

# Tata Institute of Fundamental Research

Answers for Chemistry GS2025 Written Examination

Examination Date: 08 December 2024

(The correct answers are highlighted in yellow)

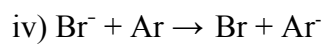
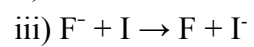
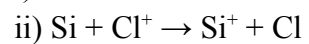
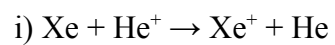
1. The energy of a  $K_{\alpha}$  X-ray from an element having atomic number  $Z$  is:

$$E(K_{\alpha}) = (10.2 \text{ eV})(Z - 1)^2$$

Which element has a  $K_{\alpha}$  X-ray line with a wavelength of 0.180 nm?

- A) Ti ( $Z = 22$ )
- B) Co ( $Z = 27$ )**
- C) Zn ( $Z = 30$ )
- D) Cu ( $Z = 29$ )

2. Which of these reactions are spontaneous in gas phase?



A) iii and iv

**B) i and ii**

C) i, ii and iv

D) only ii

3. Atomic nuclear diameter is approximately 5 femtometer. What would be the approximate velocity of an electron, if it was part of a nucleus with the weight of the electron being  $9.109 \times 10^{-31}$  kg?

(Note:  $c$  = velocity of light in vacuum)

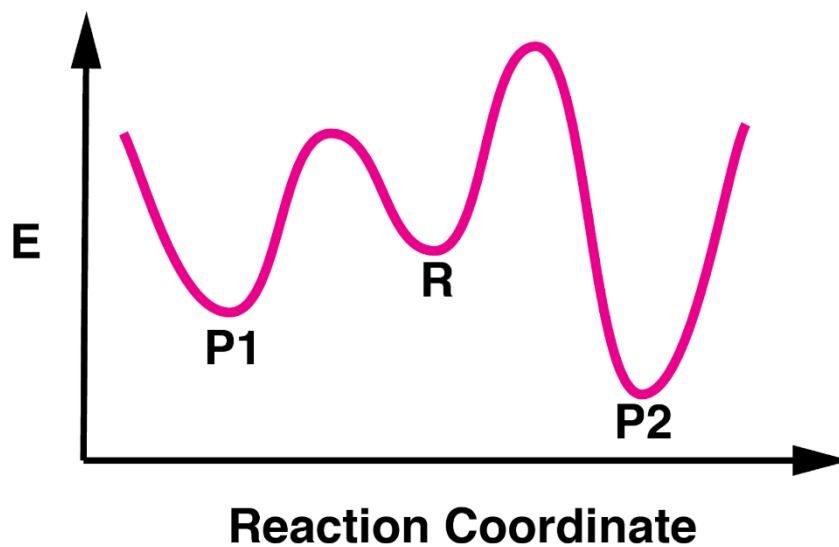
A)  $40 c$

B)  $c$

C)  $c/20$

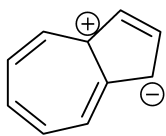
D)  $2 c$

4. The reactant (R) can convert into products P1 or P2 as can be seen in reaction profile shown below. If you want R to be converted mostly into P1 you will:

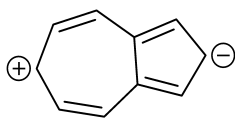


- A) Carry out the reaction at low temperature so that P1 is the major product for thermodynamic reasons.
- B) Carry out the reaction at low temperature (in a limited time) so that P1 is the major product for kinetic reasons.
- C) Carry out the reaction at high temperature so that P1 is the major product for thermodynamic reasons.
- D) Carry out the reaction at high temperature (in a limited time) so that P1 is the major product for kinetic reasons.

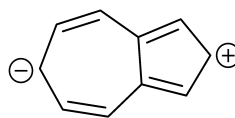
5. Among the resonance forms given below, which one is the most stable one?



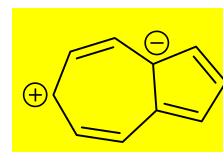
A)



B)

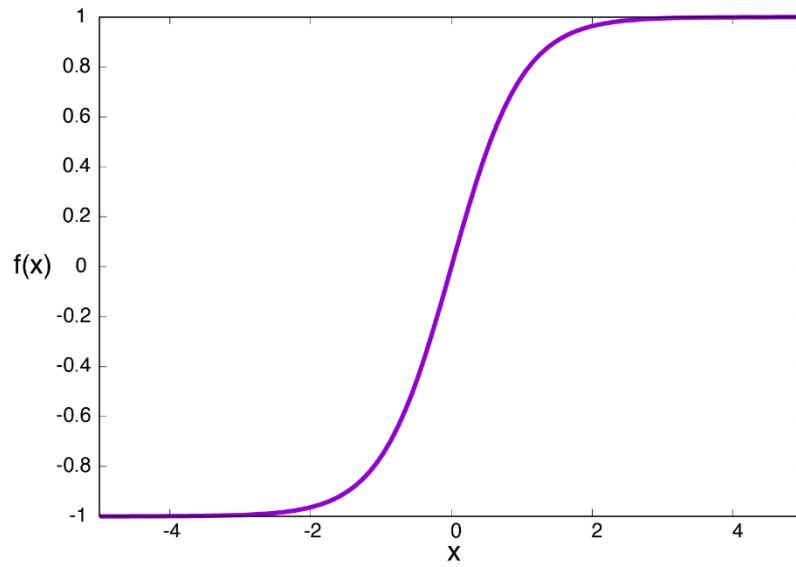


C)



D)

6) Which of functions best represents the graph shown here:



A)  $\left(\frac{e^x - e^{-x}}{e^x + e^{-x}}\right)$

B)  $\left(\frac{1}{1 + e^{-x}}\right)$

C)  $\left(\frac{e^{-x} - e^x}{e^x + e^{-x}}\right)$

D)  $\left(\frac{e^x}{e^x + 1}\right)$

7. The derivative of  $s(x) = \left(\frac{1}{1+e^{-x}}\right)$  (with respect to  $x$ ) is:

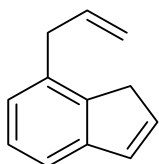
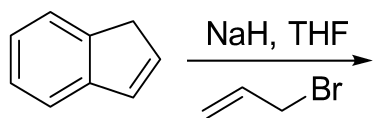
A)  $s(x)$

B)  $1 - s(x)$

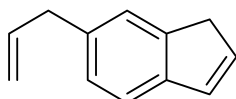
C)  $(1 - s(x))s(x)$

D)  $\left(\frac{1}{1-s(x)}\right)$

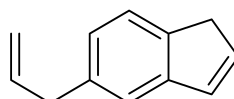
8. Predict the major product from the following reaction.



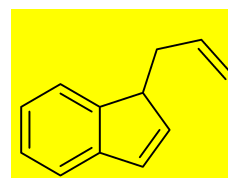
A)



B)



C)



D)



9. Equation of state of a system in canonical ensemble (N, V,  $\beta$ ) is given by:

(N is the number of particles, V is the volume, T is the temperature, Q is the partition function,  $\beta = 1/(k_B T)$ , and  $\langle P \rangle$  means the ensemble average of pressure)

$$\text{A) } \langle P \rangle = \frac{1}{\beta} \left( \frac{\delta \ln Q}{\delta V} \right)_{N, \beta}$$

$$\text{B) } \langle P \rangle = \frac{1}{V} \left( \frac{\delta \ln Q}{\delta \beta} \right)_{N, V}$$

$$\text{C) } \langle P \rangle = \frac{1}{V^2} \left( \frac{\delta \ln Q}{\delta \beta} \right)_{N, V}$$

$$\text{D) } \langle P \rangle = \frac{1}{\beta^2} \left( \frac{\delta \ln Q}{\delta V} \right)_{N, \beta}$$

10. The number of stereoisomer(s) of  $\text{trans-}[\text{CoCl}_2(\text{triethylenetetramine})]\text{Br}$  is(are)

- A) One      B) Two      C) Three      D) Four

11. Ensemble average of Gibbs entropy ( $\langle S \rangle$ ) is given by:

$$\text{A) } \langle S \rangle = -k_B \sum_k P_k \ln P_k$$

$$\text{B) } \langle S \rangle = k_B \sum_k P_k \ln P_k$$

$$\text{C) } \langle S \rangle = k_B P_k \exp(P_k)$$

$$\text{D) } \langle S \rangle = k_B P_k \exp(-P_k)$$

$k_B$  is Boltzmann constant and  $P_k$  is probability of occurrence of state  $k$  with energy  $E_k$

12. Energy of a free electron plotted as a function of its momentum will be:

- A) Hyperbolic
- B) Oscillatory
- C) **Parabolic**
- D) Linear

13. The catalyst involved in carrying out the cross metathesis of 1-butene to give ethylene and 3-hexene is:

- A)  $\text{RuCl}_2(\text{=CHPh})(\text{PCy}_3)_2$  (Cy is cyclohexyl)
- B)  $\text{Na}_2\text{PdCl}_4$
- C)  $\text{Co}_2(\text{CO})_8, \text{H}_2$
- D)  $\text{RhCl}(\text{PPh}_3)_3$

14. Ultimate spatial resolution of a microscope is related to the wavelength of the probe beam as:

- A)  $\lambda$
- B)  $1/\lambda$
- C)  $\lambda^2$
- D)  $(\lambda)^{1/2}$

15. Regarding the metal complexes  $[\text{Co}(\text{NH}_3)_6]^{3+}$  and  $[\text{Co}(\text{en})_3]^{3+}$  (en = ethylene diamine), which of the following is true?

- A) Both complexes have the same stability
- B) Stability of  $[\text{Co}(\text{NH}_3)_6]^{3+}$  is higher than  $[\text{Co}(\text{en})_3]^{3+}$
- C) Stability of  $[\text{Co}(\text{NH}_3)_6]^{3+}$  is lower than  $[\text{Co}(\text{en})_3]^{3+}$
- D) No conclusion can be made regarding the stability of the complexes

16. In a spectroscopic measurement it is found that the spectrum is broadened with Doppler broadening having the dominant contribution. Which of the following functions will best represent this spectral lineshape  $f(\nu - \nu_0)$ ?

( $\nu_0$  is the resonance frequency of the corresponding spectroscopic transition)

A)  $\exp[-k(\nu - \nu_0)]$ ;  $k$  is a constant

B)  $1/[A^2 - (\nu - \nu_0)^2]$ ;  $A$  is a constant

C)  $\exp[-a(\nu - \nu_0)^2]$ ;  $a$  is a constant

D)  $(\nu - \nu_0)^2$



17. Consider the square planar platinum (II) complex  $[\text{Pt}(\text{Py})(\text{NH}_3)(\text{Cl})(\text{NO}_2)]$ , where Py is pyridine. Based on the given facts:

1. The trans effect order:  $\text{NO}_2^- > \text{Cl}^- > \text{Py} > \text{NH}_3$
2.  $^{15}\text{N}$  NMR chemical shift of coordinated  $\text{NH}_3$ :  $\delta = -70$  ppm
3.  $^{15}\text{N}$  NMR chemical shift of coordinated  $\text{NO}_2$ :  $\delta = +140$  ppm (when N-bonded),  $\delta = -20$  ppm (when O-bonded)

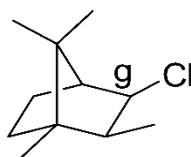
Which of the following statements is correct?

- A) The major product of the reaction of this complex with excess  $\text{NH}_3$  will have  $\text{Cl}^-$  trans to  $\text{NH}_3$ .
- B) The  $^{15}\text{N}$  NMR spectrum of the complex will show two signals: one at  $-70$  ppm and another at  $+140$  ppm.
- C) The complex is optically active.
- D) Treating the complex with  $\text{AgNO}_3$  will result in immediate and complete precipitation of  $\text{AgCl}$ .

18. A solution of two non-interacting metal complexes, X and Y, are taken in a cuvette with path length of 1 cm. The concentration of X is one micromolar ( $1 \mu\text{M}$ ) and the concentration of Y is two micromolar ( $2 \mu\text{M}$ ). The molar extinction coefficients for complexes X and Y at 500 nm are  $\epsilon_X = 1 \times 10^5 \text{ M}^{-1} \text{ cm}^{-1}$  and  $\epsilon_Y = 2 \times 10^5 \text{ M}^{-1} \text{ cm}^{-1}$ , respectively. The absorbance of the solution at 500 nm is:

- A) 1
- B) 0.3
- C) 0.4
- D) 0.5

19. Predict the approximate chemical shift and multiplicity of the  $^1\text{H}$ -NMR peak for the proton at position 'g' marked in the structure shown below.



- A) 3 ppm and double-doublet
- B) 3 ppm and triplet
- C) 5.5 ppm and double-doublet
- D) 5.5 ppm and triplet

20. How many vibrational and rotational degrees of freedom does the following molecule have?



- A) 30, 2
- B) 12, 3
- C) 30, 3
- D) 12, 2

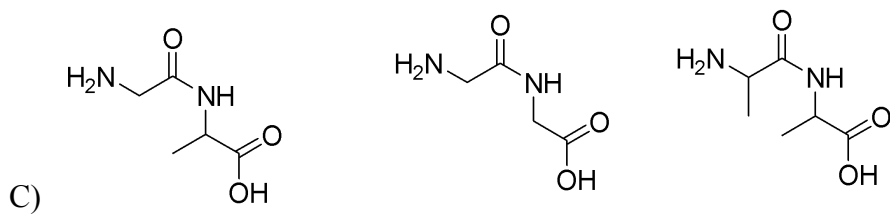
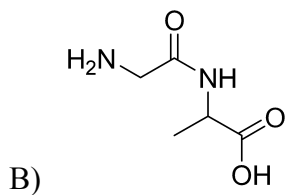
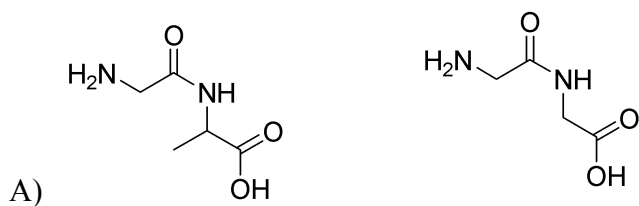
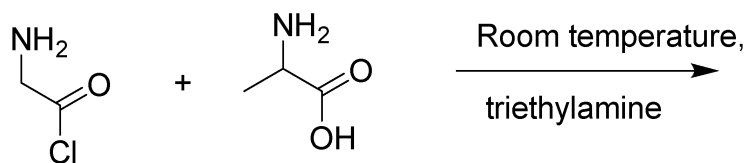
21. A protein chain with even a modest number of amino acids can theoretically fold into an astronomically large number of different conformations. If a protein were to explore each possible conformation sequentially, even at an incredibly fast rate, it would take far longer than the age of the universe to reach its native, functional state. However, consider the following simple theoretical model for protein folding:

- i) The protein is made up of only 10 amino acids
- ii) Each amino acid can exist in one of two states: one correctly and one incorrectly folded
- iii) In each second, one amino acid is randomly chosen
- iv) If the amino acid is in the incorrectly folded state, it switches to the correctly folded state
- v) If the amino acid is in the correctly folded state, nothing happens during that second

Starting from all amino acids in the incorrectly folded state, approximately how long will it take on an average for such a protein to fold correctly?

- A) 10 seconds
- B) 30 seconds**
- C) 30 minutes
- D) 30 hours

22. What would you obtain if you tried the following coupling reaction in a laboratory setting?



D) Mixture of polymers

23. The  $\Delta G^\circ$  (at 300 K) for the hydrolysis of ATP ( $\text{ATP} \rightarrow \text{ADP} + \text{phosphate}$ ) is  $-28 \text{ kJ/mole}$ . In cellular cytoplasm, the concentration of ATP, ADP, and phosphate are buffered at  $10 \text{ mM}$ ,  $10 \text{ }\mu\text{M}$  and  $10 \text{ mM}$ , respectively. This ATP hydrolysis is coupled to an enzymatic reaction (R) that has a  $\Delta G$  of  $+112 \text{ kJ/mol}$  in absence of the enzyme. What is the minimum number of molecules of ATP which must be hydrolyzed in order to have a thermodynamically favorable net reaction (ATP hydrolysis + R)?

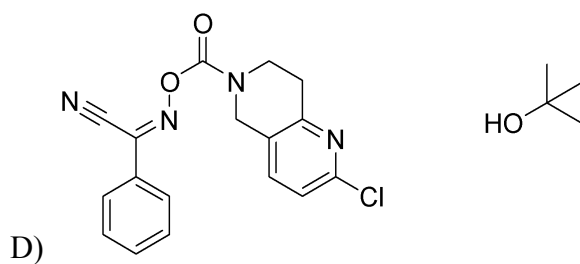
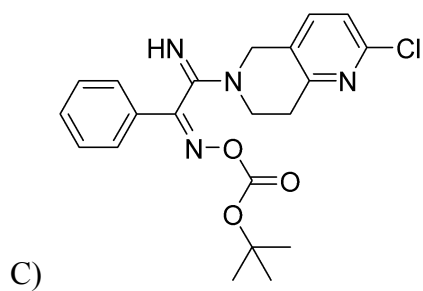
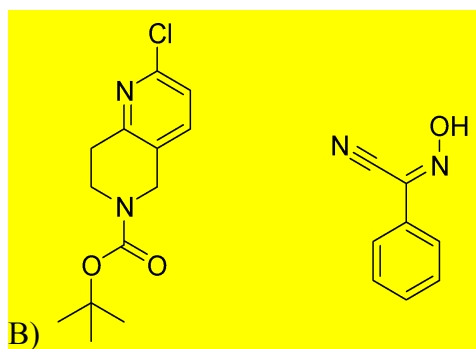
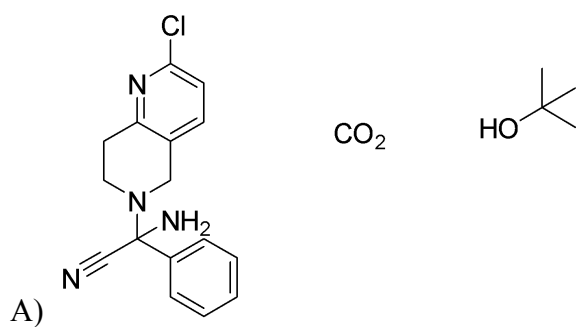
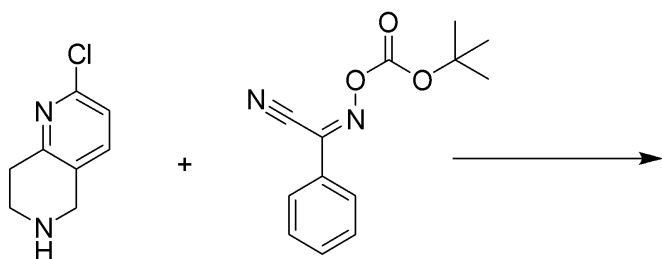
- A) 1
- B) 2**
- C) 4
- D) Cannot be determined from the given data

24. Imagine that a system is in a state  $|\alpha\rangle$ . An observation is made on this system, where the operator is represented by  $\hat{A}$  and the final state is  $|f\rangle$ . The eigenstates of  $\hat{A}$  are represented by  $\{|a_i\rangle\}$ . Which of the following statements is true?

- A) The probability of obtaining  $|a_i\rangle$  as  $|f\rangle$  is  $|\langle\alpha\rangle|^2$
- B) The probability of obtaining  $|a_i\rangle$  as  $|f\rangle$  is  $|\sum_i \langle\alpha\rangle|^2$
- C) The probability of obtaining  $|a_i\rangle$  as  $|f\rangle$  is  $|\langle\alpha\rangle|$
- D)  $|f\rangle$  can be different from any of  $\{|a_i\rangle\}$



25. Predict the product of the following reaction.



26. Consider the quantum mechanical problem of a particle inside a 1-dimensional box where the height of the well can be either infinite or finite ( $V_0 < \infty$ ). Which of the following statement is correct?

- A) All the eigenstates of the infinitely high box are lower in energy than the corresponding states in the finite counterpart
- B) All the eigenstates of the infinitely high box are higher in energy than the corresponding states in the finite counterpart
- C) The eigenfunctions are different but the energies remain the same
- D) The eigenstates can be higher or lower depending on the height of the well

27. Consider the quantum mechanical problem of a particle inside a 1-D box with infinitely high walls. Which of the following statements is correct?

- A) There is a well-defined kinetic energy,  $E_n^{kin}$ , associated with each state and hence, there is also definite momentum,  $p_n$ , since, classically,  $E^{kin} = p^2/(2m)$
- B) The standard deviation of momentum in the  $n^{th}$  state is  $2\sqrt{mE_n}$ , where  $E_n$  is the energy in the  $n^{th}$  eigenstate
- C) The expectation value of momentum in each state is positive
- D) The standard deviation of momentum in the  $n^{th}$  state is  $\sqrt{2mE_n}$ , where  $E_n$  is the energy in the  $n^{th}$  eigenstate

28. The iodine test gives a blue color due to

A) Starch –  $I_2$  complex

B) Presence of  $I_3^-$

C) Decomposition of starch

D) Starch –  $I_3^-$  complex

29. For a system with  $N$  indistinguishable particles and a normalized wavefunction  $\psi$ , the probability of finding a single particle at position  $r_1$  is given as,

$$P(r_1) = N \int dr_2 dr_3 \dots dr_N |\psi(r_1 r_2 \dots r_N)|^2$$

such that the integral over  $P$  reduces to the number of particles, i.e.  $\int P(r_1) dr_1 = N$ . In a similar fashion, how would you define the probability of finding two particles, one at position  $r_1$  and the other at  $r_2$ .

A)  $G(r_1, r_2) = N \int dr_3 \dots dr_N |\psi(r_1 r_2 r_3 \dots r_N)|^2$

B)  $G(r_1, r_2) = N(N - 1)/2 \int dr_3 \dots dr_N |\psi(r_1 r_2 r_3 \dots r_N)|^2$

C)  $G(r_1, r_2) = N(N - 1) \int dr_3 \dots dr_N |\psi(r_1 r_2 r_3 \dots r_N)|^2$

D)  $G(r_1, r_2) = P(r_1) \times P(r_2)$

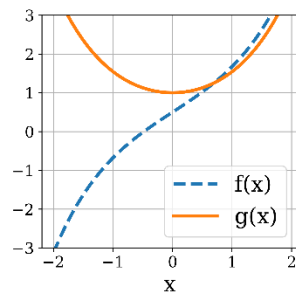
30. Consider the following functions:

$$f(x) = \frac{e^x - e^{-x}}{2}$$

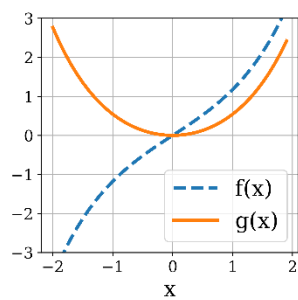
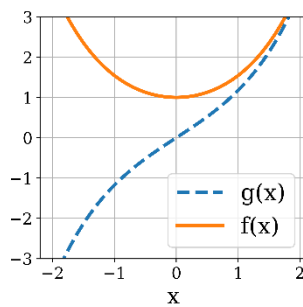
$$g(x) = \frac{e^x + e^{-x}}{2}$$

Which of the plots shown below correctly represents the above functions?

A)

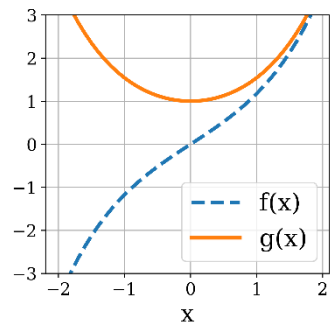


B)



C)

D)



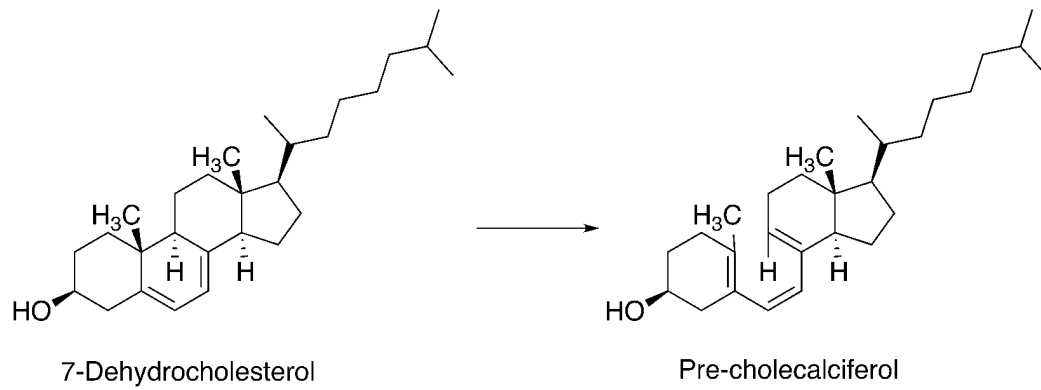
Correct Answer: D

31. A typical lithium-ion battery (4 Volt output) in a phone, powered using a 5-Watt charger can fully charge in 1.5 hours. While using the phone if the average current drawn is 50 mA and a with a single charging the phone runs for about 20 hours after which the battery fully drains, which of the following is a reasonable estimate of the efficiency of the phone battery? (efficiency = output power delivered / power consumed in charging)

- A) 74%
- B) 23%
- C) 53%
- D) 84%



32. Vitamin D3 precursor pre-cholecalciferol is produced from 7-dehydrocholesterol. Predict the reaction condition used for the transformation.



- A) acid
- B) base
- C) heat
- D) light**

33. D<sub>2</sub>O is heated using an electric heater in contact with it under a pressure of 1.0 atm such that it boils. When an electric current of 0.8 A from a 10 V supply is passed for 210 seconds it is observed that 0.8 g of D<sub>2</sub>O is vaporized. Which of the following values of molar enthalpy and molar internal energy changes at the boiling point (374 K) are correct?

A)  $\Delta H_m = +42 \text{ kJ/mol}$ ,  $\Delta U_m = +39 \text{ kJ/mol}$

B)  $\Delta H_m = +11 \text{ kJ/mol}$ ,  $\Delta U_m = 0 \text{ kJ/mol}$

C)  $\Delta H_m = +39 \text{ kJ/mol}$ ,  $\Delta U_m = +42 \text{ kJ/mol}$

D)  $\Delta H_m = -42 \text{ kJ/mol}$ ,  $\Delta U_m = -39 \text{ kJ/mol}$

34. Ground state wavefunction of the hydrogen atom can be written in the following form:

$$\psi(r) \propto \exp(-r/a_0)$$

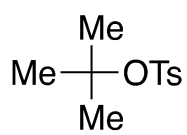
And that for He<sup>+</sup> ion can be written as:

$$\Phi(r) \propto \exp(-2r/a_0)$$

What is the ratio of probabilities (expressed in percentage) of finding the electron in a small volume shaped as a cube with dimensions  $1 \times 10^{-12}$  m at  $r = a_0$  and at the nucleus for both cases?

- A) H-atom: 36%, He<sup>+</sup> ion: 5%
- B) H-atom: 23%, He<sup>+</sup> ion: 8%
- C) H-atom: 14%, He<sup>+</sup> ion: 2%
- D) H-atom: 11%, He<sup>+</sup> ion: 14 %

35. Arrange the following molecules in decreasing rate of solvolysis.



**A**



**B**



**C**

A) A > B > C

B) B > C > A

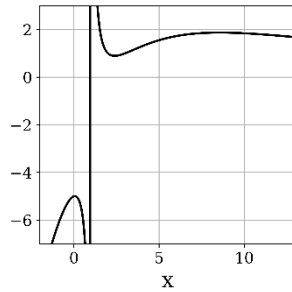
C) C > A > B

D) C > B > A

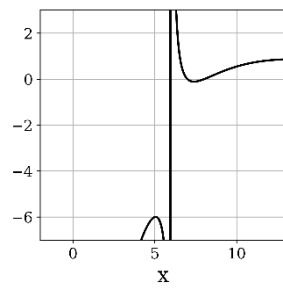
36. Which of the following plots correctly represents the function  $h(x)$  defined below:

$$h(x) = \left( \frac{x^2 - 5x + 6}{x - 1} \right) e^{-x/5}$$

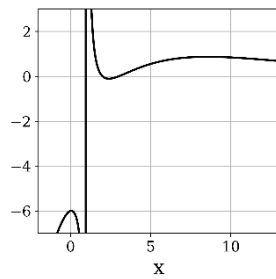
A)



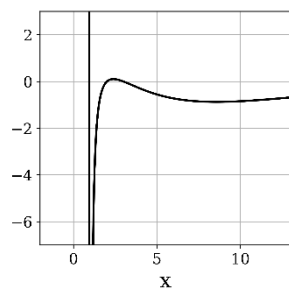
B)



C)

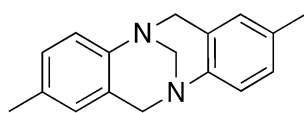


D)



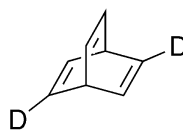
**Correct Answer: C**

37. Which of the following statements is correct?



Troger's base

**A**



2,5-dideuterio barrelene

**B**

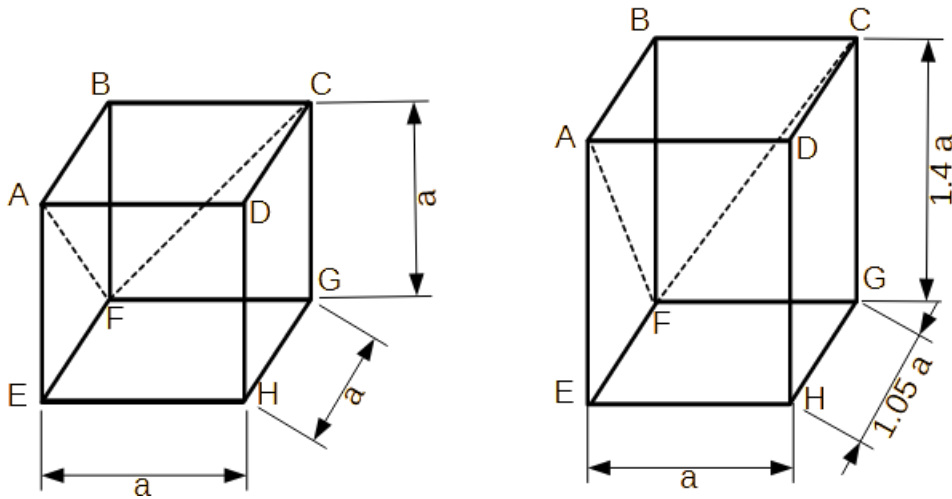
A) A is chiral and B is achiral

B) B is chiral and A is achiral

**C) Both are chiral**

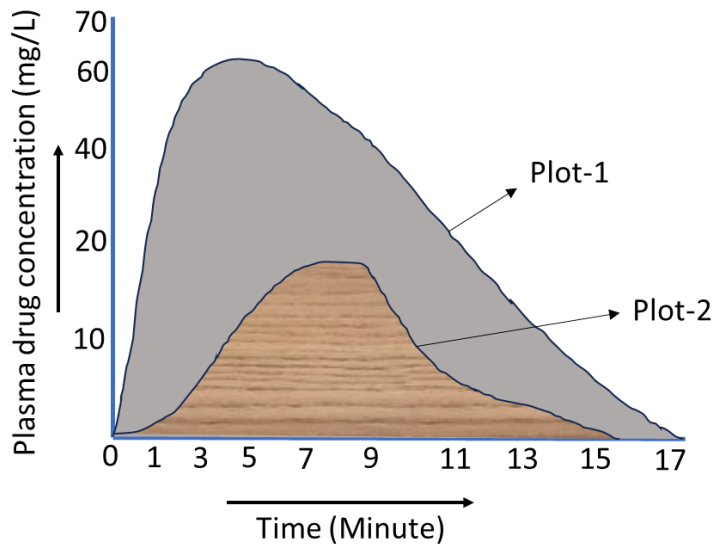
D) Both are achiral

38. Consider the cubic and orthorhombic unit cells, with internal angles =  $90^\circ$ , as shown below. What is the angle between the face diagonals (AF and FC, marked by dashed lines) in each of the cases?



- A) Orthorhombic:  $29.6^\circ$ , Cubic:  $60^\circ$
- B) Orthorhombic:  $45^\circ$ , Cubic:  $60^\circ$
- C) Orthorhombic:  $33.3^\circ$ , Cubic:  $109.5^\circ$
- D) Orthorhombic:  $49.4^\circ$ , Cubic:  $60^\circ$

39. The plots 1 and 2 represent changes in the concentration of a drug in the plasma as a function of time. This drug was administered at the same dose to a patient either intravenously or orally.



Identify which plots correctly represent the two administration modes:

- A) Plot-1 is oral and Plot-2 is intravenous
- B) Plot-1 is intravenous and Plot-2 is oral**
- C) Can not be determined as it depends on the nature of the drug molecule
- D) Can not be determined as it depends on the dose of the drug administered



40. A compactly folded globular protein in an aqueous buffer consists of a single chain of  $N$  amino acids. The radius ( $r$ ) of the protein molecule scales with  $N$  as:

A)  $r \propto N$

B)  $r \propto N^2$

C)  $r \propto N^{1/2}$

D)  $r \propto N^{1/3}$