (TLC) over paper and column chromatography.

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

$5 \times 3 = 15$

- (a) Discuss with an example how the strength of an acid can be determined by pH metric titration against a standard base.
- (b) A mixture of CaO and CaCO_3 is analysed by TGA. The result indicates that mass of the sample decreases from 250.6 mg to 190.8 mg only between 600°C and 900°C . Calculate the percentage of calcium carbonate in the mixture.
- (c) Discuss how Job's method of continuous variation can be used to determine the composition of the Ferric-thiocyanate complex.

(d) Analyses 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.

$$1+2+2=5$$

(e) What are the different techniques used in solvent extraction ? Elaborate *any one* of the techniques.

$$1+4=5$$

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

$$10 \times 3 = 30$$

(a) (i) Discuss how thermogravimetric analysis (TGA) can be utilized for the quantitative estimation of calcium (Ca) and magnesium (Mg) from a mixture of CaCO_3 and MgCO_3 .

5

(ii) Discuss the principle of colorimetric estimation of metal ions from aqueous solution. 5

(b) (i) Discuss the effect of temperature, nature of ions, concentration of ions and size of the electrodes on the conductance of a solution. 5

(ii) Discuss with an example how pK_a of an acid can be determined by electroanalytical methods. 5

(c) (i) What are the advantages of Fourier-Transform Infrared spectrometer over dispersive Infrared spectrometer ? 2

(ii) Vibrational frequency of HCl molecule is found at 2885 cm^{-1} . If the hydrogen atom of this molecule is substituted with deuterium, what will be the vibrational frequency of the molecule ? 2

(iii) How can we differentiate primary, secondary and tertiary amines using IR spectroscopy ? 2

- (iv) What is the effect and importance of isotopic substitution in IR spectroscopy? 2
- (v) What is the fingerprint region in IR spectroscopy? Why it is called so? 1+1=2
- (d) (i) 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
- (ii) What is the purpose of monochromator and nebulizer in Inductively coupled plasma atomic emission spectroscopy (ICP-AES)? What are the advantages of ICP-AES over AAS? 3+2=5
- (e) (i) What is meant by development of a chromatogram? Discuss the different methods used for development of a chromatogram. 1+6=7

- (ii) A sample of S-(+) enantiomer of a compound has an observed rotation of $+19.2^\circ$. If the specific rotation of the pure enantiomer is $+24^\circ$ then what is the optical purity of the sample? What is the composition of the mixture? 3

- (f) (i) Discuss the principle of conductometric titration for the determination of equivalence points of acid-base reaction. 5
- (ii) What is a chiral shift reagent? Discuss its role in NMR spectroscopy with a suitable example. 1+4=5