B.Sc./6th Sem (G)/CHEM/23(CBCS)

2023

6th Semester Examination

CHEMISTRY (General)

Paper : DSE 1B/2B/3B-T

[CBCS]

Full Marks : 40 Time : Two Hours

The figures in the margin indicate full marks.
Candidates are required to give their answers in their own words as far as practicable.

[Applications of Computers in Chemistry]

Group - A

Answer any ***five*** questions : 2×5=10

1. Write this mathematical expression in any computer Language :

$$\sec^2 x - \text{cosec}^2 x$$

2. "a > = b". What is meant by this command?

3. What is in built functions? Explain with example.

4. Write the importance of the iterative method?

5. What is probability distribution?

6. Write the limitations of extrapolation.

P.T.O.

7. Write the importance of molecular modelling in chemistry.

8. Write the name of two molecular visualization software.

Group - B

Answer any ***four*** questions : 5×4=20

9. (a) How do you convert binary to ASCII? Explain with example. 3

   (b) 5 Bytes equal to how much Bits? 2

10. (a) Write any five fundamental elements of programming? 2

    (b) Write a note on BASIC key words and its functions. 3

11. (a) Write six keywords of any programming language. 2

    (b) How one can include graphics in any programme? 3

12. Explain the procedure of finding roots of a differential equation by using Newton-Raphson method. 5

13. (a) Mention qualitative difference between extrapolation and interpolation of a graph. 3

    (b) Write the importance of curve fitting of a set of experimental data. 2

14. (a) What are the differences between Trapezoidal and Simpson rule of numerical integration? 3

(b) Which method is more accurate between above two methods? Give reason. 2

Group - C

Answer any ***one*** question : 10×1=10

15. (a) Differentiate between logical and relational operations. 3

(b) Write a program for numerical differentiation of F(I). 7

$X(I)$	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
$F(I)$	1.0	1.143	1.173	1.214	1.327	1.431	1.549	1.681	1.802

16. (a) A and B are 25 × 25 matrix. Write a program for multiplication of these matrices. 8

(b) What are the primary criteria of two matrix multiplication? 2

বঙ্গানুবাদ

বিভাগ - ক

যে কোনো পাঁচটি প্রশ্নের উত্তর দাও। ২×৫=১০

১। কম্পিউটার ল্যাঙ্গুয়েজে নিম্নলিখিত অঙ্কটিকে প্রকাশ কর।

$$\sec^2 x - \operatorname{cosec}^2 x$$

P.T.O.

OR

[Green Chemistry]

Group - A

Answer any ***five*** questions : 2×5=10

1. What are bioplastics? Explain with example.
2. What do you mean by supercritical fluids?
3. What do you understand by the term Inherently Safer Design (ISD)?
4. What are immobilized solvents? Give one example.
5. What is synthetic azo-pigment? Give example.
6. Is methane gas a renewable feedstock? Give reason.
7. Mention disadvantages of TBTO as antifoulant.
8. What is trans-fat?

Group - B

Answer any ***four*** questions : 5×4=20

9. How do you prepare DSIDA by MONSONTO's method? What are the advantages of this process?
10. Discuss the importance and mechanism of sonochemical Simmons-Smith Reaction.
11. Synthesize glucose to adipic acid through green route.

P.T.O.

12. Write down the twelve principles of Green Chemistry.

13. Discuss on microwave assisted synthesis of benzoic acid from methyl benzoate.

14. What is rightfit pigment? What are the criteria of rightfit pigments?

Group - C

Answer any ***one*** question : 10×1=10

15. Give the synthetic schemes for the conventional and green synthesis of catechol. What are the advantages of the green synthetic method over the conventional method for the catechol synthesis? What do you mean by cradle to cradle carpeting? 5+3+2

16. What are marine antifoulants or anti-fouling agent? Give one example of environmentally benign antifoulant and draw the structure of its main ingredients. Discuss briefly on 'sonoluminescence'. 2+4+4

বঙ্গানুবাদ

বিভাগ - ক

যে কোনো পাঁচটি প্রশ্নের উত্তর দাও। ২×৫=১০

১। বায়োপ্লাস্টিক কি? উদাহরণসহ ব্যাখ্যা কর।

২। সুপারক্রিটিক্যাল ফ্লুইড বলতে কি বোঝ?

OR

[Industrial Chemicals and Environment]

Group - A

Answer any ***five*** questions : 2×5=10

1. What is chemical oxygen demand?
2. Write down the four reasons of Water Pollution.
3. Write down the difference between Nuclear fission and Nuclear fusion.
4. How metallic Nickel can be purified by Mond's process?
5. Describe the production of acetylene gas in industry.
6. What is Eutrophication?
7. What is biocatalysis? Give example.
8. Describe the method of Industrial waste management.

Group - B

Answer any ***four*** questions : 5×4=20

9. Write an explanatory note on "Global Warming".
10. What are the uses of the following industrial gases :

    (i) Carbon monoxide (ii) Phosgene.
11. Describe the method of water purification by reverse osmosis.

P.T.O.

12. What are major sources of air pollution? How carbon monoxide in air can be estimated?

13. How Tidal and Hydel act as a source of energy — explain.

14. Describe activated sludge process with a sketch.

Group - C

Answer any ***one*** question : 10×1=10

15. (a) What are the hazards in handling the following industrial chemicals : 2½×2

    (i) Potassium Permanganate.

    (ii) Nitric acid.

    (b) Describe briefly on biochemical Nitrogen cycle. 5

16. Write short notes on (any ***two***) : 5×2

    (i) Green house effect.

    (ii) Kroll process.

    (iii) Caustic Soda.

বঙ্গানুবাদ

বিভাগ - ক

যে কোনো পাঁচটি প্রশ্নের উত্তর দাও। ২×৫=১০

১। কেমিক্যাল অক্সিজেন চাহিদা বলতে কি বোঝ?

OR

[Quantum Chemistry, Spectroscopy and Photochemistry]

Group - A

Answer any ***five*** questions : 2×5=10

1. How many nodes are present in 3s and 2p orbitals?
2. State and explain Heisenberg Uncertainty principle.
3. What are the physical significances of wave function ψ if and $|\psi|^2$.
4. Justify the statement that the number of molecular orbitals obtained in LCAO is equal to number of atomic orbitals involved.
5. What is zero point energy in harmonic oscillator?
6. On the basis of Einstein law, justify: Whether quantum yield may be greater or less than 1.
7. Explain Larmor frequency in NMR.
8. What is the unit of molar extinction coefficient and absorbance?

Group - B

Answer any ***four*** questions : 5×4=20

9. Write down the Schrödinger wave equation for particle

P.T.O.

in 1D box. How can this equation be solved for wave function (ψ) and energy (E)? 2+3

10. (a) What do you understand by (i) bonding (ii) nonbonding and (iii) anti-bonding orbitals?

    (b) What is a rigid rotator model ? 3+2

11. (a) Explain Franck-Condon principle.

    (b) Why is the phosphorescence lifetime greater than fluorescence lifetime? 3+2

12. (a) Describe the symmetric top, spherical top and asymmetric top molecules with examples.

    (b) The first line in the rotational spectra of CO has a frequency 3.842 cm^{-1}. Calculate the moment of inertia. 3+2

13. (a) What are hot bands?

    (b) The fundamental vibrational frequency of HCl is 2989 cm^{-1}. Find the force constant of HCl. 2+3

14. (a) Why anti-Stokes lines are less intense than Stokes lines in Raman scattering?

    (b) Explain the principle of ESR. 2+3

Group - C

Answer any ***one*** question : 10×1=10

15. (a) State and explain the postulates of quantum mechanics.

(b) Write down the Schrödinger wave equation.

(c) Show graphically the number of node(s) present in 1s and 2s orbital by plotting radial distribution function $4\pi r^2 |R|^2 dr$ against the radius.

(d) Draw the molecular orbitals formed by the linear combination of atomic orbitals (i) 2s-2s (ii) $2p_x$-$2p_x$ (iii) $2p_z$-$2p_z$. 3+2+2+3

16. (a) Explain chemical shift in NMR spectra with examples.

(b) Name two NMR solvents.

(c) Write notes on (i) Fluorescence (ii) Phosphorescence

(d) What is photosensitized reaction? Discuss its utility with a suitable example. 2+2+3+3

বঙ্গানুবাদ

বিভাগ - ক

যে কোনো পাঁচটি প্রশ্নের উত্তর দাও। ২×৫=১০

১। 3s এবং 2p অরবিটালে কয়টি করে নোড রয়েছে?

২। হাইজেনবার্গ অনিশ্চয়তা নীতির বর্ণনা কর এবং ব্যাখ্যা কর।

৩। তরঙ্গ ফাংশন ψ এবং $|\psi|^2$-এর তাৎপর্য কি?

P.T.O.

OR

[Molecular Modeling and Drug Design]

Group - A

Answer any ***five*** questions : 2×5=10

1. What is molecular modeling?
2. What are the forces involved in drug receptor interaction?
3. What do you mean by receptor?
4. What is energy minimization in molecular docking?
5. What is Monte Carlo simulation?
6. Discuss briefly the receptor polymorphism and dimerization.
7. What do you mean by molecular graphics?
8. Explain how ion channels act as drug targets.

Group - B

Answer any ***four*** questions : 5×4=20

9. Write a note on QSAR.
10. Discuss the principles involved in the design of pro-drug.
11. What are the basic steps of molecular docking?
12. Discuss on isosterism in relation to biological action and drug design.

P.T.O.

13. Write the principles of computer aided drug design.

14. How does Metropolis algorithm work?

Group - C

Answer any ***one*** question : $10\times1=10$

15. How computer aided drug design is useful in new drug discovery and development?

16. What is Molecular Dynamics? Discuss its applications.

বঙ্গানুবাদ

বিভাগ - ক

যে কোনো **পাঁচটি** প্রশ্নের উত্তর দাও। ২×৫=১০

১। আণবিক মডেলিং কি?

২। ড্রাগ-রিসেপ্টর মিথস্ক্রিয়া-এর জন্য কি কি বল জড়িত?

৩। রিসেপ্টর বলতে কি বোঝ?

৪। আণবিক ডকিং-এ শক্তির লঘিষ্টকরণ বলতে কি বোঝ?

৫। মন্টে কার্লো সিমুলেশন কি?

৬। রিসেপ্টর বহুরূপতা এবং দ্বিমাত্রিকরণ-এর উপর সংক্ষেপে আলোচনা কর।

৭। আণবিক গ্রাফিক্স বলতে কি বোঝ?