Total number of printed pages–16

3 (Sem–5/CBCS) CHE RE 1/RE2/RE3

2021

(Held in 2022)

CHEMISTRY

(Regular Elective)

OPTION – A

Paper : CHE–RE–5016

(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 are data processing operations ?

   (b) What is interpolation method ?

   (c) How many bits make a byte ?

   (d) What is variable ?

   (e) What is keyword ?

   (f) What is a string constant ?

   (g) What is iterative method ?

Contd.

2. Answer ***all*** questions : 2×4=8

(a) What are library functions ? Give example.

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

(c) What are structured programming and debugging ?

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

(i) Chemical reaction (evolution of concentrations with time)

(ii) Vibrational frequencies.

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 odd numbers less than 500.

(b) Describe the different types of operators with examples in BASIC language.

(c) Write a BASIC program to find the smallest of three input numbers.

(d) Write a BASIC program to find average of n input numbers.

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

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

(a) Explain Newton-Raphson 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 vapor pressure of liquid acetonitrile (CH_3CN) at three temperatures are :

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

Estimate the vapor pressure at 280.15K using *(i)* linear interpolation *(ii)* quadratic interpolation.

(d) Explain the functions of following BASIC statements with examples : *(any two)*

(i) DEF

(ii) CALL

(iii) SUB

(e) Write a BASIC program to fit a straight line for the following data relating the enthalpy of methane at 1 *atm* pressure with temperature :

Enthalpy (*Btu/lb*)	630	650	824	851	875	1050	1110	1200
Temperature (°*F*)	−200	−100	0	100	200	300	400	500

(f) What are interpolation and extrapolation ? Explain.

OPTION – B

CHE–RE–5026

(Analytical Method in Chemistry)

Full Marks : 60

Time : Three hours

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

Answer ***either*** *in English* ***or*** *in Assamese.*

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

নির্দেশ অনুসৰি তলৰ প্ৰশ্নবোৰৰ উত্তৰ দিয়া ঃ

(a) What is chiral shift reagent ?

কাইৰেল স্থানান্তৰ বিকাৰক কি?

(b) Why are quartz cuvettes used for UV-visible spectroscopy ?

UV-ভিজিবল্ স্পেক্ট্ৰ'স্কোপিত কিয় কোৱার্ট্য কিউৱেট ব্যৱহাৰ কৰা হয়?

(c) What is the relationship between wavelength and wavenumber ?

তৰংগদৈর্ঘ্য আৰু তৰংগসংখ্যাৰ মাজত সম্পৰ্ক কি?

(d) What is the stationary phase in chromatography ?

ক্ৰমেট'গ্ৰাফীত ষ্টেচনাৰী ফেজ বুলিলে কি বুজা?

(e) Which instrument is used to convert sample in mist or aerosol ?

(i) Atomizer

(ii) Hollow cathode lamps

(iii) Nebulizer

(iv) Detector

(Choose the correct answer)

নমুনা এটাক কুহেলিকা বা এৰ'চললৈ ৰূপান্তৰ কৰিবলৈ কোনটো যন্ত্ৰ ব্যৱহাৰ কৰা হয়?

(i) এট'মাইজাৰ

(ii) হ'ল কেথড্ লেম্প

(iii) নেবুলাইজাৰ

(iv) সংসূচক

(শুদ্ধ উত্তৰটো বাছি উলিওৱা)

(f) What is the unit of specific conductance ?
নির্দিষ্ট পৰিবাহিতাৰ একক কি?

(g) What is the applicability of Q-test in data analysis ?
তথ্য বিশ্লেষণত Q-টেষ্টৰ প্রয়োজনীয়তা কি?

2. Answer ***any four*** of the following questions : 2×4=8

তলৰ *যিকোনো চাৰিটা* প্রশ্নৰ উত্তৰ লিখা ঃ

(a) If the diatomic molecule HCl, with ^{1}H and ^{35}Cl were substituted with ^{37}Cl, what change occurs to the reduced mass ?

(d) (i) Define confidence interval. 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. The value of t for the 95% confidence level with three degrees of freedom is 3.18. 2+3=5

কনফিডেনচ্ ইনটাৰভেলৰ সংজ্ঞা দিয়া। এটা সংকৰ ধাতুৰ নমুনাত থকা কপাৰৰ পৰিমাণৰ চাৰিটা নিৰ্ণয়ৰ মধ্যমা হ'ল 8.27% আৰু প্ৰামাণিক বিচ্যুতি হ'ল 0.17%। শুদ্ধ উত্তৰৰ 95% কনফিডেনচ্ লিমিত নিৰ্ণয় কৰা। তিনিটা ডিগ্ৰীচ্ অফ্ ফ্ৰিডমৰ সৈতে 95% কনফিডেনচ্ লেভেলৰ বাৰে t ৰ মান হ'ল 3.18।

(ii) What is the basic principle of atomic absorption spectroscopy ? What are the different atomization processes commonly employed in the atomic absorption spectroscopy (AAS) ? 5

এট'মিক এবযৰ্বছন স্পেক্ট্ৰ'স্কোপীৰ মৌলিক কাৰ্যনীতি কি? এট'মিক এবযৰ্বছন স্পেক্ট্ৰ'স্কোপীত সাধাৰণতে কি কি এট'মাইজেছন প্ৰক্ৰিয়া ব্যৱহাৰ কৰা হয়?

(e) (i) Discuss the factors on which conductance of a solution depends. 5

এটা দ্রৱৰ পৰিবাহীতা নির্ভৰ কৰা কাৰকবোৰ আলোচনা কৰা।

(ii) Discuss the principle used in HPLC. 5

HPLC ত ব্যৱহাৰ হোৱা কার্য্যনীতি আলোচনা কৰা।

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

প্রামাণিক ক্ষাৰক এটা ব্যৱহাৰ কৰি pH মেট্রিক টাইট্রেছন পদ্ধতিৰে অম্ল এটা গাঢ়তা কেনেদৰে নিৰূপণ কৰা হয়? আলোচনা কৰা।

(ii) Discuss the application of ion exchange chromatography with an example. 5

উদাহৰণসহ আয়ন বিনিময় ক্রমেট'গ্রাফীৰ প্রয়োগ আলোচনা কৰা।

OPTION - C

CHE-RE-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 : 2×4=8

(a) Describe briefly the Born-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 : 5×3=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=5

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

4. Answer ***any three*** questions from the 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) : 5+5=10

(i) *ab initio* molecular orbital methods

(ii) Semiempirical molecular orbital methods.

(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
