I N D E X

SECTION - I

"PHYSICAL CHEMISTRY"

NUMBER OF QUESTIONS ASKED IN GATE EXAM (2000 - 2025)

Units	2025	2024	2023	2022	2021	2020	2019	2018	2017	2016	2015	2014	2013	2012	2011
Structure : Quantum Chemistry	7	5	4	5	3	3	4	6	6	3	3	3	4	5	3
Group Theory	2	3	2	1	1	1	1	-	-	1	-	1	1	1	1
Molecular Spectroscopy	1	2	1	4	4	4	1	3	-	2	1	1	1	2	2
Equilibrium : 1. Chemical Thermodynamics	2	3	1	1	3	3	2	2	2	5	6	4	2	3	-
2. Chemical Equilibrium	-	-	-	-	2	-	1	-	-	1	-	1	1	-	-
3. Electrochemistry	1	2	2	1	2	2	1	3	3	1	4	1	3	1	2
4. Phase Equilibrium	2	2	2	1	3	1	2	1	1	1	1	1	1	2	3
5. Statistical Thermodynamics	3	-	1	2	-	-	2	1	1	1	1	2	1	1	-
Kinetics	2	3	4	3	2	4	2	3	5	4	2	1	3	2	4
Surfaces and Interfaces	-	1	2	1	-	1	2	1	1	1	1	1	1	-	-

Units	2010	2009	2008	2007	2006	2005	2004	2003	2002	2001	2000
Structure : Quantum Chemistry	3	7	1	5	6	7	3	1	5	3	1
Group Theory	1	2	2	-	7	-	2	-	1	1	-
Molecular Spectroscopy	2	2	6	3	1	2	3	2	5	3	1
Equilibrium : 1. Chemical Thermodynamics	5	4	4	3	6	5	9	7	3	8	4
2. Chemical Equilibrium	1	-	-	-	1	-	2	1	-	2	1
3. Electrochemistry	1	1	1	4	2	3	1	4	3	3	1
4. Phase Equilibrium	3	3	1	2	4	5	4	2	4	-	3
5. Statistical Thermodynamics	-	-	1	2	1	-	-	2	-	-	-
Kinetics	1	5	3	7	3	3	5	5	3	-	2
Surfaces and Interfaces	-	-	1	-	-	1	-	1	-	-	-

STRUCTURE & QUANTUM CHEMISTRY

Previous Year Exam Question & Solutions

[GATE 2000]

1. $^2P_{3/2}$ is the ground state of
   (a) H (b) Li
   (c) B (d) F

[GATE 2001]

2. As per the uncertainty principle, $\Delta x \cdot \Delta p_y$ =
   (a) h (b) $h / 2\pi$
   (c) λ (d) zero

[GATE 2001]

3. The second lower state of particle in a cubic box is
   (a) non degenerate
   (b) doubly degenerate
   (c) triply degenerate
   (d) six-fold degenerate

[GATE 2001]

4. Given than, $\Psi_{n,l,m}$ (r,θ, ϕ) = $R_{n,l}$ (r) (θ, ϕ); R_{20} (r) α (2 − r / a_0) $e^{-r/ao}$, $Y_{0,0}$ (θ, ϕ) = 1 / $\sqrt{4\pi}$ .The position of radial node in the 2s orbital is at
   (a) r =a_0 (b) r =2a_0
   (c) r =a_0 / 2 (d) r =a_0 / 4

[GATE 2002]

5. The ground state of aluminium atom is
   (a) $^2P_{1/2}$ (b) $^2P_{3/2}$
   (c) $^4P_{5/2}$ (d) $^4P_{3/2}$

[GATE 2002]

6. The velocity of the electron in the hydrogen atom
   (a) increases with increasing principal quantum number
   (b) decreases with increasing principal quantum number
   (c) is uniform for any value of the principal quantum number
   (d) first increases and then decreases with principal quantum number

[GATE 2002]

7. In allene, hybridization of the central and terminal carbons respectively are
   (a) sp^2 and sp^2 (b) sp^2 and sp^3
   (c) sp and sp^2 (d) sp and sp^3

[GATE 2002]

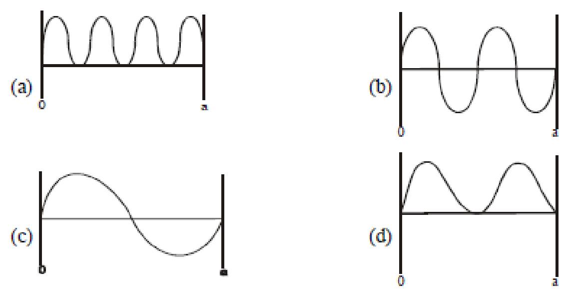
8. The probability of finding a free particle inside the left half of a 1-dimensional box of length L is
   (a) L/2 (b) $\sqrt{(2/L)}$
   (c) 2/L (d) 1/2

[GATE 2002]

9. The force between two electrons separated by 0.1 nm in vacuum ($\varepsilon_0 = 8.854 \times 10^{-12} J^{-2} C^{-2} m^{-1}$) is
   (a) 2.31×10^{-8}N (b) -2.31×10^{-8} N
   (c) -1.15×10^{-8} N (d) 1.155×10^{-8}N

[GATE 2003]

10. For the energy level ($2h^2/ma^2$) the probability for a particle of mass 'm' over the length 'a' of a one-dimensional box is depicted by



[GATE 2004]

11. In units of $\frac{h^2}{8m^2}$, the energy difference between levels corresponding to 3 and 2 node eigenfunctions for a particles of mass in a one dimensional box of length ℓ is
    (a) 1 (b) 3
    (c) 5 (d) 7

[GATE 2004]

12. On the basis o LCAO-MO theory, the magnetic characteristics of N_2 and N_2^+ are
    (a) both diamagnetic
    (b) both paramagnetic
    (c) N_2 dimagnetic and N_2^+ paramagnetic
    (d) N_2 paramegnetic and N_2^+ diamagnetic

[GATE 2004]

13. Match the following:

P. 4n+2 rule	I. Woodward-Hoffmann ruleII.
Q. single valued	II. Bound system
R. <P >=0	III. Hurtree-Fock Theory
S. photochemically allowed	IV. Huckeltheory
	V. Wave function
	VI. unbound system

Codes:
(a) P-I. Q-III, R-IV, S-VI (b) P-II, Q-VI, R-III, S-I
(c) P-IV, Q-V, R-II, S-VI (d) P-IV, Q-V, R-II, S-I

[GATE 2005]

14. The set of eigenfunctions $\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}\,(0 \leq a, n = 1,2,3 \ldots.)$ is
(a) orthogonal
(b) normalized
(c) both orthogonal and normalized
(d) unnormalized

[GATE 2005]

15. The function $e^{ax^2}(\alpha > 0)$ is not an acceptable wave function for bound system, because
(a) it is not continuous (b) it is multivalued
(c) it is not normalisable (d) all of these

[GATE 2005]

16. First order perturbation correction $\Delta\varepsilon_n^{(1)}$ to energy level ε_n of a simple harmonic oscillator due to the anharmonicity perturbation γx^3 is given b.
(a) $\Delta\varepsilon_n^{(1)}=\gamma$ (b) $\Delta\varepsilon_n^{(1)}=\gamma^2$
(c) $\Delta\varepsilon_n^{(1)}=\gamma^{-1}$ (d) $\Delta\varepsilon_n^{(1)}=0$

[GATE 2005]

17. The 2s orbital of H-atom has radial node at $2a_0$ because Ψ_{2s} is proportional to
(a) $\left(\frac{1}{2}+\frac{r}{a_0}\right)$ (b) $\left(2+\frac{r}{a_0}\right)$
(c) $\left(2-\frac{r}{a_0}\right)$ (d) $\left(2-\frac{r}{2a_0}\right)$

[GATE 2005]

18. The orbital $\Psi = 1_{S_{H_A}} - 1_{S_{H_B}}$ of water belongs to the irreducible representation
(a) A_1 (b) B_1
(c) A_2 (d) B_2

[GATE 2005]

19. As per Huckel theory, π--electron energy levels of cyclobutadiene are
(a) $\alpha + 2\beta, \alpha + \beta, \alpha - \beta, \alpha + 2\beta$,
(b) $\alpha + 2\beta, \alpha - \beta, \alpha - \beta, \alpha - 2\beta$,
(c) $\alpha + 2\beta, \alpha, \alpha, \alpha - 2\beta$,
(d) $\alpha + \beta, \alpha - \beta, \alpha - \beta, \alpha - 2\beta$,

[GATE 2005]

20. Given β = -75 kJ/mol,
(a) paramagnetic and its lowest absorption energy is 150 kJ
(b) paramagnetic and its lowest absorption energy is 75 kJ
(c) diamagnetic and its lowest absorption energy is 75 kJ
(d) diamagnetic and its lowest absorption energy is 150 kJ.

[GATE 2006]

21. In the Huckel model for benzene, the π electronic transitions from the occupied to the unoccupied molecular orbitals do NOT occur at
(a) 4β (b) 3β
(c) 2β (d) 1β

[GATE 2006]

22. To demonstrate the variational principle, a trial function $\psi=C_1+\frac{\Psi_{2s}+\Psi_{3s}}{\sqrt{2}}$ + $C_2+\frac{\Psi_{2s}+\Psi_{3s}}{\sqrt{2}}$ where C_1 and C_2 are the variational parameters and$\psi_{2s}\psi_{3s}$ and are the 2s, and 3s orbitals of the hydrogen atom, is constructed. The corresponding secular determinant for the hydrogen atom (in eV) is
(a) $\begin{vmatrix} 3.4\left(1+\frac{4}{9}\right)2-E & 3.4(1-4/9)/2 \\ 3.4(1-4/9)/2 & 3.4\left(1+\frac{4}{9}\right)2-E \end{vmatrix}$
(b) $\begin{vmatrix} 3.4\left(1+\frac{4}{9}\right)2-E & 3.4(1-4/9)/2 \\ 3.4(1-4/9)/2 & 3.4\left(1-\frac{4}{9}\right)2-E \end{vmatrix}$
(c) $\begin{vmatrix} 3.4\left(1+\frac{4}{9}\right)2-E & 3.4(1+4/9)/2 \\ 3.4(1-4/9)/2 & 3.4\left(1-\frac{4}{9}\right)2-E \end{vmatrix}$
(d) $\begin{vmatrix} 3.4\left(1+\frac{4}{9}\right)2-E & 0 \\ 0 & 3.4\left(1+\frac{4}{9}\right)2-E \end{vmatrix}$

[GATE 2006]

23. Which of the following pairs of operators commute?
(a) x and d/dx (b) d/dx and d^2/dx^2+ 2d/dx
(c) x^2d/dx and d^2/dx^2 (d) x^2 and d/dx

[GATE 2006]

24. The zero-point energy of the vibration of $^{35}Cl_2$ mimicking a harmonic oscillator with a force constant k = 2293.8 Nm^{-1} is
(a) 10.5×10^{-21} J (b) 14.8×10^{-21} J
(c) 20×10^{-21} J (d) 29.6×10^{-21} J

[GATE 2006]

25. The first excited state wavefunction for a particle in a box that spans from –a to +a is
(a) $\sqrt{\frac{1}{a}}cos\left(\frac{\pi x}{a}\right)$ (b) $\sqrt{\frac{1}{a}}sin\left(\frac{\pi x}{a}\right)$
(c) $\sqrt{\frac{2}{a}}cos\left(\frac{2\pi x}{a}\right)$ (d) $\sqrt{\frac{2}{a}}sin\left(\frac{2\pi x}{a}\right)$

[GATE 2006]

26. A perturbation V=δ(x-a/2) is introduced in the box. The first order energy correction to the first excited state is
(a) 0 (b) 2/a
(c) 1/a (d) 1/2a

[GATE 2007]

27. For a homonuclear diatomic molecule, the bonding molecular orbital is
(a) σ_u oflowest energy
(b) σ_u of second lowest energy
(c) π_g of lowest energy
(d) π_u oflowest energy

[GATE 2007]

28. The ionisation potential of hydrogen atom is 13.6 eV. The first ionisation potential of a sodium atom, assuming that the energy of its outer electron can be represented by a H-atom like model with an effective nuclear charge of 1.84, is

(a) 46.0 Ev (b) 11.5 eV
(c) 5.1 eV (d) 2.9 eV

[GATE 2007]

29. The quantum state of a particle moving in a circular path in a plane is given by $\Psi_m(\phi) = \left(\frac{1}{\sqrt{2\pi}}\right) e^{im\phi}$, m = O, ±1, ±2, ... When a perturbation H$_1$= P cos ¢ is applied (P is a constant), what will be the first order correction to the energy of Ihemth state

(a) 0 (b) P/(2 π)
(c) P/(4 π) (d) Pm^2/(4 π^2)

[GATE 2007]

30. Consider a particle of mass m moving in a one-dimensional box under the potential V=0 for 0 ≤ x ≤ a and V = ∞ outside the box. When the partial is in its lowest energy state the average momentum ($<p_x>$) of the particle is

(a) $<p_x> = 0$ (b) $<p_x>= h/a$
(c) $<p_x>= h/2a$ (d) $<p_x> = h/2\pi a$

[GATE 2007]

31. The uncertainty in the momentum (Δpx) of the particle in its lowest energy state is

(a) $\Delta p_x= 0$ (b) $\Delta p_x = h/a$
(c) $\Delta p_x =h/2a$ (d) $\Delta p_x = h/2\pi a$

[GATE 2008]

32. The wave function of a diatomic molecule has the form = $0.89\ \varphi_{covalent} + 0.45\ \varphi_{ionic}$.The chance that both electrons of the bond will be found on the same atom in 100 inspections of the molecule approximately is

(a) 79 (b) 20
(c) 45 (d) 60

[GATE 2009]

33. The minimum number of electrons needed to form a chemical bond between two atoms is

(a) 1 (b) 2
(c) 3 (d) 4

[GATE 2009]

34. The ground state electronic energy (Hartree) of a helium atom, neglecting the inter-electron repulsion, is

(a) - 1.0 (b) - 0.5
(c) - 2.0 (d) - 4.0

[GATE 2009]

35. A particle is confined to a one-dimensional box of length 1 mm. If the length is changed by 10^{-9} the % change in the ground state energy is

(a) 2 x 10^{-4} (b) 2 x 10^{-7}
(c) 2 x 10^{-2} (d) 0

[GATE 2009]

36. The operation of the commutator [x, d/dx] on a function f(x) is equal to

(a) 0 (b) f(x)
(c) -f(x) (d) x df/dx

[GATE 2009]

37. The lowest allowed energy is equal to zero for

(a) the hydrogen atom
(b) a rigid rotor
(c) a harmonic oscillator
(d) a particle in a 3-dimensional box

[GATE 2009]

38. The degeneracy of a quantum particle in a cubic box having energy four times that of the lowest energy is

(a) 3 (b) 6
(c) 1 (d) 4

[GATE 2009]

39. The de Broglie wavelength for a He atom travelling at 1000 ms^{-1} (typical speed at room temperature) is

(a) 99.7 x 10^{-12} m (b) 199.4 x 10^{-12} m
(c) 199.4 x 10^{-18} m (d) 99 x 10^{-6} m

[GATE 2010]

40. For eigen functions $\Psi_1 = \sqrt{\frac{1}{b} sin\left(\frac{\pi x}{b}\right)}$ and $\Psi_2 = \sqrt{\frac{2}{b} sin\left(\frac{2\pi x}{b}\right)}$ of particle in a 1-D box of length b(0 ≤ x ≤b)

(a) Ψ_1 is normalized and orthogonal to Ψ_2
(b) Ψ_1 is normalized but not orthogonal to Ψ_2
(c) Ψ_2 is nonnalized and orthogonal Ψ_1
(d) $\Psi_2$is neither normalized nor orthogonal to Ψ_1

[GATE 2010]

41. The commutator [x^3, p$_x$] is equal to

(a)-$\frac{3hx^2}{2\pi i}$ (b) $\frac{hx}{2\pi i}$
(c) $\frac{hx^2}{2\pi i}$ (d) $\frac{3hx^2}{2\pi i}$

[GATE 2010]

42. An electron of mass 'm' is confined to a one dimensional box of length. 'b'. If it makes a radiative transition from second excited state to the ground state. The frequency of the photon emitted is

(a) 9h/8mb^2 (b) 3h/8mb^2
(c) h/mb^2 (d) 2h/mb^2

[GATE 2011]

43. The wave function for a Harmonic oscillator described by $N\,x\,\exp(-ax^2/2)$ has

(a) one maximum only
(b) one maximum, one minimum only
(c) two maxima, one minimum only
(d) two maxima, two minima only

[GATE 2011]

44. If an arbitrary wave function is used to calculate the energy of a quantum mechanical system, the value calculated is never less than the true energy. The above statement relates to
(a) perturbation theory
(b) variation principle
(c) Heisenberg's uncertainty principle
(d) quantization of energy

[GATE 2011]

45. The wave function for a quantum mechanical particle in a 1-dimensional box of length 'a' is given by $\Psi = A\sin\frac{\pi x}{a}$. The value of 'A' for a box of length 200 nm is
(a) 4×10^4 (nm)^2 (b) $10\sqrt{2}$ (nm)$^{1/2}$
(c) $\sqrt{2}/10$ (nm)$^{-1/2}$ (d) 0.1 (nm)$^{-1/2}$

[GATE 2012]

46. Let ϕ_x^C and ϕ_z^C denote the wavefunctions of the 2px and 2pz orbitals of carbon, respectively, and ϕ_x^O and ϕ_z^O represent the wavefunctions of the 2px and 2pz orbitals of oxygen, respectively. If C_1 and C_2 are constants used in linear combinations and the CO molecule is oriented along the z axis, then, according to molecular orbital theory, the π-bonding molecular orbital has a wavefunction given by
(a) $C_1\phi_z^C + C_2\phi_x^O$ (b) $C_1\phi_z^C + C_2\phi_z^O$
(c) $C_1\phi_x^C + C_2\phi_z^O$ (d) $C_1\phi_x^C + C_2\phi_x^O$

[GATE 2012]

47. The wavefunction of a 1-D harmonic oscillator between x = +∞ and x = -∞ is given by $\Psi(x) = N(2x^2 - 1)e^{-x^2/2}$. The value of N that normalizes the function $\Psi(x)$ is (Given: $\int_{-\infty}^{+\infty} x^{2n} e^{-x^2} dx = \frac{1.3.5...(2n-1)}{2^n}\sqrt{\pi}$)
(a) $\left(\frac{1}{8\sqrt{\pi}}\right)^{1/2}$ (b) $\left(\frac{1}{3\sqrt{\pi}}\right)^{1/2}$
(c) $\left(\frac{1}{2\sqrt{\pi}}\right)^{1/2}$ (d) $\left(\frac{1}{4\sqrt{\pi}}\right)^{1/2}$

Statement for Linked Answer Questions 48 and 49: Hückel molecular orbital theory can be applied to the allene radical. $CH_2{=}CH{-}\dot{C}H_2$

[GATE 2012]

48. The secular determinant (where α, β and E have their usual meanings) is given by
(a) $\begin{vmatrix} \alpha - E & \beta & 0 \\ \beta & \alpha - E & \beta \\ 0 & \beta & \alpha - E \end{vmatrix}$
(b) $\begin{vmatrix} \alpha - E & 0 & 0 \\ 0 & \alpha - E & \beta \\ 0 & \beta & \alpha - E \end{vmatrix}$
(c) $\begin{vmatrix} \alpha - E & \beta & 0 \\ \beta & \alpha - E & 0 \\ 0 & 0 & \alpha - E \end{vmatrix}$
(d) $\begin{vmatrix} \alpha - E & -\beta & 0 \\ -\beta & \alpha - E & -\beta \\ 0 & -\beta & \alpha - E \end{vmatrix}$

[GATE 2012]

49. The possible values of E are
(a) $\alpha + \sqrt{2\beta}$, α, $\alpha - \sqrt{2\beta}$ (b) $\alpha + \sqrt{2\beta}$, α, $\alpha - \sqrt{2\beta}$
(c) α +β, α, α - β (d) α +2β, α, α - 2β

[GATE 2012]

50. If Δy and Δp_y are the uncertainties in the y-coordinate and the y component of the momentum of a particle respectively, then, according to uncertainty principle $\Delta y \Delta p_y$ is ($\hbar = \frac{h}{2\pi}$ and h is Planck's constant)
(a) $\geq \hbar$ (b) $>\hbar/2$
(c) $>\hbar$ (d) $\geq \hbar/2$

[GATE 2013]

51. Two trial wave functions $\phi_1 = c_1x(a-x)$ and $\phi_2 = c_1x(a-x) + c_1x^2(a-x)^2$ give ground state energies E_1 and E_2, respectively, for the microscopic particle in a 1-D boxby using the variation method. If the exact ground state energy is E_0, the correct relationship between E_0, E_1 and E_2 is
(a) $E_0 = E_1 = E_2$ (b) $E_0 < E_1 < E_2$
(c) $E_0 < E_2 < E_1$ (d) $E_0 > E_2 = E_1$

[GATE 2013]

52. The ground state energies of H atom and H_2 molecule are –13.6 eV and –31.7 eV, respectively. The dissociation energy of H_2 is _______ eV.

[GATE 2013]

53. e^{-2x^2} is an eigen function of the operator $\left(\frac{d^2}{dx^2} - 16x^2\right)$. The corresponding eigen value is
(a) + 4 (b) – 4
(c) + 2 (d) – 2

[GATE 2013]

54. The angular part of the wavefunction for the electron in a hydrogen atom is proportional to $\sin^2\theta \cos\theta e^{2i\phi}$. The values of the azimuthal quantum number (l) and the magnetic quantum number (m) are, respectively
(a) 2 and 2 (b) 2 and –2
(c) 3 and 2 (d) 3 and –2

[GATE 2014]

55. The value of the magnetic quantum number of a p_x orbital is
(a) – 1 (b) 0
(c) +1 (d) undefined

[GATE 2014]

56. $\psi = N\, r\, (6 - Z\, r)\, e^{-Zr/3} \cos\theta$, is a proposed hydrogenic wavefunction, where Z = Atomic number, r = radial distance from the nucleus, θ = azimuthal angle, N is a constant. The INCORRECT statement about ψ is
(a) $\psi = 0$ in the xy-plane
(b) two radial nodes are present in ψ
(c) one angular node is present in ψ
(d) the size of the orbital decreases with increase in atomic number

[GATE 2025]

106. If a particle's state function is an eigenfunction of the operator $\hat{L}^2$ with eigenvalue $30\hbar^2$, then the possible eigenvalue(s) of the operator $\hat{L}^2 z$ for the same state function is/are

(a) $10\hbar^2$ (b) $16\hbar^2$

(c) $25\hbar^2$ (d) 0

Answer Key									
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
d	d	c	b	a	b	a	d	a	a
11	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
d	c	d	c	c	d	c	d	c	a
21	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**
d	a	b	b	b	c	d	c	a	a
31	**32**	**33**	**34**	**35**	**36**	**37**	**38**	**39**	**40**
c	b	a	d	a	b	b	c	a	c
41	**42**	**43**	**44**	**45**	**46**	**47**	**48**	**49**	**50**
a	c	b	b	d	d	c	a	a	d
51	**52**	**53**	**54**	**55**	**56**	**57**	**58**	**59**	**60**
c	4.4 to 4.6	b	c	d	b	a	d	a	896 to 900
61	**62**	**63**	**64**	**65**	**66**	**67**	**68**	**69**	**70**
d	b	b	b	a	899 to 901	225 to 240	33.30 to 36.90	0.80 to 0.84	a
71	**72**	**73**	**74**	**75**	**76**	**77**	**78**	**79**	**80**
c	4.4 to 4.6	a	0.55 to 0.65	210 to 216	c	0.5	0	2.8 to 3.0	b
81	**82**	**83**	**84**	**85**	**86**	**87**	**88**	**89**	**90**
c	a	c,d	2000	39.5 to 40.5	d	5	b,d	0.18 to 0.20	2
91	**92**	**93**	**94**	**95**	**96**	**97**	**98**	**99**	**100**
c	a	b	a	2	c	b,c	3	8	74.10 to 74.30
101	**102**	**103**	**104**	**105**	**106**				
3.110 to 3.200	b	b, c	c	a, c	b, c, d				

Solutions

1. **Solution:** Correct answer is (d).
$^2P_{3/2}$ is the ground state for p^5 systems, i.e. systems with one unpaired electron and more than half – filled p orbitals.
H and Li are s^1 systems, B is a p^3 system, while F is a p^5 system.

2. **Solution:** Correct answer is (d).
The uncertainty principle applied to uncertainties in the same direction. Hence, if the uncertainties in x and p_y are in two different directions, then the product of the uncertainties is zero.

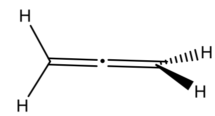
3. **Solution:** Correct answer is (c).
The second lowest energy state of a particle in a cubic box has quantum numbers
$(n_x, n_y, n_z) = (1,1,2), (1,2,1), (2,1,1)$
All of these states have energy
$$E^{3D} = (1^2 + 1^2 + 2^2)\frac{h^2}{8ma^2} = 6\frac{h^2}{8ma^2}$$
Hence, the second lowest state has degeneracy = 3.

4. **Solution:** Correct answer is (b).
The value of r where the radial part of the wave function becomes zero is the radial node. The given radial part is
$$R_{20}(r) \propto \left(2 - \frac{r}{a_0}\right) e^{-r/a_0}$$
This can be zero only if
$$\left(2 - \frac{r}{a_0}\right) = 0$$
$$\therefore r = 2a_0$$
Hence, correct answer is (B).

5. **Solution:** Correct answer is (a).
Aluminium has electronic configuration $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$, i.e. aluminium is a p^1 system. The ground state term symbol will have $L = 1$, i.e. Term Symbol P and $S = +1/2$. Thus, spin multiplicity will be $2S + 1 = 2$.
Also the J values range from $(L + S)$ to $|L - S|$.
$$\therefore J = \frac{3}{2}, \frac{1}{2}$$
As the system is less than half-filled, the lowest J value has lower energy.
Hence, the ground state term symbol is $^2P_{1/2}$.

6. **Solution:** Correct answer is (b).
According to Bohr's theory,
$$v = \frac{n\hbar}{mr}$$
and
$$r = \frac{n^2}{Z} \times a_0$$
$$\therefore v = \frac{Z\hbar}{ma_0} \times \frac{1}{n}$$
$$\therefore v \propto \frac{1}{n}$$
Thus, at higher quantum numbers, velocity is lower.

7. **Solution:** Correct answer is a.
Structure of allene is



It can be clearly seen that all carbons have a planar geometry, and hence, are sp^2 hybridized.

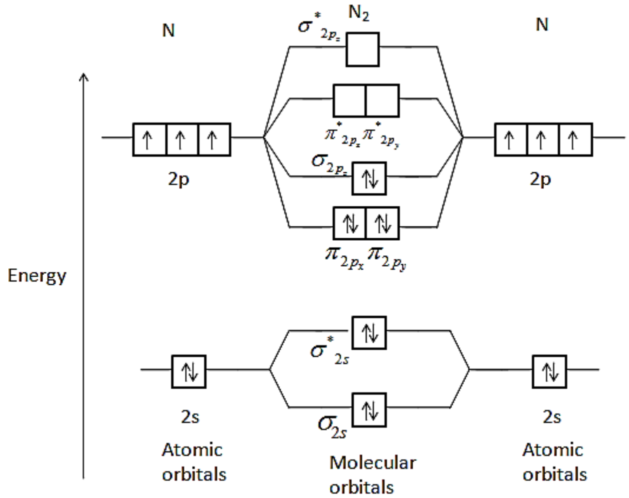
8. **Solution:** Correct answer is (d).
The probability of a free particle in a one – dimensional box is symmetric about the center of the box. Hence, the probabilities in the left half and the right half are equal. As the total probability is one, the probability in the left half will be 1/2.

9. **Solution:** Correct answer is (a).
According to the Coulomb's law,
$$F = \frac{q_1 q_2}{4\pi\varepsilon_0 r^2}$$
$$= \frac{(-1.6 \times 10^{-19}) \times (-1.6 \times 10^{-19})}{4 \times \pi \times 8.854 \times 10^{-12} \times (0.1 \times 10^{-9})^2}$$
$$= 2.3 \times 10^{-8}\ N$$

10. **Solution:** Correct answer is (a).
$$E_n = \frac{n^2 h^2}{8ma^2} = \frac{2h^2}{ma^2}$$
$$\therefore \frac{n^2}{8} = 2$$
$$\therefore n = 4$$
For this energy level, number of nodes= $n - 1 = 3$.
Also, probabilty density functions will always be positive, i.e. above the X – axis. Hence, (B) and (C) cannot be the answers. Also, (C) has only one node.

11. **Solution:** Correct answer is (d).
For a particle in a one – dimensional box, if number of nodes is 2, then quantum number $n = 3$, and if number of nodes is 3, then quantum number $n = 4$.
$$\therefore \Delta E = E_4 - E_3 = (4^2 - 3^2)\frac{h^2}{8ml^2}$$
$$= 7\frac{h^2}{8ml^2}$$

12. **Solution:** Correct answer is (c).
The LCAO – MO energy level diagram for N_2 is



As there are no unpaired electrons, N_2 is diamagnetic. However, during formation of N_2^+, an electron from σ_2p_z will be removed, thus, resulting in an unpaired electron. Hence, N_2^+ is paramagnetic.

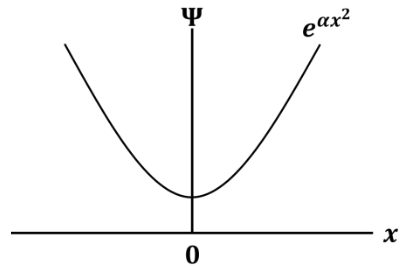
13. **Solution:** Correct answer is (d).
The Huckel theory gives the $(4n+2)$ electron rule for aromaticity.
For a wavefunction to be acceptable, it must be single valued.
The average value of momentum, <P>, is zero for bound systems.
The Woodward – Hoffmann rules give the photochemically allowed transitions.

14. **Solution:** Correct answer is (c).
The given set of eigenfunctions is eigenfunctions of a one dimensional box. According to the theorems of Quantum Mechanics, the eigenfunctions of a given system form an orthonormal set. Hence, the given eigenfunctions are both orthogonal and normalized.
The set of eigen function is $\sqrt{\frac{2}{a}}\, sin\, \frac{n\pi x}{a}$
is normalized.

$$\int_0^a \sqrt{\frac{2}{a}} sin \frac{n\pi x}{a} \sqrt{\frac{2}{a}} sin \frac{n\pi x}{a} dx = 1 \rightarrow normalized\ if\ n = 1$$

$$\int_0^a \sqrt{\frac{2}{a}} sin \frac{\pi x}{a} \sqrt{\frac{2}{a}}\, sin\, \frac{2\pi x}{a} dx = 0 \rightarrow orthogonal$$

15. **Solution:** Correct answer is (c).



For a wavefunction to be acceptable, it MUST (a) be continuous, (b) be single valued, (c) be finite (normalisable) and (d) have a continuous derivative. As can be seen in the graph, the function $e^{\alpha x^2}$ is continuous, single-valued, and has a continuous derivative, but is NOT finite (NOT normalisable).

16. **Solution:** Correct answer is (d).
For a simple harmonic oscillator, an odd perturbation function results in the first order energy correction being zero.
i.e. $\Delta\varepsilon_n^{(1)} = 0$.

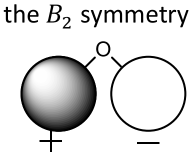
17. **Solution:** Correct answer is (c).
If a radial nodes exists at $r = 2a_0$, it means that $r - 2a_0 = 0$.
If we divide by a_0 on both sides, we get

$$\frac{r}{a_0} - 2 = 0\ OR\ \left(2 - \frac{r}{a_0}\right) = 0$$

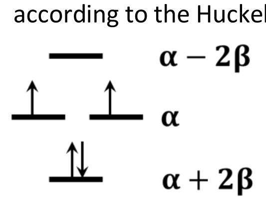
Thus, a radial node will exist at $r = 2a_0$ if the wavefunction

$$\Psi_{2s} \propto 2 - \frac{r}{a_0}$$

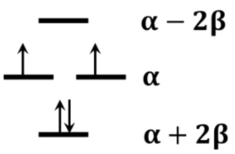
18. **Solution:** Correct answer is d.
The given molecular orbital will lose the rotational $\hat{C}_2$ and the reflection $\hat{\sigma}_v$ (perpendicular plane) symmetries, but the identity $(\hat{E})$ and $\hat{\sigma}_v{}'$ (molecular plane) symmetries will be intact. Hence, this orbital will transform according to the B_2 symmetry of the C_{2v} point group.



19. **Solution:** Correct answer is (c).
The π – electron energy level diagram of cyclobutadiene, according to the Huckel theory, is given by

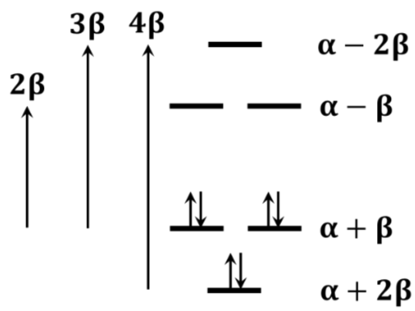


20. **Solution:** Correct answer is (a).
The π – electron energy level diagram of cyclobutadiene, according to the Huckel theory, is given by



It can be seen that there are two π – electrons. Hence, cyclobutadiene is paramagnetic.
Also, the lowest absorption energy is given by
$\Delta E = (\alpha - 2\beta) - \alpha = -2\beta$
$= (-2) \times (-75) = 150\ kJ\ mol^{-1}$

21. **Solution:** Correct answer is (D).



According to Huckel model for benzene, the energy level diagram is as shown in the figure. The six π electrons are arranges in the two lowest levels. Thus, it can be seen from the diagram that the π electronic transitions from the occupied to the unoccupied levels will have energy 2β, 3β and 4β.
As a transition with energy β is not possible,

22. **Solution:** Correct answer is (a).
The energy of a hydrogen atom wavefunction is given by

$$E_n = -\frac{13.6}{n^2}$$

$$\therefore E_{2s} = -\frac{13.6}{2^2} = -\frac{13.6}{4}\quad E_{3s} = \frac{13.6}{3^2} = -\frac{13.6}{9}$$

$$H_{11} =< \varphi_{2S} + \varphi_{3S}|H|\varphi_{2S} + \varphi_{3S} = -\frac{13.6}{4} - \frac{13.6}{9}$$

$$H_{22} =< \varphi_{2S} - \varphi_{3S}|H|\varphi_{2S} + \varphi_{3S} = -\frac{13.6}{4} - \frac{13.6}{9}$$

$$H_{12} = H_{21} =< \varphi_{2S} - \varphi_{3S}|H|\varphi_{2S} + \varphi_{3S} = -\frac{13.6}{4} - \frac{13.6}{9}$$

$$S_{21} = S_{12} =< \varphi_{2S} + \varphi_{3S}|\varphi_{2S} - \varphi_{3S} = 1 - 1 = 0$$

$$S_{12} =< \varphi_{2S} + \varphi_{3S}|\varphi_{2S} + \varphi_{3S} = 1 + 1 = 2$$

$$S_{22} =< \varphi_{2S} - \varphi_{3S}|\varphi_{2S} - \varphi_{3S} = 1 + 1 = 2$$

$$\begin{vmatrix} H_{11} - ES_{11} & H_{12} - ES_{12} \\ H_{21} - ES_{21} & H_{22} - ES_{22} \end{vmatrix}$$

$$= \begin{vmatrix} -3.4\left(1 + \frac{4}{9}\right)2 - E \times 1 & -3.4\left(1 - \frac{4}{9}\right)/2 - E \times 0 \\ -3.4\left(1 - \frac{4}{9}\right)/2 - E \times 0 & -3.4\left(1 + \frac{4}{9}\right)2 - E \times 1 \end{vmatrix}$$

$$= \begin{vmatrix} 3.4\left(1 + \frac{4}{9}\right)2 - E & 3.4\left(1 - \frac{4}{9}\right)/2 \\ 3.4\left(1 - \frac{4}{9}\right)/2 & 3.4\left(1 + \frac{4}{9}\right)2 - E \end{vmatrix}$$

23. **Solution:** Correct answer is (b).
(a) $\left[\hat{x}, \frac{d}{dx}\right] = x\frac{d}{dx} - \frac{d}{dx}(\hat{x}) = x\frac{d}{dx} - \left(x\frac{d}{dx} + 1\right) = -\hat{1} \neq 0$
(b) $\left[\frac{d}{dx}, \left(\frac{d^2}{dx^2} + 2\frac{d}{dx}\right)\right] = \frac{d}{dx}\left(\frac{d^2}{dx^2} + 2\frac{d}{dx}\right) - \left(\frac{d^2}{dx^2} + 2\frac{d}{dx}\right)\frac{d}{dx} = \frac{d^3}{dx^3} + 2\frac{d^2}{dx^2} - \frac{d^3}{dx^3} - 2\frac{d^2}{dx^2} = 0$
(c) $\left[x^2\frac{d}{dx}, \frac{d^2}{dx^2}\right] = x^2\frac{d}{dx}\frac{d^2}{dx^2} - \frac{d^2}{dx^2}\left(x^2\frac{d}{dx}\right) = x^2\frac{d^3}{dx^3} - \frac{d}{dx}\left(x^2\frac{d^3}{dx^3} - \frac{d}{dx}\left(\frac{d^2}{dx^2}x^2\right)\right) \neq 0$
(d) $\left[x^2, \frac{d}{dx}\right] = x^2\frac{d}{dx} - \frac{d}{dx}(x^2) = x^2\frac{d}{dx} - 2x \neq 0$

24. **Solution:** Correct answer is (b).
Zero point energy is given by

$$ZPE = \frac{1}{2}h\nu = \frac{1}{2}h \times \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} = \frac{h}{4\pi}\sqrt{\frac{k}{\mu}}$$

Given: $k = 2293.8\ N\ m^{-1}$
Reduced mass is given by
$\mu = \frac{m_{Cl} \times m_{Cl}}{M_{Cl} + M_{Cl}} = \frac{35\times35}{35+35} = 17.5\ amu = \frac{17.5\times10^{-3}}{6.022\times10^{23}} = 2.91 \times 10^{-26}\ kg\ mol^{-1}$
$\therefore ZPE = \frac{h}{4\pi}\sqrt{\frac{k}{\mu}} = \frac{6.62\times10^{-34}}{4\times3.14} \times \sqrt{\frac{2293.8}{2.91\times10^{-26}}} = 14.8 \times 10^{-21}\ J$

25. **Solution:** Correct answer is (b).
For a one-dimensional box of length L, the first excited state wavefunction is fiven by

$$E_{ES} = \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)$$

For a box of length $L = 2a$, this energy will be

$$E_{ES} = \sqrt{\frac{2}{2a}}\sin\left(\frac{2\pi x}{2a}\right) = \sqrt{\frac{1}{a}}\sin\left(\frac{\pi x}{a}\right)$$

26. **Solution:** Correct answer is (c).
A property of the Dirac delta function $\delta(x - m)$ is

$$\int_{-\infty}^{+\infty} f(x)\,\delta(x - m)\,dx = f(m)$$

This property also applies to any other symmetric limits, as long as the point $x = m$ is within these limits.
$\therefore \int_{-a}^{+a}\sin^2\left(\frac{\pi x}{a}\right)\delta\left(x - \frac{a}{2}\right)dx = \int_{-\infty}^{+\infty}\sin^2\left(\frac{\pi x}{a}\right)\delta\left(x - \frac{a}{2}\right)dx$
$= \sin^2\left(\frac{\pi}{a} \times \frac{a}{2}\right) = \sin\frac{\pi}{2} = 1$

Hence, the first order energy correction to the first excited state is given by

$$E_{ES}^{(1)} = \int_{-a}^{+a} \sqrt{\frac{1}{a}} \sin\left(\frac{\pi x}{a}\right) \delta\left(x - \frac{a}{2}\right) \sqrt{\frac{1}{a}} \sin\left(\frac{\pi x}{a}\right) dx$$

$$= \frac{1}{a}\int_{-a}^{+a} \sin^2\left(\frac{\pi x}{a}\right) \delta\left(x - \frac{a}{2}\right) dx$$

$$= \frac{1}{a} \times 1 = \frac{1}{a}$$

27. **Solution:** Correct answer is (d).
The bonding molecular orbitals are either σ_g or π_u.

28. **Solution:** Correct answer is (c).
The energy of single electron atomic species is given by

$$E_n = -\frac{Z^2}{n^2} \times 13.6$$

If we approximate the sodium atom as a single electron in the 3s orbital ($n = 3$) and replace the atomic number Z by the effective nuclear charge, then we can use this formula to calculate ground state energy of a sodium atom.

$$\therefore E_{GS} = -\frac{{Z_{eff}}^2}{n^2} \times 13.6 = -\frac{1.84^2}{3^2} \times 13.6 = 5.1\ eV$$

29. **Solution:** Correct answer is (a).
The first order perturbation correction to the mth state is given by

$$E_m^{(1)} = \int \Psi_m^*(\phi)\, H_1\, \Psi_m(\phi)\, d\phi$$

The limits of ϕ are from 0 to 2π. Hence, for the given wavefunction, the first order correction is

$$E_m^{(1)} = \int_0^{2\pi} \left(\frac{1}{\sqrt{2\pi}}\right) e^{-im\phi} \cdot P\cos\phi \cdot \left(\frac{1}{\sqrt{2\pi}}\right) e^{im\phi}\, d\phi$$

$$= \frac{P}{2\pi}\int_0^{2\pi} \cos\phi\ d\phi$$

$$= \frac{P}{2\pi}[\sin\phi]_0^{2\pi} = \frac{P}{2\pi}[\sin 2\pi - \sin 0] = \frac{P}{2\pi}[0 - 0]$$

$$= 0$$

30. **Solution:** Correct answer is (a).
For a one-dimensional box with infinite potential barriers, average value of linear momentum,

$$\langle \hat{p}_x \rangle = 0$$

for all energy levels.

31. **Solution:** Correct answer is (c).
The uncertainty in momentum is calculated as follows.

$$\Delta\hat{p}_x = (\langle \hat{p}_x^2\rangle - \langle \hat{p}_x\rangle^2)^{1/2}$$

$$= \left(\frac{n^2h^2}{4a^2} - 0^2\right)^{1/2} \quad \ldots\left(\because \langle \hat{p}_x^2\rangle = \frac{n^2h^2}{4a^2} \text{ and } \langle \hat{p}_x\rangle = 0\right)$$

$$= \frac{nh}{2a}$$

For the lowest energy state, $n = 1$.

32. **Solution:** Correct answer is (b).
If both electrons are found on the same atom, then the molecule will be ionic, as the charge will be concentrated on one atom only. Hence, probability that both electrons will be found on the same atom in 100 inspections is the same as the probability of the wavefunction being ionic.

$$\therefore P(\Psi = \varphi_{ionic}) = \frac{0.45^2}{0.89^2 + 0.45^2} \times 100 \approx 20$$

Hence, correct answer is (B).

33. **Solution:** Correct answer is (a).
The molecule with the least number of electrons is the H_2^+ molecular ion, which contains only one electron.

34. **Solution:** Correct answer is (c).
The energy of an electron in the He atom, if inter-electron repulsion is neglected, is given by

$$E = -\frac{Z^2}{n^2} \times 0.5\ hartrees$$

For He atom ground state, $Z = 2$ and $n = 1$.

$$\therefore E = -\frac{2^2}{1^2} \times 0.5 = -2.0\ hartrees.$$

This is the energy of one electron. Thus, the energy of both electrons of the He atom combined, is

$$E = 2 \times (-2.0) = -4.0\ hartrees$$

Hence, correct answer is (D).

35. **Solution:** Correct answer is (a).
For a one-dimensional box,

$$E \propto \frac{1}{L^2}$$

$$\therefore \frac{dE}{dL} \propto -\frac{2}{L^3}$$

$$\therefore dE \propto \frac{2\,dL}{L^3}$$

$$\therefore \frac{dE}{E} = \frac{\frac{2\,dL}{L^3}}{\frac{1}{L^2}} = \frac{2\,dL}{L} = \frac{2 \times 10^{-9}}{10^{-3}} = 2 \times 10^{-6}$$

$$\therefore \%\ \text{change in energy} = \frac{\text{dE}}{\text{E}} \times 100 = 2 \times 10^{-4}$$

36. **Solution:** Correct answer is (b).

$$\left[x, \frac{d}{dx}\right] f(x) = x\frac{d}{dx} f(x) - \frac{d}{dx}(x\, f(x))$$

$$= x\frac{d}{dx} f(x) - \left(x\frac{d}{dx} f(x) + f(x)\frac{d}{dx}(x)\right)$$

$$= f(x)$$

37. **Solution:** Correct answer is (b).
The ground state energy for hydrogen atom is – 13.6 eV.
The ground state energy of a harmonic oscillator is $0.5h\nu$.
The energy of a three dimensional box is

RADIOACTIVITY

Previous Year Exam Question & Solutions

[GATE 2004]

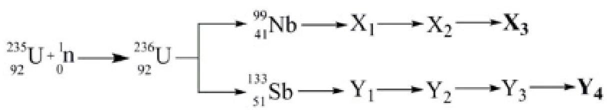
1. The number of hyperfine split lines observed in ESR spectrum of methyl radical is
(a) 1 (b) 4
(c) 6 (d) 8

[GATE 2016]

2. Among the following, the most stable isotope to radioactive decay is
(a) $^{206}_{82}Pb$ (b) $^{210}_{82}Pb$
(c) $^{212}_{82}Pb$ (d) $^{214}_{82}Pb$

[GATE 2020]

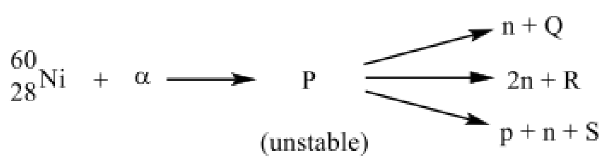
3. The fission reaction of $^{235}_{92}U$ with thermal neutron is represented below.



$^{99}_{41}Nb$ and $^{133}_{51}Sb$ are the primary fission fragment pair, which undergo series of radioactive decay to form stable nuclei X_3 and Y_4 (chain enders). The X_3 and Y_4, respectively are:
(a) $^{96}_{41}Nb$ and $^{130}_{51}Sb$ (b) $^{99}_{44}Ru$ and $^{133}_{55}Cs$
(c) $^{93}_{38}Sr$ and $^{127}_{35}Ag$ (d) $^{87}_{35}Br$ and $^{124}_{43}Tc$

[GATE 2023 MSQ]

4. The choice(s) that correctly identify radioisotopes (P, Q, R, S) shown in the following nuclear reaction is (are)



(a) $P = ^{64}_{30}Zn$ (b) $Q = ^{63}_{30}Zn$
(c) $R = ^{62}_{29}Cu$ (d) $S = ^{62}_{29}Cu$

Answer Key			
1	2	3	4
(b)	(a)	(b)	(a),(b),(d)

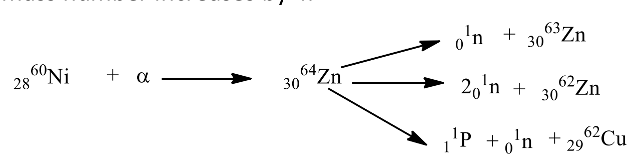
:: SOLUTIONS ::

1. **Solution:** Correct answer is
$\dot{C}H_3 \Rightarrow Hypertone = (2NI + 1) = (2^*3^*1/2 + 1) = 4lines$

2. **Solution:** Correct answer is (a)
Lead (Pb) has four stable isotopes:
^{204}Pb, ^{206}Pb, ^{207}Pb, ^{208}Pb, ^{204}Pb, is entering a primordial nuclide and is not a radiologenic nuclide

3. **Solution:** Correct answer is (b)
The radioactive series of fission fragment ^{99}Nb (mass number $A = 4 \times 24 + 3$) gives only those daughter nuclei (or stable end product) which have mass number A=4n+3, where n is an integer. Thus, daughter nuclei may have mass number A= 99, 95, 91, 87, 83, 79,……..etc. from the given options, ^{87}Br and ^{99}Ru Nuclei are the only two possibilities for stable nuclei X_3. similarly, the radioactive series of fission fragment ^{133}Sb gives only those daughter nuclei (or stable end product) which have mass number A=4n+1. Where, n is an integer. Thus, daughter nuclei may have mass numbers A=133,129,125,121, etc.
From the given options, ^{133}Cs is the only possibility for stable nucleus Y
Hence, X_3 and Y_4 are ^{99}Ru and ^{133}Cs respectively.

4. **Solution:** Correct answer is (a), (b), (d)
α-particle ($^4_2$He)
When α particle emit atomic number increases by 2 and mass number increases by 4.



BIOINORGANIC

Previous Year Exam Question & Solutions

[GATE 2001]

1. The metals involved in nitrogenase are
(a) Fe and Mg (b) Mo and K
(c) Mo and Fe (d) Fe and K.

[GATE 2003]

2. "Matching" exercises. choose the correct one from the alternatives A, B, C and D.

Column-I	**Column-II**
P. $ZnSO_4(aq)+K_4[Fe(CN)_6[aq]\rightarrow$Products	1. Enzymatic reaction
Q. $Zn(s)+CuSO_4(aq)]\rightarrow$Products	2. Chain reaction
R. $H_2+Cl_2\xrightarrow{\Delta}$ Products	3. Redox reaction
S. Fischer-Tropsch synthesis of hydrocarbons	4. Precipitation reaction
	5. Surface reaction
	6. Hydrolysis reaction

(a) P-2, Q-4, R-5, S-6 (b) P-1, Q-3, R-2, S-4
(c) P-4, Q-3, R-2, S-5 (d) P-1, Q-6, R-2, S-5

[GATE 2004]

3. Match the following:

P: Ferritin	I electron transport
Q: Vitamin B12	II. Ionophore
R: Cytochromes	III. Oxygen transport
S: Valinomycin	IV. Nitrogen fixation
	V. Organometallic enzyme
	VI. Iron storage

(a) P-VI, Q-IV, R-II, S-I (b) P-I, Q-III, R-VI, S-IV
(c) P-III, Q-V, R-IV, S-VI (d) P-VI, Q-V, R-I, S-II

[GATE 2005]

4. The metal present at the active site of the protein carboxypeptidase A is
(a) Zinc (b) molybdenum
(c) magnesium (d) cobalt

[GATE 2005]

5. Match the column:-

Column-I	**Column-II**
(P) Cytochromec	(I) Molybdenum
(Q) Calmodulin	(II) Potassium
(R) Chlorophyll	(III) Magnesium
(Q) Alcohol dehydrogenase	(IV) Zinc
	(V) Iron
	(VI) Calcium

(a) P-V, Q-VI, R-III, Q-V (b) Q-II, Q-III, Q-IV, Q-VI
(c) R-III, R-IV, R-VI, R-III (d) S-IV, S-V, S-II, S-IV

[GATE 2005]

6. Matals used in automobile catalytic converters are:
(a) Pt and Pd (b) Pt and Rh
(c) Pd and Rh (d) Rh and Ni

[GATE 2005]

7. **Statement**: D-Glucose and D-mannose give the same phenylosazone.
Reason: Osazone formation results in a loss of the stereocentre at C2 but does not affect other stereo centers.
Assertion: D-Glucose and D-mannose are enantiomers.
(a) Both Reason and Assertion are correct
(b) Both Reason and Assertion are wrong.
(c) Reason is correct but Assertion is wrong.
(d) Reason is wrong but Assertion is correct.

[GATE 2006]

8. Iron-sulphur clusters in biological systems are involved in
(a) proton transfer (b) atom transfer
(c) group transfer (d) electron transfer

[GATE 2006]

9. The amino acid side chain high affinity for Ca^{2+} and Cu^{2+} in metallo-proteins is:
(a) carboxylate in both the cases.
(b) imidazole in both the cases.
(c) caboxylatefor Ca^{2+} and imidazole for Cu^{2+}.
(d) imidazole for Ca^{2+} and carboxylate for Cu^{2+}.

[GATE 2006]

10. In biological systems, the metal ion involved in the dioxygen transport besides Fe is
(a) Co (b) Zn
(c) Mg (d) Cu

[GATE 2007]

11. In photosynthesis, the predominant metal present in the reaction centre of photosystem II is
(a) Zn (b) Cu
(c) Mn (d) Fe

[GATE 2007]

12. Zn in carbonic anhydrase is coordinated by three histidine and one water molecule. The reaction of CO_2 with this enzyme is an example of
(a) electrophilic addition
(b) electron transfer
(c) nucleophilic addition
(d) electrophilic substitution

[GATE 2007]

13. The catalyst used in the conversion of ethylene to acetaldehyde using Wacker process is
(a) HCo(CO)4
(b) [PdCl4]2-
(c) V2O5
(d) TiCl4 in the presence of Al(C2H5)3

[GATE 2008]

14. In biological systems, the metal ions involved in electron transport are
(a) Na+ and K+ (b) Zn2+ and Mg2+
(c) Ca2+ and Mg2+ (d) Cu2+ and Fe3+

[GATE 2009]

15. In the transformation of oxy-haemoglobin to deoxyhaemoglobin
(a) Fe2+ in the low spin state changes to Fe2+ in the high spin state
(b) Fe2+ in the low spin state changes to Fe3+ in the low spin state
(c) Fe2+ in the high spin state changes to Fe2+ in the low spin state
(d) Fe2+ in the high spin state changes to Fe3+ in the high spin state

[GATE 2009]

16. Among 1he following pair of metal ions present in Nature. The first one functions as an Electron transfer agent and the second one catalyzes the hydrolysis reactions. The correct pair is
(a) Fe and Zn (b) Mg and Fe
(c) Co and Mo (d) Ca and Cu

[GATE 2011]

17. A well-known naturally occurring organometallic compound is
(a) vitamin B12 coenzyme (b) chlorophyll
(c) cytochrome P-450 (d) myoglobin

[GATE 2011]

18. The red color of oxy-haemoglobin is mainly due to the
(a) d-d transition
(b) metal to ligand charge transfer transition
(c) ligand to metal charge transfer transition
(d) intraligan dπ-π* transition

[GATE 2012]

19. Haemoglobin is an oxygen carrying protein. The correct statement about oxy-hemoglobin is that
(a) the metal is low-spin in +3 oxidation state while dioxygen is in O2– form
(b) the metal is high-spin in +3 oxidation state while dioxygen is in O2– form
(c) the metal is low-spin in +3 oxidation state while dioxygen is in neutral form
(d) the metal is high-spin in +3 oxidation state while dioxygen is in neutral form

[GATE 2013]

20. Oxymyoglobin Mb(O2) and oxy-haemoglobin Hb(O2)4, respectively, are
(a) paramagnetic and paramagnetic
(b) diamagnetic and diamagnetic
(c) paramagnetic and diamagnetic
(d) diamagnetic and paramagnetic

[GATE 2014]

21. Mg^{2+} is preferred in photosynthesis by chlorophyll because
(a) it has strong spin-orbit coupling
(b) it has weak spin-orbit coupling
(c) it is a heavy metal
(d) it binds strongly with chlorophyll

[GATE 2014]

22. In Monosanto acetic acid process shown below, the role of HI is

$$CH_3OH + CO \xrightarrow[180°C, 30\ bar]{Rh(I) catalyst/HI} CH_3CO_2H$$

(a) to covert CH_3OH to a stronger nucleophile (CH_3O^-)
(b) to reduce the Rh(I) catalyst to a Rh(0) species
(c) to reduce a Rh(III) active species to a Rh(I) species in the catalytic cycle
(d) to convert CH_3OH to CH_3I

[GATE 2015]

23. Among the given pH values, the O2 binding efficiency of hemoglobin is maximum at
(a) 6.8 (b) 7.0
(c) 7.2 (d) 7.4

[GATE 2015]

24. Identify the function of hemocyanin and the metal responsible for it.
(a) O2 transport and Fe
(b) O2 transport and Cu
(c) electron transport and Fe
(d) electron transport and Cu

[GATE 2016]

25. During oxygen transport by hemerythrin, oxygen is bound as
(a) O2– to one Fe(III) only
(b) HO2–to one Fe(III) only
(c) O22–to one Fe(II) and one Fe(III)
(d) O22–to two Fe(II)

[GATE 2016]

26. At pH 7.2 and 10 Torr oxygen partial pressure, the extent of O2 binding is
(a) high for both haemoglobin and myoglobin
(b) high for haemoglobin and low for myoglobin
(c) high for myoglobin and low for haemoglobin
(d) low for both haemoglobin and myoglobin

ANSWER KEY									
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
(c)	(c)	(d)	(a)	(d)	(a)	(a)	(d)	(c)	(d)
11	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
(c)	(c)	(b)	(d)	(a)	(a)	(a)	(d)	(a)	(b)
21	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**
(b)	(d)	(d)	(b)	(b)	(c)	(a)	(c)	(a)	(b)
31	**32**	**33**	**34**	**35**	**36**	**37**	**38**		
(c)	(b)	(c)	(b)	(a),(d)	(d)	(b),(c)	(a)(b)(d)		

:: SOLUTIONS ::

1. Solution: Correct answer is (c)

The metals involved in nitrogenase are Mo and Fe

Nitrogenase is an enzyme complex responsible for nitrogen fixation, which converts atmospheric nitrogen (N_2) into ammonia (NH_3). It contains two important metal-containing components: one with **molybdenum (Mo)** and the other with **iron (Fe)**. These metals play a crucial role in the enzyme's activity.

2. Solution: Correct answer is (c)

(P) ZnSO4 (aq)+K4 [Fe(CN)6](aq) → K2SO4+ Zn_2 [Fe(CN),]
Precipitation reaction

(Q) Zn(s)+CuSO4(aq) → ZnSO4 + Cu(s)
Redox reaction

(R) H_2+Cl_2HCl (chain reaction due to formation of free radical)

(S) Fischer tropsch synthesis of hydrocarbons→ it involve conversion of CO and H2 into liquid hydrocarbon. The reaction occurs in presence of certain metal catalyst which provides surface for reaction. Hence, it is a surface reaction.

3. Solution: Correct answer is (d)

- **Ferritin**: **Iron storage**
  Ferritin is a protein complex that stores iron in a bioavailable form in cells. It helps regulate iron homeostasis in the body.
- **Vitamin B12**: **Organometallic enzyme**
  Vitamin B12 (cobalamin) contains a cobalt ion in its structure and acts as a coenzyme in various biochemical reactions, including DNA synthesis and fatty acid metabolism. It is considered an organometallic compound because of the metal-carbon bond in its structure.
- **Cytochromes**: **Electron transport**
  Cytochromes are heme-containing proteins that play a critical role in electron transport chains, particularly in mitochondria during cellular respiration, facilitating the transfer of electrons.
- **Valinomycin**: **Ionophore**
  Valinomycin is a cyclic molecule that acts as an ionophore, facilitating the transport of potassium ions (K^+) across biological membranes.
  Ferritin → Iron storage
  Vitamin B12 → Organometallic enzyme
  Cytochromes → Electron transport
  Valinomycin → Ionophormoduloas

4. Solution: Correct answer is (a)

The metal present at the active site of the protein carboxypeptidase A is zinc

Carboxypeptidase A is a metalloprotease enzyme that uses a zinc ion at its active site to catalyze the hydrolysis of peptide bonds at the carboxyl end of proteins and peptides. The zinc ion plays a crucial role in the enzyme's catalytic mechanism.

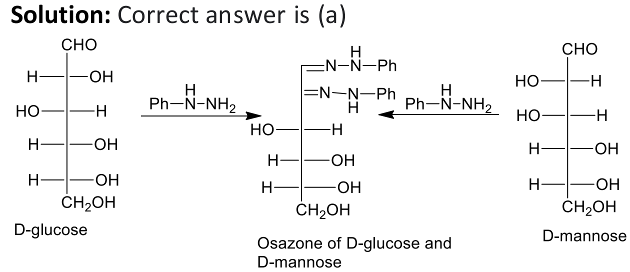
5. Solution: Correct answer is (d)

- **Cytochrome-C → Iron**
  Cytochrome C contains heme groups, where the iron (Fe) in the heme is crucial for its electron transfer function in the electron transport chain.
- **Calmodulin → Calcium**
  Calmodulin is a calcium-binding messenger protein. It undergoes conformational changes upon binding to calcium ions, allowing it to regulate various enzymes and cellular processes.
- **Chlorophyll → Magnesium**
  Chlorophyll, the green pigment in plants responsible for photosynthesis, contains a magnesium ion (Mg^{2+}) at its center. This metal ion is essential for the molecule's ability to absorb light and convert it into chemical energy.
- **Alcohol Dehydrogenase → Zinc**
  Alcohol dehydrogenase (ADH) is an enzyme that contains zinc ions at its active site, which are critical for its catalytic activity in the conversion of alcohols to aldehydes or ketones.

6. Solution: Correct answer is (a)

Pd and Rh are two precious metal that is used in autocatalytic convertor.

7. Solution: Correct answer is (a)



During Osazone formation stereocentre of C, is lost. D-glucose and D-mannose are distereomers

8. Solution: Correct answer is (d)

Iron sulphur cluster in biological systems are involved in electron transfer reaction.

These clusters consist of iron (Fe) and sulfur (S) atoms and play a crucial role in electron transfer processes, particularly in the electron transport chain and various redox reactions within cells. The iron-sulfur clusters facilitate the movement of electrons by undergoing reversible oxidation and reduction. They are key components in enzymes and proteins involved in cellular energy production, such as in the mitochondria and photosynthesis.

9. Solution: Correct answer is (c)

Carboxylate for Ca^{2+} and imidazole for Cu^{2+}.

10. Solution: Correct answer is (d)

In biological systems, the Cu involved in the dioxygen transport besides Fe

Copper plays a role in dioxygen transport and binding in certain proteins, such as **hemocyanin**, which is an oxygen-carrying molecule found in some arthropods and mollusks. Unlike hemoglobin (which contains iron), hemocyanin uses copper ions to bind oxygen.

11. Solution: Correct answer is (c)

In photosynthesis, Mn is the predominant metal present in the reaction centre of photosystem-11.

Manganese is a crucial component of the oxygen-evolving complex (OEC) in photosystem II, where it plays a key role in the splitting of water molecules to release oxygen during the light-dependent reactions of photosynthesis.

12. Solution: Correct answer is (c)

Zn in carbonic anhydrase, the CO_2 undergoes nucleophilic addition reaction.

In carbonic anhydrase, the zinc ion (Zn^{2+}) at the active site facilitates the conversion of carbon dioxide (CO_2) into bicarbonate (HCO_3^-) by coordinating with a water molecule. The water molecule becomes deprotonated, and the hydroxide ion (OH^-) formed acts as a nucleophile, attacking the electrophilic carbon of CO_2, leading to the formation of bicarbonate.

13. Solution: Correct answer is (b)

Wacker's process

$C_2H_4 + H_2O + [PdCl_4]^{-2} \rightarrow CH_3CHO + Pd + 2HCl + 2CI^-$

$Pd + 2CuCl_2 + 2Cl \rightarrow [Pd(Cl_4)]^{-2} + 2CuCl$

$2CuCl + \frac{1}{2}O_2 + 2HCI \rightarrow 2CuCl_2 + H_2O$

Net reaction $C_2H_4 + \frac{1}{2}O_2 \rightarrow CH_3CHO$

14. Solution: Correct answer is (d)

In biological systems, Cu^{2+} and Fe^{2+} metal ion involve in electron transport. This is due their variable oxidation state.

Both copper (Cu) and iron (Fe) play crucial roles in electron transport. Copper is involved in proteins like cytochrome c oxidase, while iron is part of iron-sulfur clusters and heme groups in cytochromes, which are essential components of the electron transport chain, particularly in mitochondria and chloroplasts.

15. Solution: Correct answer is (a)

The transformation of oxyhaemoglobin to deoxyhaemoglobin Fe^{2+} involves change in low spin state to high spin state.

In deoxyhaemoglobin, Fe^{2+} is in high spin state.

In oxyhaemoglobin, iron of heme group bind with oxygen molecule, and Fe become low spin

16. Solution: Correct answer is (a)

Fe act as electron transfer agent in many reaction. Zn act as catalyst in hydrolysis reaction specially enzymatic reaction by carboxypeptidase.

17. Solution: Correct option (a)

Vitamin B_{12} co-enzyme is a naturally occurring organometallic compound.

18. Solution: Correct answer is (d)

Red colour of oxyhemoglobin is mainly due to $\pi - \pi^*$ transition in porphyrin system.

The red color of **oxyhemoglobin** is primarily due to the electronic transitions involving the iron ion in the heme group. In particular, the iron undergoes a **d-d transition** in which electrons in the d-orbitals of the iron ion move between different energy levels, absorbing light in the visible spectrum. This absorption contributes to the red color observed in oxygen-bound hemoglobin.

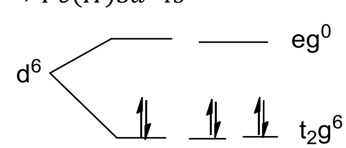
19. Solution: Correct answer is (a)

In oxyhaemoglobin the metal is low-spin in $+3$ oxidation state while dioxygen is in O.

20. Solution: Correct answer is (b)

Oxymyoglobin Mb(O2)

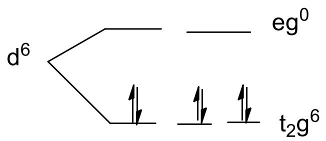
$\Rightarrow Fe(II)3d^6 4s^0$



Low spin, Diamagnetic

Oxyhemoglobin Hb(O2)4

$\Rightarrow Fe(II)3d^6 4s^0$



Low spin, Diamagnetic

21. **Solution:** Correct answer is (b)
In photosynthesis, Mg^{2+} is preferred and it is present in chlorophyll. It has small spin-orbit coupling. So, inter system crossing is inhibited which favours the energy transfer from the excited singlet state.

22. **Solution:** Correct answer is (d)
In Monsanto acetic acid process role of HI is to convert CH_3OH to CH_3I
$CH_3OH + HI \rightarrow CH_3I + H_2O$

23. **Solution:** Correct answer is (d)
The O_2 binding efficiency of hemoglobin is maximum at blood pH is 7.4

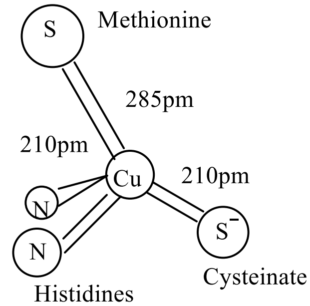
24. **Solution:** Correct answer is (b)
hemocyanin is a copper containing protein which is responsible for oxygen transport in some invertebrates

25. **Solution:** Correct answer is (b)
During oxygen transport by hemerythrin, oxygen is bound as HO_2^- to one Fe(III) only

26. **Solution:** Correct answer is (c)
At low pH and low pressure Hb has less oxygen binding tendency. While for Mb this is hight.

27. **Solution:** Correct answer is (a)
Chlorophylls are complexes of Mg^{2+} with porphyrin ring in which one of the pyrrole rings has been reduced. A porphyrin ring with one double bond reduced is called a chlorin. Therefore, chlorophylls are the complexes of Mg^{2+} metal ion with substituted chlorin (macrocyclic skeleton).

28. **Solution:** Correct answer is (c)
Plastocyanin is important bioinorganic complex, they help in electron transfer during photosynthesis. They are present between Photosystem I and Photosystem II. It changes oxidation state from +1 to +2 or vice versa during electron transfer. The oxidised form of copper contain the active site Cu+2 ions, thus the copper ion forms a trigonal pyramidal and tetrahedral structure with methionine, Cysteine, and two histidine residues, here the copper ion is forming a structure that is distorted and tetrahedral because of the geometry of the protein.



29. **Solution:** Correct answer is (a)
Oxy-myoglobin is formed when myoglobin which is globular protein binds with it. Oxy-myoglobin store oxygen in muscles. So, oxygen is present in O2- which is superoxide ion state in oxy-myoglobin. Oxy-hemocyanin is formed by the oxygenation of hemocyanin. Hemocyanin is a protein that contains copper and is generally found in crustaceans. Oxy-hemocyanin is blue in colour and used for binding and storage of oxygen. O22- which is peroxide ion in Oxyhemocyanin.

30. **Solution:** Correct answer is (b)

Ferritin	metal storage
Rubredoxin	electron transfer
Cobalamin	methyl transfer
Carbonic anhydrase	acid-base catalysis

- **Ferritin → Metal storage**
Ferritin is a protein that stores iron in a non-toxic, bioavailable form, helping regulate iron levels in the body.
- **Rubredoxin → Electron transfer**
Rubredoxin is a small iron-containing protein involved in electron transfer reactions, typically in anaerobic microorganisms.
- **Cobalamin → Methyl transfer**
Cobalamin (Vitamin B12) acts as a coenzyme in methyl transfer reactions, important for DNA synthesis and metabolism.
- **Carbonic anhydrase → Acid-base catalysis**
Carbonic anhydrase is an enzyme that catalyzes the reversible conversion of carbon dioxide and water to bicarbonate and protons, playing a role in regulating pH and CO_2 levels.

31. **Solution:** Correct answer is (c)